
WORK EXTRACTION FROM ACTIVE MATTER SYSTEMS

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Statement of originality

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For Sinéad.

Abstract

This thesis examines active matter, a particular class of non-equilibrium systems consisting of agents that autonomously extract energy from their surroundings to sustain their dynamics. Examples include biological systems, such as molecular motors and bacteria, as well as synthetic counterparts, such as Janus particles.

Active matter defies “equilibrium” thermodynamics by breaking the principle of detailed balance. While this renders much of the *standard* statistical mechanics toolkit ineffective, the upside is that it leads to a rich array of phenomena with no equilibrium counterpart. Perhaps the most familiar is the ability of active matter to spontaneously perform useful work. With growing interest in this phenomenon, I explore how active matter can be modelled and leveraged to perform useful work, especially in the context of “active engines”, i.e. microscale machines powered by active matter.

This thesis comprises two main parts. The first presents various minimal models of work extraction from active particles. These demonstrate how particle currents can be channelled to perform work, while also considering key concepts like autonomy and efficiency. These models roughly increase in complexity as the chapters progress, culminating in the design of a protocol that extracts *optimal* power from active particles with hidden internal states.

The next part addresses the role of dense active matter in the development of active engines. I characterise one such class of dense active matter, namely active crystals, through exact calculations of its thermodynamic properties, including fluctuations, energy, and entropy production. I also investigate foundational principles, such as how activity affects the crystalline order of these regularly arranged condensates.

Aside from providing insight into the fundamental properties of active matter, the framework presented in this thesis is easily extensible to more complex systems, and thus offers a pathway to harnessing the unique properties of active matter for practical use.

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1

Introduction

The world around us is constantly on the move. Abundant examples of this can be found across Nature, ranging from the molecular motors that facilitate intracellular transport to the pattern-forming murmurations of starlings. More generally, *non-equilibrium* systems can be found at all levels of complexity and across a wide range of spatial scales. Over the last couple of decades, the scientific endeavour to systematically characterise non-equilibrium systems has been one of the key driving forces behind the study of the closely related “active matter”. As its name suggests, *active* matter is distinguished from its passive counterpart by the ability to liberate free energy for practical use. For instance, many organisms deploy metabolic processes to repurpose the chemical free energy they obtain from food into the kinetic energy of self-propelled motion.

The recent success of active matter models in mimicking the behaviour of a wide variety of living systems has established them as the cutting edge in the study of non-equilibrium systems [1–5]. Though the distinction between the two is somewhat blurred, in this thesis, I will use “active matter” to refer exclusively to the class of systems who sustain their dynamics autonomously, while using “non-equilibrium systems” to also encompass those systems whose dynamics need to be sustained by constant or repeated application of an *external* force.¹ However, restricting the term “active matter” in this way does not restrict its applicability only to living systems. In fact, a wealth of synthetic active matter systems are at the forefront of experiments, the most prominent example being Janus particles [8–12].

Unless acted on by a force, passive matter is said to exist in, or be relaxing towards, an *equilibrium* steady state. As a result, passive matter is well described by the “equilibrium” thermodynamic principles formulated just after the Industrial Revolution over 200 years ago [13]. These principles allow one to characterise an ensemble of passive matter, such as an everyday gas, by just a few of its macroscopic properties—such as pressure (P), temperature (T), and volume (V)—which can be understood as some manifestation of the *average* behaviour of the constituent particles. For instance, these quantities combine in the equation of state for an ideal gas as $PV = Nk_B T$, where N is the number of particles in the gas and $k_B \approx 1.38 \times 10^{-23} JK^{-1}$ is the Boltzmann constant. To quantify fluctuations about the average behaviour, arising from the microscopic degrees of freedom, requires the more rigorous toolkit of statistical mechanics. These tools take into account the probabilistic nature of individual particles, and thus provide a deeper understanding

¹There are other non-equilibrium systems that escape even this categorisation. Spin glasses are one such example because of their *very* slow approach to equilibrium below a critical temperature [6, 7]. However, such systems will not be considered in this thesis.

of a system’s thermodynamic properties, such as at the onset of a phase transition [14, 15].

In contrast, by operating out of equilibrium, active matter breaks so-called “detailed balance”, which requires each elementary process to be in equilibrium with its corresponding reverse process, i.e. each process satisfies the detailed balance condition $p_i W(i \rightarrow j) = p_j W(j \rightarrow i)$, where p_s is the steady-state probability to be in state s and $W(s_1 \rightarrow s_2) \geq 0$ is the transition probability from state s_1 to s_2 . Breaking this notion of *microscopic* reversibility invalidates the use of the equilibrium statistical mechanics toolkit mentioned before. For instance, it is not possible in general to define an equation of state for an active fluid, due to the lack of a well-defined temperature and pressure [16, 17].² As a result, finding a systematic way of characterising non-equilibrium systems to the same degree of success as equilibrium thermodynamics and statistical mechanics have done for passive systems is more challenging. Far from being a coherent framework, the ongoing efforts to do so collectively come under a branch of mathematics coined *non-equilibrium* statistical mechanics. So far, these efforts have yielded great success in modelling many interesting phenomena with no equilibrium counterpart, including: autonomous ratcheting [20–24], aggregation of particles at surfaces [19, 25–28], motility-induced phase separation [29–32], and flocking [33–36].

Non-equilibrium systems are driven by an irreversible flow of energy, since the once-useful free energy flowing into their constituents is eventually dissipated back into their environment as thermal energy, or “heat”, that cannot be recycled into a useful form. As a result, the entropy of the system—i.e. the amount of energy (per unit temperature) that cannot be converted into useful work—increases. This degradation of useful energy is linked to the irreversibility of a system’s underlying dynamics by the entropy production *rate* (which I will simply call “entropy production” for brevity) [37–39].

The entropy production of a system formally quantifies the irreversibility of its dynamics.³ More qualitatively, if some series of system states across time is equally likely to occur both forward and in reverse then its associated entropy production vanishes. On the other hand, if a series is significantly more likely to occur either forward *or* in reverse, then its entropy production is positive. An example of the latter is dropping a ceramic mug on a hard surface. The series of states of the mug going forward in time could be described by i) being held at rest, ii) free fall, and iii) at rest on the surface and likely broken into pieces. The flow of energy here is from (gravitational) potential $\rightarrow$ kinetic $\rightarrow$ thermal. The mug initially dissipates a small amount of heat during its free fall due to friction from the air. The remainder of the mug’s initial potential energy is then dissipated into thermal motion of the air and the surface shortly after coming into contact with the latter. It is clear here that the reverse series of states would be impossible to observe in practise. Hence, a positive rate of entropy production represents that time-reversal symmetry in a system has been broken. In fact, this is the hallmark of a system operating out-of-equilibrium. Correspondingly, a vanishing rate of entropy production indicates no time-reversal symme-

²Some counterexamples of active fluids with well-defined pressures do exist [18, 19].

³Mathematically, the entropy production is given by the Kullback-Leibler divergence (see Ref. [40]) of the densities of forward and time-reversed trajectories.

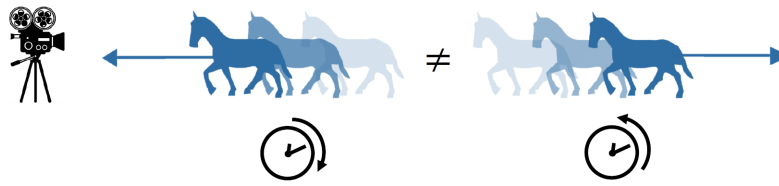


Figure 1.1: Illustration of how the breaking of time-reversal symmetry by a system can be viewed as the ability to distinguish whether a recording of that system is being played forward or backward in time. In other words, whether the arrow of time can be ascertained from the recording. The greater the confidence in determining whether a recording is being played forwards or backwards mirrors the inherent irreversibility of the system’s dynamics, which is formally quantified by the entropy production rate.

try breaking and that the system is at equilibrium. These statements are synthesised by The Second Law of Thermodynamics, which states that—on average—the total entropy of an isolated system does not decrease over time. An equivalent statement is that thermal energy cannot be spontaneously converted into useful work.

Entropy production is a powerful tool in demonstrating a certain level of universality between different models of active matter. For instance, many models have identical algebraic expressions for their entropy productions despite drastic differences in their underlying dynamics [41, 42]. This will be demonstrated later in Chapter 2, where I calculate the entropy production of the different canonical active particle models. Entropy production is also useful for exploring in what limits the dynamics of a non-equilibrium system become fully irreversible or reversible. The latter, in particular, informs us what specific parameter values or attributes of these systems are the ones that actually make the system non-equilibrium.

Since entropy production formally quantifies irreversibility, it is often said that it can also quantify the *distance* of a system from equilibrium [43]. However, what it means precisely for one system to be further from equilibrium than another is rather ambiguous (aside from the arbitrary assignment of entropy production as the yardstick). For instance, many non-equilibrium systems have greater entropy production than others simply by virtue of their greater size and/or self-propulsion speed (consider a car being driven on a motorway, which has much greater entropy production than a self-propelling bacterium). However, there is arguably nothing else that makes these systems inherently more “non-equilibrium” than those with smaller entropy production. This ambiguity can be avoided entirely by defining there to be only two discrete classes of systems: non-equilibrium and equilibrium. With these definitions, we care about entropy production in terms of “equilibriumness” only so far as a positive value indicates a system is non-equilibrium.

A more grounded way of comparing non-equilibrium systems is by a tangible observable that can be unambiguously classified as greater for one system over another. One such observable is a system’s ability to perform useful thermodynamic work. Work extraction from a system is still intimately related to entropy production [44]. For instance, a vanishing rate of entropy production also implies that it is impossible to extract work from

a (Markovian) system.⁴ Similarly, positive entropy production indicates the possibility of work extraction, as only through the breaking of time-reversal symmetry can a system have internal currents that can be channelled to perform work. The relation between entropy production, time-reversal symmetry, and work extraction can be visualised with the aid of Figure 1.1. The horse illustrated in this figure breaks time-reversal symmetry because if its motion were recorded and played in reverse then it would appear to be galloping backwards, which would be an obvious indicator that the recording is being played in reverse. This ability to ascertain the “arrow of time” is what allows us to exploit the horse’s self-propelled motion to perform useful work. For instance, a cargo can be attached to the horse, which the horse then reliably transports in the direction it is facing.

In comparison, consider now the motion of a single colloidal particle suspended in a solution. Constant bombardment from other particles in the solution result in random fluctuations in the position of the colloidal particle known as “Brownian motion”—named after the botanist Robert Brown, who was the first person to systematically study this kind of motion [45]. Since Brownian motion is completely random, it does not break time-reversal symmetry, nor can it be used to perform useful work. In the case of the colloidal particle, its unbiased random movements would prevent transport of an attached cargo with any predictability. In short, time-reversal symmetry breaking is indicated by a positive rate of entropy production and this, in turn, bounds the rate of work that can be extracted from a system. Since entropy production is essentially the amount of useful energy being wasted, while work extraction is the amount of energy that is effectively utilised, the ratio of the latter to the former roughly quantifies a system’s thermodynamic efficiency. This will be made more explicit in Chapter 2.

The inability of equilibrium systems to perform useful work was challenged by the “Brownian ratchet” thought experiment devised by Marian Smoluchowski [46], and popularised by Richard Feynman [47]. In this experiment, a paddle—which is coupled to a heat bath—is connected along its axis of rotation to a ratchet and pawl, which are coupled to a different heat bath of the same temperature. I have schematised the setup in Figure 1.2. The ratchet and pawl are supposed to act as a mechanical diode by preventing the paddle, and by extension the axle connecting the paddle to the ratchet, from rotating in a particular direction. If this were the case, then collisions from particles in the paddle’s heat bath would drive a unidirectional rotation of the paddle and axle in the opposite direction. By also incorporating a mass that gets raised by this rotation, the system appears to break The Second Law by spontaneously converting thermal energy from the particle collisions into useful work. This should be impossible. The reason the Brownian ratchet does not actually break The Second Law is due to other effects that need to be considered [47]. Chiefly, collisions from particles in the ratchet and pawl’s heat bath lead to thermal motion of the pawl itself, and thus there are transient periods where the pawl slips, al-

⁴I will show in Chapter 7 that it is still possible to extract work from certain non-Markovian systems that do not break time-reversal symmetry. A Markovian system is one in which its probabilities for changing state depend only on the state at the current moment in time t and not on any state at an earlier time $t' < t$.

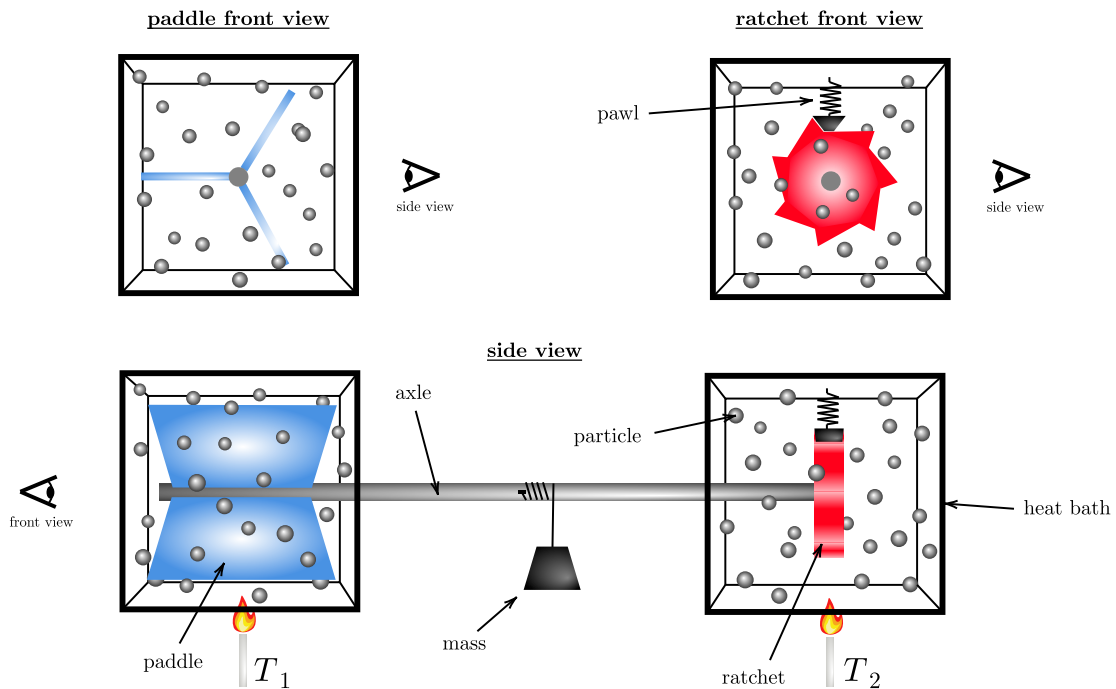


Figure 1.2: Schematic of the “Brownian ratchet” thought experiment. Collisions from particles cause the paddle to rotate. The frictional force between the ratchet and pawl generally causes the paddle, which is connected to the ratchet by an axle, to rotate in a preferred direction. However, the pawl itself is subject to random “Brownian” motion and so it occasionally loses contact with the ratchet, allowing the paddle, axle, and ratchet to rotate in the opposite direction. If the paddle and ratchet are coupled to heat baths of the same temperature, i.e. $T_1 = T_2$, then the average rates of rotation in either direction exactly cancel, and so the system tends to rotate randomly, preventing work extraction. If $T_1 \neq T_2$, then the resulting flow of heat from the hotter to the cooler bath can be harnessed to perform useful work, such as by increasing the gravitational potential energy of a mass.

lowing the ratchet, axle, and paddle to rotate backwards. When these additional effects are incorporated, the rates of forward and backward rotation exactly cancel, resulting in no net work extraction [48]. The slipping rate, in fact, depends on the temperature of the ratchet and pawl’s heat bath. Hence, the setup could be used to extract work simply by setting the two heat baths to different temperatures. However, this would still comply with The Second Law because heat would now flow from the hotter to the cooler bath via the axle [49]. The Brownian ratchet thought experiment demonstrates that, even when we attempt to force random motion into a particular direction, work extraction in an equilibrium system is still an impossibility.

This is in contrast to a recent real-life experiment where *Escherichia coli* bacteria suspended in solution were shown to drive the rotation of a ratchet wheel [50]. Even in the absence of temperature gradients, self-propelling active matter such as *E. coli* can

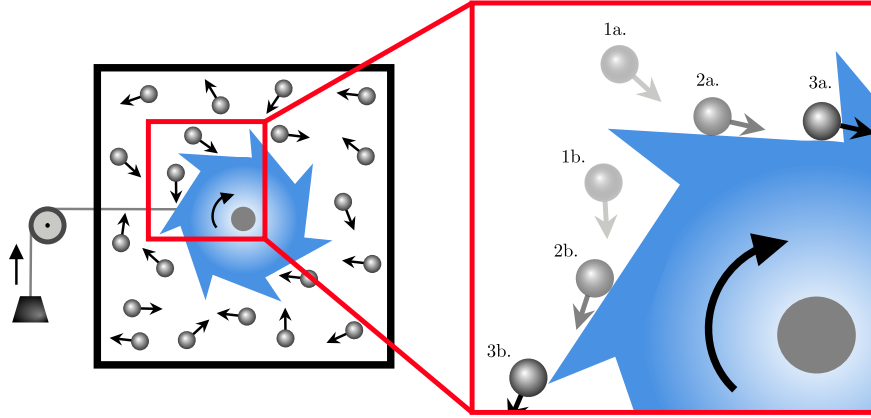


Figure 1.3: Schematic illustration of the experiment performed in Ref. [50]. *Escherichia coli* bacteria are represented by self-propelling particles whose self-propulsion directions, indicated by arrows, diffuse over time. By propelling into the sides of the ratchet wheel, the *E. coli* become pinned for brief periods of time and subsequently use their self-propulsion to drive an in-plane rotation of the wheel, see sequence 1a→3a above. The ratchet’s broken spatial symmetry results in a preference to the average rotation, as illustrated by sequence 1b→3b where particles do not become pinned against the ratchet for certain incident angles. The average rotation can be used to perform useful work, such as by increasing the gravitational potential energy of a mass.

spontaneously perform useful work because they are out of equilibrium. In this particular example, the combination of the ratchet’s broken spatial symmetry and the *E. coli*’s broken time-reversal symmetry result in a unidirectional rotation of the wheel. More precisely, the *E. coli* propel into the wheel for a period of time that depends on their angle of incidence. This angular dependence is what breaks the rotational symmetry. I have illustrated this idea in Figure 1.3.

The above examples demonstrate that the ability to spontaneously perform useful work is a distinguishing feature of non-equilibrium systems. However, this is not a recently discovered phenomenon, rather an everyday occurrence. For instance, similarly to the *E. coli* in Ref. [50], hamsters are well known to drive the persistent rotation of an exercise wheel. So what distinguishes *E. coli* from hamsters in terms of work extraction? First, the work extraction from *E. coli* in Ref. [50] occurs at a microscopic scale ruled by fluctuations. Fluctuations make extracting work at the microscopic scale inherently more impractical and therefore more impressive. Second, is a question of autonomy. Hamsters want to exercise and so—in a sense—*voluntarily* perform work, whereas an *E. coli*’s only motivation is chemotaxis. Yet, *E. coli* can be harnessed in such a way that they involuntarily drive the rotation of the ratchet wheel. This is important for achieving controllable work extraction from active matter that is independent of the constituents’ autonomy.

The growing relevance of work extraction in the field of active matter was highlighted in a major review article, “The 2020 motile active matter roadmap” [3], published a few months before I began my doctoral studies. This article dissected the important questions

in the still emerging field of active matter. In one section, it was suggested that a “timely and exciting [research area] is to design machines that are powered by active matter. [...] Can we usefully exploit the principles designed by evolution, and will dense active matter have a part to play in this development?” In another, it was identified that “Synthetic active particles also have possible applications as micro-engines. [...] Maybe even more fundamentally, the role of entropy production and efficiency of such active engines has recently moved into the focus.” The importance of work extraction is highlighted in this article as the desire to power microscale machines with active matter, which I will refer to as “active engines”. This aim of this thesis is to contribute towards this goal by showcasing a variety of minimal models of work extraction from active matter systems, as well as addressing the foundational principles of dense active matter.

Before delving into the main research topic, Part 1 of this thesis will briefly review some of the key methods used in later chapters. I first provide an overview of active particle models in Chapter 2, before introducing Doi-Peliti field theory in Chapter 3—which will be particularly useful for understanding the main derivation in Chapter 4.

Two main parts follow. In Part 2, I present several toy models of work extraction from active matter and other non-equilibrium systems. Work extraction in such systems is typically achieved by harnessing a steady-state net current to either push obstacles [23], or increase the gravitational potential energy of a mass [51], see Figures 1.2 and 1.3. To avoid the work extraction depending on the fine details of the system on which the work is being performed, the latter will be abstracted to an unspecified external force, thereby also keeping the work extraction as general as possible for each model. The progression of the chapters in Part 2 roughly mirrors the complexity of the systems under consideration, culminating in a calculation and proposal of *optimal* work extraction from active particles in Chapter 7. The exactly solvable nature of these models makes them important for obtaining deeper and quicker insight than for a model that is amenable only to numerical solutions. Moreover, the apparent simplicity of these models makes them easily extensible to more complicated dynamics and they are thus, in some sense, foundational. A brief overview of each chapter in this part is given below.

In Chapter 4, the first of Part 2, Doi-Peliti field theory is used to solve a one-dimensional model of a drift-diffusive particle that changes the sign of its drift only through interacting with the boundaries of the finite domain on which it resides. This is a modification of the “run-and-tumble” active particle model, where “tumbling” is restricted to occur only at boundaries. Hence, the active particles of this model are referred to as “boundary tumbling”. Work extraction enters by mapping this system to a one-dimensional ring geometry, whence one can channel the resulting net current to perform useful work. As it turns out, only through the interplay of fluctuations, self-propulsion, and boundary tumbling does the system permit a non-uniform steady-state density. Interestingly, in certain parameter regimes, a boosted rate of work extraction beyond the diffusionless case is found.

In Chapter 5, the relatively recent notion of “stochastic resetting” is applied to a

diffusive particle moving in a spatially asymmetric “ratchet” potential. Here, the system undergoes cyclic switching between a freely diffusive phase and a resetting phase where the potential facilitates the return of the particle to the origin. On average, the asymmetry of the potential biases the particle’s motion, resulting in a net current which could be used to perform useful work. As the particle is purely diffusive, this is not a model of active matter but rather an example of a non-equilibrium system whose dynamics need to be sustained by repeated application of an external force. Hence, this chapter provides an example of work extraction from non-equilibrium systems other than active matter.

Contrast this with Chapter 6, in which a *static* ratchet potential is used to rectify the motion of a run-and-tumble particle without the need for an external controller. Together, Chapters 5 and 6 demonstrate a key difference between work extraction from externally forced non-equilibrium systems and active matter is that the latter can be sustained autonomously. For the model in Chapter 6, I perform exact calculations of the power and efficiency of the resulting work extraction, as well as the system’s entropy production rate.

Equipped with a thorough overview of work extraction in active matter systems, Part 2 concludes with Chapter 7. In this chapter, the optimal rate of work extraction from unbiased active particles is calculated under the realistic assumption that the particles’ self-propulsion is not an observable degree of freedom. Furthermore, a novel feedback protocol based on first-passage statistics is shown to saturate this bound of optimal work extraction.

The shorter Part 3 is focused on addressing the role dense active matter will play in the development of active engines, as highlighted in “The 2020 motile active matter roadmap” [3]. In particular, realistic active engines must be compatible with active matter rarely coming in single units, but rather as an ensemble of interacting particles. In the singular chapter of Part 3 (Chapter 8), one such class of interacting active matter is explored in detail, namely “active crystals”. These regularly arranged condensates form from active particles undergoing motility induced phase separation. In this chapter, one- and two-dimensional crystals are characterised through exact calculations of their key properties, including average particle separation, instantaneous energy, and entropy production. One of the key results of this chapter is that the exact calculations give a definitive answer to whether activity supports long-range crystalline order according to the original criterion developed by David Mermin [52].

Finally, I conclude with a summary of this thesis in Chapter 9. Suggestions for future work are provided at the end of each chapter. As an interesting aside, in Appendix A, I show how the properties of certain systems can depend on the interpretation of the noise term in their governing stochastic equations of motion.

The content of this thesis is based on several published papers and some manuscripts currently being prepared for submission. The chapters to which these works correspond are outlined in Table 1.1. The permissions to reproduce these works as part of my thesis are given in Appendix B. The author contributions to the original work on which a chapter is based are given at the beginning of said chapter. The material drawn from these original

works has been edited to align with the narrative of this thesis. However, being based on different works, each chapter is largely self-contained and has its own set of notation. While every effort has been made to homogenise the notation, the definitions of certain mathematical symbols may still differ between chapters.

Chapter/Appendix	Status of corresponding publication	Authorship
4	Phys. Rev. Res. 4 , 033234 (2022) [28]	First author
5	J. Phys. A: Math. Theor. 57 , 325001 (2024) [53]	First author*
6	Phys. Rev. E 108 , 014139 (2023) [21]	First author*
7	Phys. Rev. Lett. 131 , 188301 (2023) [54]	Not first author
8	In preparation	First author
A	arXiv 2410.04124 (2024) [55]	First author

Table 1.1: Overview of chapters associated with work I have published. Asterisks * indicate that first authorship was shared with a coauthor.

~ Part 1 ~

Methods

2

Active particle models—a brief overview

In this chapter, I will introduce some of the main concepts that will feature frequently throughout the rest of this thesis focusing, in particular, on the equations describing the canonical active particle models.

2.1 Langevin equation

Before tackling the more complicated dynamics of active particles, we begin with the stochastic differential equation describing Brownian motion of a single particle in one dimension [56, 57],

$$m\ddot{x}(t) = -\gamma\dot{x} + F(x, t) + \gamma\tilde{\xi}(t), \quad (2.1)$$

where m is the mass of the particle, $x(t)$ is its time-dependent position, γ is the (Stokes) friction coefficient due to the surrounding medium, and $F(x, t)$ is a generic space- and time-dependent force. Equation (2.1) is known as the “Langevin equation” and generalises Newton’s Second Law through the addition of a stochastic term $\tilde{\xi}(t)$. The purpose of this term is to incorporate, in a coarse-grained sense, the effect of the random collisions a particle experiences from other particles in its surrounding medium. This “thermal noise” can therefore be understood in terms of its statistics,

$$\langle \tilde{\xi}(t) \rangle = 0, \quad (2.2a)$$

$$\langle \tilde{\xi}(t_2)\tilde{\xi}(t_1) \rangle \sim e^{-\frac{|t_2-t_1|}{\tau_c}}, \quad (2.2b)$$

where $\langle \bullet \rangle$ represents the ensemble average of a quantity $\bullet$, and τ_c is the typical timescale on which a collision takes place. Equation (2.2a) tells us that the stochastic term is drawn from a distribution with zero mean. Physically, this means the collisions do not impart any preferential direction on the particle’s motion. The collision time τ_c is usually much smaller than other relevant timescales. In particular, the effect of any single collision is quickly forgotten due to the sheer frequency of collisions the particle experiences. In other words, collisions can be assumed to be independent. Mathematically, this amounts to replacing Equation (2.2b) with the following autocorrelation function

$$\langle \tilde{\xi}(t_2)\tilde{\xi}(t_1) \rangle = 2D\delta(t_2 - t_1), \quad (2.3)$$

where $\delta(t)$ is the Dirac delta function and D is the diffusion constant, quantifying the rate that the particle’s probability density spreads over time. When $\tilde{\xi}(t)$ is completely characterised by Equations (2.2a) and (2.3), it is known as “white noise”. White noise is

not a differentiable function, and so the position $x(t)$ itself is an everywhere-continuous nowhere-differentiable function that can be understood only through the machinery of stochastic calculus.

Many active systems operate in high-viscous environments where inertial effects are less relevant, i.e. at small Reynold's number. Such systems can be modelled by the simpler “overdamped” regime of the Langevin equation. This regime is equivalent to assuming the typical timescale τ_{obs} of interest is much larger than the inertial timescale, i.e. $\tau_{\text{obs}} \gg m/\gamma$. In the overdamped regime, the inertial term on the left-hand side of Equation (2.1) vanishes, and so the Langevin equation reduces to

$$\dot{x}(t) = F(x, t) + \tilde{\xi}(t), \quad (2.4)$$

where we have set $\gamma = 1$ without loss of generality. In the overdamped regime, velocities have the same interpretation as forces, as the time it takes a particle to accelerate to terminal velocity is negligible. Furthermore, for an overdamped system at equilibrium, diffusion satisfies the Einstein relation $\gamma D = k_B T$, where $k_B \approx 1.38 \times 10^{-23} \text{ JK}^{-1}$ is the Boltzmann constant and T is the average temperature of the surrounding medium.

The trajectory of a single particle can be simulated by iteratively integrating the Langevin equation in small time increments Δt . First, we rewrite Equation (2.4) in a form that will be more illustrative for the subsequent discussion,

$$\dot{x}(t) = F(x, t) + \sqrt{2D}\xi(t), \quad (2.5)$$

where we have redefined $\tilde{\xi}(t) = \sqrt{2D}\xi(t)$ such that the white noise in Equation (2.5) is now of unit variance, i.e. $\langle \xi(t_2)\xi(t_1) \rangle = \delta(t_2 - t_1)$. From integrating Equation (2.5), we obtain

$$x(t + \Delta t) = x(t) + \int_t^{t+\Delta t} dt' F(x, t') + \sqrt{2D} \int_t^{t+\Delta t} dt' \xi(t'), \quad (2.6)$$

where the “Wiener increments” $\int_t^{t+\Delta t} dt' \xi(t')$ are normally distributed with mean zero and variance Δt . This can be shown explicitly,

$$\left\langle \int_t^{t+\Delta t} dt' \xi(t') \right\rangle = \int_t^{t+\Delta t} dt' \langle \xi(t') \rangle = 0, \quad (2.7)$$

using Equation (2.2a), and

$$\begin{aligned}
 \left\langle \int_t^{t+\Delta t} dt' \xi(t') \int_t^{t+\Delta t} dt'' \xi(t'') \right\rangle &= \int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' \langle \xi(t') \xi(t'') \rangle \\
 &= \int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' \delta(t' - t'') \\
 &= \int_t^{t+\Delta t} dt' \Theta(t' - t) \Theta(t + \Delta t - t') \\
 &= \int_t^{t+\Delta t} dt' 1 \\
 &= \Delta t,
 \end{aligned} \tag{2.8}$$

using Equation (2.3), recalling $\tilde{\xi}(t) = \sqrt{2D}\xi(t)$. The ability to exchange the ordering of ensemble averages and time integration in the above requires us to assume the system we are modelling is ergodic. This is generally the case for the systems that will be considered in this thesis.

The approximate numerical solution to Equation (2.5) can be found using the Euler-Maruyama method, i.e.

$$x(t + \Delta t) \approx x(t) + F(x, t)\Delta t + \sqrt{2D\Delta t} \mathcal{N}(0, 1), \tag{2.9}$$

where $\mathcal{N}(\mu, \sigma^2)$ is a random number drawn from a normal distribution of mean μ and variance σ^2 , and we have used that the statistics of $\sigma\mathcal{N}(\mu, 1)$ are the same as $\mathcal{N}(\mu, \sigma^2)$. Iterating Equation (2.9) for small time increments Δt allows one to simulate the trajectory of a particle described by Equation (2.5).

So far, we have assumed diffusion D is independent of the position of the particle. If diffusion is not space dependent, then the noise term $\sqrt{2D}\xi(t)$ in Equation (2.5) is known as “additive” noise. A space-dependent diffusion, on the other hand, makes the noise term “multiplicative”, and introduces several complications. The main complication is that multiplicative noise presents a choice in how the Langevin equation is integrated. More specifically, the choice comes down to which value the random variable $x(t)$ takes in the interval $[x(t), x(t + \Delta t)]$ when evaluating the space-dependent diffusion at each timestep. To see this, we return to Equation (2.5) and replace the diffusion constant with a space-dependent diffusion. The resulting numerical solution for the Langevin equation with space-dependent diffusion is given by

$$x(t + \Delta t) \approx x(t) + F(x, t)\Delta t + \sqrt{2D[(1 - \alpha)x(t) + \alpha x(t + \Delta t)]} \int_t^{t+\Delta t} dt' \xi(t'), \tag{2.10}$$

where $\alpha \in [0, 1]$. Each α represents a different convention. The most commonly chosen are Itô ($\alpha = 0$) [58], Stratonovich ($\alpha = 1/2$) [59], and isothermal/Hänggi-Klimontovich ($\alpha = 1$) [60, 61]. Importantly, each convention results in different physical properties. This is illustrated in greater detail in Appendix A, where I present a case study of using a

metamaterial of spatially varying diffusivity to cloak a region of space from an ensemble of diffusing particles.

In the remainder of this thesis, we will encounter only additive noise. For additive noise, the dynamics described by a Langevin equation are independent of the chosen convention. Hence, for the remainder of this thesis, we will be able to simulate particle trajectories using the Euler-Maruyama method presented in Equation (2.9).

2.2 Fokker-Planck equation

The evolution of a particle's position described by a Langevin equation can be equivalently encoded by the probability density $P(x, t)$ to observe the particle at a position x at time t . The evolution of a probability density is governed by a ‘‘Fokker-Planck equation’’ [62]. The Fokker-Planck equation describing the same dynamics as the Langevin equation (2.5) is

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial J(x, t)}{\partial x}, \quad (2.11)$$

where

$$J(x, t) = F(x, t)P(x, t) - D\frac{\partial P(x, t)}{\partial x}, \quad (2.12)$$

is the particle current.

I will now present the solution to the Fokker-Planck equation for two well-known cases.

2.2.1 Drift-diffusive particle

First, we consider a constant force $F(x, t) = v \in \mathbb{R}$. This describes a drift-diffusive particle with drift speed v . In this case, the Fokker-Planck equation (2.11) is most easily solved by making the coordinate transformation $x' = x + vt$. This brings the Fokker-Planck equation into a form describing freely diffusive motion, which has a well-known solution. In any case, the solution to the drift-diffusive Fokker-Planck equation is

$$P(x, t|x_0, t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left(-\frac{(x-x_0-v(t-t_0))^2}{4D(t-t_0)}\right), \quad (2.13)$$

for a particle initialised at position x_0 at time t_0 , i.e. $P(x, t_0) = \delta(x-x_0)$. By comparing Equation (2.13) to the standard form for a Gaussian distribution of mean μ and variance σ^2 ,

$$G(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right), \quad (2.14)$$

we identify that the particle's average position drifts away from its initial position with time, i.e. $\langle x(t) \rangle = x_0 + v(t-t_0)$, while its variance around this average position (also known as the mean square displacement) increases linearly with time, i.e. $\langle (x(t) - \langle x(t) \rangle)^2 \rangle = 2D(t-t_0)$. More generally, the time-dependent n^{th} moment of particle position is given by

$$\langle x^n(t) \rangle = \int_{-\infty}^{\infty} dx x^n P(x, t|x_0, t_0). \quad (2.15)$$

The mean and variance of the particle position could equally have been derived from

the Langevin equation in the following way. Starting from Equation (2.6), we obtain the following solution to the drift-diffusive Langevin equation,

$$x(t) = x_0 + v(t - t_0) + \sqrt{2D} \int_{t_0}^t dt' \xi(t'). \quad (2.16)$$

Taking an ensemble average of Equation (2.16), the noise term proportional to $\sqrt{2D}$ vanishes, see Equation (2.7), whence we immediately obtain $\langle x(t) \rangle = x_0 + v(t - t_0)$. The variance is then calculated from

$$\langle (x(t) - \langle x(t) \rangle)^2 \rangle = 2D \left\langle \int_{t_0}^t dt' \int_{t_0}^t dt'' \xi(t') \xi(t'') \right\rangle = 2D(t - t_0), \quad (2.17)$$

where we have used the result of Equation (2.8) to evaluate the ensemble average, recognising here that $\Delta t = t - t_0$.

2.2.2 Ornstein-Uhlenbeck process

The second case we will consider is the Ornstein-Uhlenbeck process [63], where a particle diffuses in a harmonic potential, i.e. $F(x, t) = -U'(x)$, where $U(x) = kx^2/2$ and $k > 0$ is the strength of the potential $U(x)$. The Ornstein-Uhlenbeck process is particularly important because it is the only non-trivial process that is stationary, Gaussian, and Markovian. Here, “stationary” means the Ornstein-Uhlenbeck process can attain a non-trivial steady-state density. This is a consequence of the confining, or “mean-reverting”, nature of the potential. A Markov process is one in which its probabilities for changing state depend only on the state at the current moment in time t and not on any state at an earlier time $t' < t$.

The solution to the Fokker-Planck equation describing the Ornstein-Uhlenbeck process is given by

$$P(x, t | x_0, t_0) = \sqrt{\frac{k}{2\pi D (1 - e^{-2k(t-t_0)})}} \exp \left(-k \frac{(x - x_0 e^{-k(t-t_0)})^2}{2D (1 - e^{-2k(t-t_0)})} \right), \quad (2.18)$$

whence we identify the average particle position as $\langle x(t) \rangle = x_0 \exp(-k(t - t_0))$, and its variance as $\langle (x(t) - \langle x(t) \rangle)^2 \rangle = D (1 - \exp[-2k(t - t_0)]) / k$. The latter tells us that a stronger potential tends to confine the particle closer to the origin while greater diffusion allows the particle to explore a larger region of space. Dependence on the initial conditions is seen to decay with a rate depending only on the strength of the potential k . Any memory of initial conditions is completely lost in the steady-state limit $t - t_0 \rightarrow \infty$, which is a consequence of the system’s ergodicity. In this limit, the system has a steady-state density given by the simple expression

$$P(x) = \sqrt{\frac{k}{2\pi D}} e^{-\frac{kx^2}{2D}}. \quad (2.19)$$

Equation (2.19) is an example of a Boltzmann distribution. A Boltzmann distribution

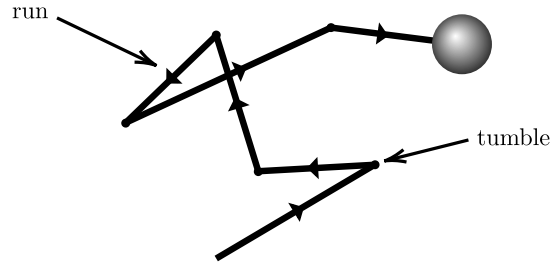


Figure 2.1: Schematic illustration of a particle undergoing diffusionless run-and-tumble motion in two dimensions.

describes the steady-state probability density of an equilibrium system, and is characterised by being proportional to $\exp(-U(x)/D)$ (in units where friction $\gamma = 1$). If a system’s steady-state density does not have the same form as a Boltzmann distribution, then this indicates that the system is likely non-equilibrium.

As for the drift-diffusive case in Section 2.2.1, we could have equally derived the mean and variance of the particle position from the solution to the Langevin equation (2.6) in an analogous way.

2.3 Canonical active particle models

With the machinery of the Langevin equation and Fokker-Planck equation in place, I will now give brief overviews of the canonical active particle models. The white noise considered in this section will be of unit variance, i.e. $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$.

2.3.1 Run-and-tumble

A paradigmatic model of active motility is the run-and-tumble (RnT) particle. RnT particles idealise the piecewise-ballistic locomotion of *Escherichia coli* bacteria [64–66]. RnT particles undergo a random walk consisting of ballistic self-propelled “runs” interspersed with exponentially distributed changes in direction, known as “tumbles” [29]. I have illustrated this in Figure 2.1. Each tumble is assumed to be instantaneous and, in dimensions greater than one, draws from a continuous distribution of possible directions. In one dimension, RnT dynamics simplify significantly to that of a particle switching between two directions of motion [19, 22, 67]. In this regime, models of confined RnT particles can possess non-equilibrium steady states that are analytically accessible [19, 21, 26, 27, 42, 68, 69], making them an attractive route to studying non-equilibrium phenomena analytically.

Here, I will go over the details only for the simpler one-dimensional RnT model, as this is the case that will be mainly considered in this thesis. The Langevin equation for the position of a run-and-tumble particle in one dimension is

$$\dot{x}(t) = v\sigma(t) + \sqrt{2D}\xi(t), \quad (2.20)$$

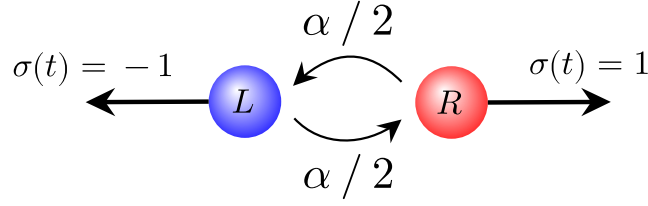


Figure 2.2: Schematic illustration of the telegraphic noise acting on a RnT particle in one dimension. The RnT particle switches between left-moving $\sigma(t) = -1$ (blue sphere marked “L”) and right-moving $\sigma(t) = 1$ (red sphere marked “R”) states with an effective rate $\alpha/2$.

where $v > 0$ is the constant self-propulsion speed of the RnT particle, and $\sigma(t) \in \{1, -1\}$ is “telegraphic noise”. The telegraphic noise switches sign with a Poissonian (i.e. average) rate $\alpha/2$. Here, α is the “tumble rate” and is conventionally twice that of the effective switching rate to account for tumbles that do not result in a change in direction. This convention is necessary if one wants to preserve the correct mapping between the one-dimensional and higher-dimensional RnT models [70]. I have schematised the telegraphic noise acting on a one-dimensional RnT particle in Figure 2.2.

As stated above, RnT motion in one dimension is essentially the switching of a particle’s self-propulsion between two different directions. If we refer to $\sigma(t) = 1$ as a “right-moving state” and $\sigma(t) = -1$ as a “left-moving state”, then we can equivalently represent the one-dimensional RnT particle model by the following coupled Fokker-Planck equations,

$$\frac{\partial P_R(x, t)}{\partial t} = D \frac{\partial^2 P_R(x, t)}{\partial x^2} - v \frac{\partial P_R(x, t)}{\partial x} - \frac{\alpha}{2} (P_R(x, t) - P_L(x, t)), \quad (2.21a)$$

$$\frac{\partial P_L(x, t)}{\partial t} = D \frac{\partial^2 P_L(x, t)}{\partial x^2} + v \frac{\partial P_L(x, t)}{\partial x} - \frac{\alpha}{2} (P_L(x, t) - P_R(x, t)), \quad (2.21b)$$

where $P_{R/L}(x, t)$ is the probability density to observe the RnT particle in the right/left-moving state at a position x at time t .

2.3.2 Active Brownian

The active Brownian particle (ABP) is the only canonical active particle model that does not admit a one-dimensional description. Similarly to RnT particles, ABPs have a constant self-propulsion speed. However, rather than experiencing *abrupt* changes in their self-propulsion direction, their direction instead diffuses *continuously* over time [30, 70, 71]. Using bold characters to represent vectors, the time evolution of the position of an ABP in two dimensions is described by the following Langevin equation,

$$\dot{\mathbf{x}}(t) = v \mathbf{n}(t) + \sqrt{2D} \boldsymbol{\xi}(t), \quad (2.22)$$

where $v > 0$ is the particle self-propulsion speed, $\mathbf{n} = (\cos(\theta), \sin(\theta))^T$ is the unit director specifying the orientation of the ABP, and θ is the two-dimensional polar angle. In two

dimensions, the statistics of the white noise $\boldsymbol{\xi}(t) = (\xi_1(t), \xi_2(t))^T$ are generalised to

$$\langle \boldsymbol{\xi}(t) \rangle = \mathbf{0}, \quad (2.23a)$$

$$\langle \boldsymbol{\xi}(t_2) \boldsymbol{\xi}^T(t_1) \rangle = \mathbb{1}_2 \delta(t_2 - t_1), \quad (2.23b)$$

where $\mathbb{1}_2$ is the 2×2 identity matrix. The angular dynamics are themselves specified by another Langevin equation,

$$\dot{\theta} = \sqrt{2D_{\text{rot}}} \eta(t), \quad (2.24)$$

where D_{rot} is the *rotational* diffusion constant and $\eta(t)$ is another white-noise term, i.e.

$$\langle \eta(t) \rangle = 0, \quad (2.25a)$$

$$\langle \eta(t_2) \eta(t_1) \rangle = \delta(t_2 - t_1). \quad (2.25b)$$

The two different white-noise terms are uncorrelated, i.e. $\langle \eta(t_2) \xi_i(t_1) \rangle = 0$ for any $i \in \{1, 2\}$.

The equivalent Fokker-Planck equation for ABPs is

$$\frac{\partial P(\mathbf{x}, \theta, t)}{\partial t} = D \nabla^2 P(\mathbf{x}, \theta, t) + D_{\text{rot}} \frac{\partial^2 P(\mathbf{x}, \theta, t)}{\partial \theta^2} - v \mathbf{n} \cdot \nabla P(\mathbf{x}, \theta, t), \quad (2.26)$$

where ∇ is the differential operator.

The more complicated dynamics of ABPs means their steady-state distributions in confining potentials are less amenable to a fully analytic treatment. However, one particular example of an exactly solvable ABP model can be found in Ref. [72].

Aside from modelling synthetic Janus particles [11, 12], ABP dynamics are often adopted for the constituent particles of the Vicsek model [33]. The Vicsek model attempts to capture aspects of flocking behaviour by allowing the orientation vectors of nearest neighbouring particles (or particles within a certain radius of another) to align.

2.3.3 Active Ornstein-Uhlenbeck

Lastly, active Ornstein-Uhlenbeck particles (AOUPs) are a generalisation of the Ornstein-Uhlenbeck process presented in Section 2.2.2, where the particle's self-propulsion undergoes an Ornstein-Uhlenbeck process [73], i.e.

$$\dot{x}(t) = v(t) + \sqrt{2D} \xi(t), \quad (2.27)$$

with

$$\dot{v}(t) = -\mu v(t) + \sqrt{2D_v} \eta(t), \quad (2.28)$$

where μ^{-1} assumes the role of a typical persistence time, and D_v (which has units of velocity squared per unit time) quantifies the size of the fluctuations in the particle's self-propulsion speed $v(t)$. As for the ABP model above, the zero-mean white-noise terms $\xi(t)$ and $\eta(t)$ are independent and have unit variance.

The equivalent Fokker-Planck equation for AOUPs is

$$\frac{\partial P(x, v, t)}{\partial t} = D \frac{\partial^2 P(x, v, t)}{\partial x^2} + D_v \frac{\partial^2 P(x, v, t)}{\partial v^2} - v \frac{\partial P(x, v, t)}{\partial x} + \mu \frac{\partial}{\partial v} (v P(x, v, t)). \quad (2.29)$$

AOUPs are a particularly attractive route for modelling non-equilibrium systems due to their simplicity compared to ABPs. For instance, the solution to the AOUP model in higher dimensions merely factorises into products of the one-dimensional solution [74]. In the absence of an external force, AOUPs are also equivalent to inertial Brownian particles, i.e. Brownian particles described by the underdamped Langevin equation (2.1).

2.3.4 Mappings to other non-equilibrium systems

Often, the dynamics of a non-equilibrium system can be mapped to another simply by reimagining the meaning of the system’s parameters. This can sometimes afford a better vantage point, which I will make use of in Chapter 6. However, to briefly illustrate this idea, consider the Langevin equation for a run-and-tumble particle in a harmonic potential

$$\dot{x}(t) = v\sigma(t) - kx(t) + \sqrt{2D}\xi(t), \quad (2.30)$$

where $k > 0$ is the strength of the harmonic potential and all other symbols retain the same meanings from Section 2.3.1. By rewriting the first two terms on the right-hand side of Equation (2.30) as $-k(x(t) - v\sigma(t)/k)$, the Langevin equation can be seen to also represent a (non-active) Brownian particle diffusing in a harmonic potential whose trap centre switches stochastically between the two positions $\pm v/k$.¹ Though their interpretations are different, this mapping demonstrates that the dynamics of the two systems are exactly the same in spite of the constituent particles of one system being passive and that of the other being active. The Brownian particle in a fluctuating potential perspective arguably offers a more intuitive view as to why particles tend to accumulate at positions $\pm v/k$, as originally found for RnT particles subject to a stationary harmonic potential in Ref. [42].

2.4 Mean square displacement

Consider now that each of the Langevin equations for the canonical active particle models in Section 2.3 can be written in the general form

$$\dot{x}(t) = w(t) + \sqrt{2D}\xi(t), \quad (2.31)$$

where $w(t)$ is a generic “active noise” that can be specialised to represent any of the canonical active particle models, e.g. $w(t) = v\sigma(t)$ for RnT particles in one dimension, where $\sigma(t)$ is telegraphic noise. Equation (2.31) also readily generalises to higher dimensions, such as for ABPs, by replacing each time-dependent quantity with a corresponding vector. For simplicity, I will continue to consider only the one-dimensional case, but note that the

¹I thank Emir Sezik for drawing my attention to this.

results of this section easily generalise to higher dimensions in a manner similar to that described above for Equation (2.31).

The similarities between the active particle models also extend to the statistics of the active noise. In particular, the active noises for the canonical models all satisfy

$$\langle w(t) \rangle = 0, \quad (2.32a)$$

$$\langle w(t_2)w(t_1) \rangle = \bar{w}^2 e^{-\frac{|t_2-t_1|}{\tau_p}}, \quad (2.32b)$$

where $\bar{w}^2$ is the typical magnitude squared of the self-propulsion speed, i.e. $\bar{w}^2 = v^2$ for RnT and ABPs, and $\bar{w}^2 = D_v/\mu$ for AOUPs, while τ_p is the typical persistence time of the active particle, i.e. $\tau_p = 1/\alpha$ for RnT particles, $\tau_p = 1/D_{\text{rot}}$ for ABPs, and $\tau_p = 1/\mu$ for AOUPs.

The solution to Equation (2.31) is given by

$$x(t) = \int_0^t dt' w(t') + \sqrt{2D} \int_0^t dt' \xi(t'), \quad (2.33)$$

assuming initialisation $x(0) = 0$ for simplicity. It is easy to see that $\langle x(t) \rangle = 0$ for all t in the absence of a non-trivial initialisation due to the active and thermal noise both being mean zero. Then, the mean square displacement of an active particle governed by Equation (2.31) is

$$\langle x^2(t) \rangle = \int_0^t dt' \int_0^t dt'' \langle w(t')w(t'') \rangle + 2D \int_0^t dt' \int_0^t dt'' \langle \xi(t')\xi(t'') \rangle. \quad (2.34)$$

The second double integral on the right-hand side of Equation (2.34) was already evaluated in Equation (2.8). After inserting the expression for $\langle w(t')w(t'') \rangle$ from Equation (2.32b) into Equation (2.34), then performing the resulting integration over the active noise in a similar manner to Equation (2.8), we eventually obtain for the mean square displacement of any of the canonical active particle models,

$$\langle x^2(t) \rangle = 2Dt + 2\bar{w}^2\tau_p^2 \left(e^{-t/\tau_p} - 1 + \frac{t}{\tau_p} \right). \quad (2.35)$$

A more detailed evaluation of the integral over the active noise can be found in Section 8.C of Chapter 8. In higher dimensions, Equation (2.35) generalises by simply multiplying the contribution from the diffusion $2Dt$ by the number of dimensions d .

By expanding the exponential term as a Taylor series, we find, at short times $t \ll \tau_p$,

$$\langle x^2(t) \rangle = 2Dt + \bar{w}^2 t^2 + \mathcal{O}((t/\tau_p)^3). \quad (2.36)$$

Thus, the mean square displacement initially scales linearly with time t , due to the thermal diffusion, before scaling quadratically (ballistically) due to the self-propelled motion.

On the other hand, we find at large times $t \gg \tau_p$,

$$\langle x^2(t) \rangle \approx 2(D + \bar{w}^2 \tau_p) t, \quad (2.37)$$

corresponding to long-time diffusive behaviour with an effective diffusion constant $D + \bar{w}^2 \tau_p$.

2.5 Entropy production

As mentioned in the introduction to this thesis, a system's entropy production quantifies the degree to which its dynamics break time-reversal symmetry. In this section, I give a derivation of the average entropy production of the drift-diffusive particle introduced in Section 2.2.1 of this chapter, before generalising it to that of generic active particles. This derivation will be based off similar calculations in Refs. [21, 26, 38, 75, 76]. A drift-diffusive particle can be considered a simple model of an active particle that self-propels continuously in the same direction. As we will be interested in the steady-state entropy production, we require the system to have a non-trivial steady-state density and therefore consider the dynamics to take place on a ring of circumference $L > 0$, i.e. a one-dimensional interval with periodic boundary conditions.

There are several equivalent ways to derive the entropy production for a system, such as using path integral methods [38]. Arguably the most straightforward approach is to directly take the time derivative of the system's total entropy. The total entropy of a system involving *continuous* degrees of freedom is given by the Gibbs-Shannon entropy formula [77],

$$S(t) = - \int_0^L dx P(x, t) \log \left(\frac{P(x, t)}{P_0} \right), \quad (2.38)$$

where P_0 , which has the same dimensions as the probability density $P(x, t)$, merely exists to retain dimensional consistency in the logarithm of Equation (2.38), but will drop out of the final expression for the entropy production. Taking the time derivative of Equation (2.38) results in

$$\dot{S}(t) = - \int_0^L dx \frac{\partial P(x, t)}{\partial t} \left(\log \left(\frac{P(x, t)}{P_0} \right) + 1 \right). \quad (2.39)$$

Next, the goal is to manipulate Equation (2.39) into a form where we can readily distinguish so-called “internal” and “external” contributions. The time derivative of the probability density $\partial_t P(x, t)$ is related to the current $J(x, t)$ through Equation (2.5), i.e. $\partial_t P(x, t) = -\partial_x J(x, t)$. Inserting this expression and then integrating by parts, we obtain

$$\dot{S}(t) = - \int_0^L dx \frac{J(x, t)}{P(x, t)} \frac{\partial P(x, t)}{\partial x}, \quad (2.40)$$

where the boundary term from the integration vanishes due to the system's periodic boundary conditions. We can similarly use Equation (2.12) to rewrite $\partial_x P(x, t) = vP(x, t)/D -$

$J(x, t)/D$, whence we obtain

$$\dot{S}(t) = \int_0^L dx \left(\frac{J^2(x, t)}{DP(x, t)} - \frac{v}{D} J(x, t) \right). \quad (2.41)$$

It is convention to now decompose the time-derivative of the entropy, Equation (2.41), into two separate contributions [78], i.e. $\dot{S}(t) = \dot{S}_i(t) - \dot{S}_e(t)$, where

$$\dot{S}_i(t) = \int_0^L dx \frac{J^2(x, t)}{DP(x, t)} \geq 0 \quad (2.42)$$

is the internal entropy production, and

$$\dot{S}_e(t) = \int_0^L dx \frac{v}{D} J(x, t) \quad (2.43)$$

is the external entropy production. A more detailed calculation shows that the external entropy production is associated with changes in entropy of the reservoirs coupled to the system and is thus, as its name suggests, the entropy flux that is lost to the surroundings [38]. In contrast, the internal entropy production is always non-negative and vanishes only if the system satisfies detailed balance. Positive *internal* entropy production is therefore the signature of a non-equilibrium system. Throughout the rest of this thesis, any reference to “entropy production” can be assumed to mean the internal contribution $\dot{S}_i$.

The standard route to calculating the steady-state (internal) entropy production is to make use of $\lim_{t \rightarrow \infty} \dot{S}(t) = 0$, which is a result of $\lim_{t \rightarrow \infty} \partial_t P(x, t) = 0$ in Equation (2.39). The vanishing time-derivative of the entropy implies that $\dot{S}_i = \dot{S}_e$ at steady state, whence one can in fact use the simpler expression for the steady-state external entropy production to evaluate the steady-state internal entropy production, i.e.

$$\dot{S}_i := \lim_{t \rightarrow \infty} \dot{S}_i(t) = \int_0^L dx \frac{v}{D} J. \quad (2.44)$$

The steady-state current of the drift-diffusive system is simply $J = v/L$, as this is the average rate that the drift-diffusive particle completes a lap of the ring.² Inserting $J = v/L$ into Equation (2.44), we finally obtain

$$\dot{S}_i = \frac{v^2}{D}. \quad (2.45)$$

As we would expect, the entropy production vanishes if the particle does not self-propel, i.e. if $v = 0$. However, the entropy production also vanishes in the limit $D \rightarrow \infty$, in which the particle’s self-propulsion is completely washed out by diffusive fluctuations. Equation (2.45) also tells us that the entropy production diverges in the absence of diffusive fluctuations, i.e. $D \rightarrow 0$. This reflects that the dynamics of the system have become fully

²This could have also been deduced from Equation (2.12) by calculating the steady-state probability density, which is $P(x) = 1/L$.

irreversible—or, rather, fully deterministic. In this case, the arrow of time can always be reliably determined from a recording of the system’s dynamics, see Figure 1.1.

As it turns out, a simple generalisation of Equation (2.45) gives the entropy production for the canonical active-particle models. This generalisation is

$$\dot{S}_i = \frac{\bar{w}^2}{D}, \quad (2.46)$$

where, as in Section 2.4, $\bar{w}^2$ is the typical magnitude squared of the self-propulsion speed for any of the canonical active particle models.³ Since $\bar{w}^2 = v^2$ for RnT and ABPs, then the entropy production of these canonical active-particle models is in fact the same as that of a drift-diffusive particle for the same self-propulsion speed v and (translational) diffusion D .

2.6 Work extraction and efficiency

Lastly, I will give a brief discussion of work extraction. If a system exhibits a net current, then work can be extracted from the system by applying an external force (such as a movable obstacle or other kind of load) against the current [23, 51]. Defining the magnitude of this time-independent force as f , the average rate of work extraction $\dot{W}$ from a positive current is

$$\dot{W} = \langle \dot{x}(t) \rangle f. \quad (2.47)$$

In the case of the drift-diffusive particle subject to an external force, $\langle \dot{x}(t) \rangle = v - f$ and we thus have $\dot{W} = (v - f)f$. If $f > v$, resulting in $\dot{W} < 0$, then work is being performed *on* the system. It is easy to see that the rate of work extraction for the drift-diffusive particle is maximised for $f = v/2$, resulting in $\dot{W} = v^2/4$. This optimal external force represents a compromise between transporting as large a load as possible and not stalling the system too greatly.

For $\dot{W} > 0$, the associated thermodynamic efficiency of the work extraction is given by [21, 51]

$$\eta_{\text{th}} = \frac{\dot{W}}{\dot{E}_i} = \frac{\dot{W}}{\dot{W} + D\dot{S}_i}, \quad (2.48)$$

where $\dot{E}_i = \dot{W} + D\dot{S}_i$ is the rate that energy is dissipated by the system to sustain its dynamics. The entropy production for a drift-diffusive particle subject to an external force f is $\dot{S}_i = (v - f)^2/D$, and so its corresponding thermodynamic efficiency is $\eta_{\text{th}} = f/v$ for $f < v$. Thus, for a force resulting in optimal work extraction from a drift-diffusive particle, $f = v/2$, we find the corresponding efficiency is $\eta_{\text{th}} = 1/2$. Meanwhile, the work extraction approaches optimal efficiency of $\eta_{\text{th}} = 1$ for $f \rightarrow v^-$. In this limit, all of the particle’s self-propulsive force is being used purely to move the load, coming at the expense of an infinitesimally small rate of work extraction.

³This generalisation can be shown by an analogous derivation to that of the drift-diffusive particle [21, 26, 38]. The derivation assumes the dynamics of the systems are Markovian or, in other words, that we know the particle’s internal self-propulsion state at all times.

Harnessing an overall net current is one simple example of how to extract work from a non-equilibrium system. In Chapter 7, I will demonstrate that a feedback protocol can be used to extract work from active particle systems that do not exhibit a net current.

3

Doi-Peliti field theory—a brief derivation

The purpose of this chapter is to provide a brief overview of Doi-Peliti field theory. Since many detailed derivations of Doi-Peliti field theory already exist [79–82], this chapter acts as a more accessible alternative for readers interested only in the key details of its derivation. This chapter can also be considered a supplement to Chapter 4 for those who wish to gain a deeper understanding of the main derivation in the latter.

In Doi-Peliti field theory, the stochastic dynamics of a system are reformulated as a path integral. Path integrals were first introduced by Norbert Wiener in his pioneering work on Brownian motion [83–85], but are perhaps more commonly associated with quantum field theory due to major developments made by Paul Dirac and Richard Feynman in the 1930s and 40s [86, 87]. The more recent foundations of Doi-Peliti field theory were laid by Masao Doi in the 1970s after he repurposed the second quantisation procedure from quantum field theory to provide a compact Fock-space representation of a classical many-particle system [88, 89]. Luca Peliti then extended this idea by reformulating the Fock-space representation as a path integral for the case of birth-death processes on a lattice [90]. Since its inception, Doi-Peliti field theory has become a well-established formalism in statistical mechanics, with its most notable applications being to active matter [42, 70, 74, 91–94], and epidemiological processes such as branching [95–99].

In truth, using Doi-Peliti field theory to solve the governing equation of a system is mathematically analogous to using standard techniques. Yet, Doi-Peliti field theory, and statistical field theories more generally, offer much more than standard techniques alone. This was highlighted in the seminal paper by Martin, Siggia, and Rose [100], in which they formed the basis for what would later come to be known as MSR field theory (predating even Doi-Peliti). In this paper, the authors noted “there is not to our knowledge a satisfactory theory [of classical systems] with the utility, generality, and precision of the quantum-field theories. [...] Although a classical procedure does not exist, the value of a practical scheme would be enormous.” One of the key distinguishing features of statistical field theories is that they can make perturbative calculations more transparent. In particular, the terms of a perturbation series can be economically represented by Feynman diagrams, which offer an intuitive visualisation of the microscopic processes taking place in the system. The diagrammatic rules associated with these diagrams, in turn, make the perturbative calculations more tractable. Field theories are also readily extensible: Any new process or interaction introduced into a system can be readily accommodated in its field-theoretic description by simply treating the new interaction as a perturbation to the existing structure. Lastly, renormalisation techniques are most naturally implemented in a field-theoretic framework [81, 101–103].

Doi-Peliti field theory is particularly well-suited to describing reaction-diffusion systems, i.e. stochastic systems involving a chemical-reaction-like exchange between diffusive particles. Some examples of reaction-diffusion systems include birth-death processes [90], predator-prey (Lotka-Volterra) systems [104], and run-and-tumble motion [42, 70]. This suitability is attributed to Doi-Peliti field theory being the statistical field theory that most clearly retains particle identity [105]. Not correctly tracking particle identity in a calculation can lead to erroneous results [37], as pointed out in Ref. [106].

3.1 Master equation

A possible starting point for the derivation of a Doi-Peliti field theory is to write the dynamics of a reaction-diffusion system as a master equation [101].¹ A master equation is a linear first-order differential equation that describes the time evolution of the probability for finding a system in a particular configuration or “microstate”.

In general, the master equation is constructed from gain and loss contributions to the probability that originate from the system’s microscopic reaction-diffusion processes, i.e.

$$\dot{p}(\{n\}; t) = \sum_{\{n'\} \neq \{n\}} W(\{n'\} \rightarrow \{n\}) p(\{n'\}; t) - \sum_{\{n'\} \neq \{n\}} W(\{n\} \rightarrow \{n'\}) p(\{n\}; t), \quad (3.1)$$

where $\{n\}$ is a particular microscopic configuration, and $W(s_1 \rightarrow s_2) \geq 0$ is the transition rate to go from state s_1 to state s_2 .

In constructing the master equation for a Markovian system, we consider all the processes that contribute to the system being in state $\{n\}$ at time t when going from the infinitesimally earlier time $t - \Delta t$. We assume $\Delta t > 0$ is small enough such that only one process can occur in time Δt . For instance, for a branching-decay system, we assume Δt is small enough such that only one particle can undergo a single branching *or* decay event during this time. The probability for two branching events, or branching followed by decay, to occur in this time would be of order $(\Delta t)^2$, which vanishes to leading order in Δt .

After writing down the master equation for a system, the next step is to rewrite the equation in terms of bosonic (ladder) operators in a process analogous to second quantisation in quantum field theory.

3.2 Second quantisation

The master equation (3.1) is written in the language of second quantisation as per Doi’s original method [89]. This first involves promoting the probability $p(\{n\}; t)$ to a probability generating function $\psi(z, t)$. As an example, for multiple particles that live on a lattice,

¹One could alternatively start from a Fokker Planck equation, as in Refs. [42, 74]. However, starting from a master equation is more illustrative and provides the most intuition, as one first lists all of the system’s relevant microscopic processes.

the relation between the probability and probability generating function is given by

$$\psi(z, t) = \sum_{\{n\}} p(\{n\}; t) \dots z_{i-1}^{n_{i-1}} z_i^{n_i} z_{i+1}^{n_{i+1}} \dots, \quad (3.2)$$

where the sum is over all possible microstates $\{n\} = \{\dots n_{i-1}, n_i, n_{i+1}, \dots\}$ of the number of particles that occupy each site i , and $z_i^{n_i}$ represents that n_i particles of species z reside at site i . Each z can thus be thought of as representing a single indistinguishable particle. Equation (3.2) is easily generalised to multiple particle species (or distinguishable particles) by allowing a different symbol to represent each species, e.g. z and y in the case of two different species.

In analogy to the wavefunction from quantum mechanics, the probability generating function can be rewritten in terms of orthonormal states of a Fock space, i.e.

$$|\psi(t)\rangle = \sum_{\{n\}} p(\{n\}; t) |\dots, n_i, \dots\rangle, \quad (3.3)$$

where $|\dots, n_i, \dots\rangle$ denotes a state in which there are n_i particles at site i .

Bosonic operators can be readily applied to the probability generating function to either decrease or increase the number of particles at a particular site. The creation operator $a_i^\dagger$ has the effect of adding a particle at site i , i.e.

$$a_i^\dagger |\dots n_{i-1}, n_i, n_{i+1} \dots\rangle = |\dots n_{i-1}, n_i + 1, n_{i+1} \dots\rangle, \quad (3.4)$$

whilst the annihilation operator a_i removes a particle at site i ,

$$a_i |\dots n_{i-1}, n_i, n_{i+1} \dots\rangle = n_i |\dots n_{i-1}, n_i - 1, n_{i+1} \dots\rangle. \quad (3.5)$$

In terms of the original notation used in Equation (3.2), a creation operator is represented by z_i and an annihilation operator by ∂_{z_i} . Repeated application of the bosonic operators generalises in the expected way, e.g. $(a_i^\dagger)^k |\dots n_{i-1}, n_i, n_{i+1} \dots\rangle = |\dots n_{i-1}, n_i + k, n_{i+1} \dots\rangle$. Henceforth, to ease notation, I will omit the explicit site-dependence of the operators and occupation numbers for the rest of this section, thereby rendering the following a derivation for a spatially independent system. However, it should be emphasised that the generalisation to multiple lattice sites is easily performed in a manner analogous to Equations (3.4) and (3.5).

The number operator $\hat{N} = a^\dagger a$ is a composite operator that extracts the particle number without changing the state of the system, i.e.

$$\hat{N} |n\rangle = a^\dagger a |n\rangle = a^\dagger n |n-1\rangle = n a^\dagger |n-1\rangle = n |n\rangle. \quad (3.6)$$

The ordering of the bosonic operators in the number operator is important because they

do not commute. This can be seen from their non-vanishing commutator,

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1, \quad (3.7)$$

which can be verified by explicit operation of the commutator on a state, e.g. $[a, a^\dagger] |n\rangle = |n\rangle$.

In addition, we define the vacuum state as the state with no particles (at every lattice site in a space-dependent system), which results in the following property:

$$a |0\rangle = 0, \quad (3.8)$$

reflecting that a particle cannot be removed from the state that already has no particles. This convention is used so that the ground-state energy of a system vanishes for a “normal-ordered” Hamiltonian. An operator is in normal-ordered form if all of its constituent creation operators act after all of the constituent annihilation operators. In other words, in any product of creation and annihilation operators, all creation operators must be to the left of all annihilation operators. If an operator is not already in normal-ordered form, then it can (and must) be brought into normal ordered form through the commutation relation, i.e. one can replace any product $aa^\dagger$ with $1 + a^\dagger a$ as a result of Equation (3.7).

The second quantisation procedure is completed by obtaining a differential equation for the probability generating function in terms of the bosonic operators. To demonstrate this, I will consider a system consisting of only a single lattice site where particles residing at this site undergo radioactive decay with rate $r > 0$. As a reaction, this can be represented by $A \xrightarrow{r} \emptyset$ for a species A . The master equation for this system reads

$$\dot{p}(n; t) = r [(n + 1)p(n + 1; t) - np(n; t)]. \quad (3.9)$$

We first take a time derivative of Equation (3.3), and insert the right-hand side of the master equation (3.9) in place of the resulting $\dot{p}(n; t)$, i.e.

$$\frac{\partial |\psi(t)\rangle}{\partial t} = \sum_{n=0}^{\infty} \dot{p}(n; t) |n\rangle = \sum_{n=0}^{\infty} r [(n + 1)p(n + 1; t) - np(n; t)] |n\rangle. \quad (3.10)$$

After this, any n -dependent factors can be replaced by normal-ordered products of $a^\dagger$ and a using Equations (3.4), (3.5), and (3.7). This results in

$$\frac{\partial |\psi(t)\rangle}{\partial t} = \sum_{n=0}^{\infty} r [p(n + 1; t) a |n + 1\rangle - p(n; t) a^\dagger a |n\rangle]. \quad (3.11)$$

The sums in Equation (3.11) now need to be rewritten in terms of $|\psi(t)\rangle$. This is readily performed for the sum over terms proportional to $p(n; t)$. However, for the sum over terms proportional to $p(n + 1; t)$, we first need to make the substitution $n' = n + 1$, whence we

obtain

$$\frac{\partial |\psi(t)\rangle}{\partial t} = ra \sum_{n'=1}^{\infty} p(n'; t) |n'\rangle - ra^\dagger a \sum_{n=0}^{\infty} p(n; t) |n\rangle. \quad (3.12)$$

The first summation now runs from $n' = 1$ to infinity. However, by asserting $p(n < 0; t) = 0$, i.e. it is impossible to observe a negative number of particles, then $p(n' = 0; t) = 0$ and so the lower limit of the sum can be lowered to $n' = 0$ without changing its result. After doing this, we finally obtain

$$\frac{\partial |\psi(t)\rangle}{\partial t} = ra \sum_{n'=0}^{\infty} p(n'; t) |n'\rangle - ra^\dagger a \sum_{n=0}^{\infty} p(n; t) |n\rangle \quad (3.13a)$$

$$= ra |\psi(t)\rangle - ra^\dagger a |\psi(t)\rangle \quad (3.13b)$$

$$= r (a - a^\dagger a) |\psi(t)\rangle, \quad (3.13c)$$

where we have used the definition of the probability generating function, Equation (3.3).

Finally, we introduce the Doi shift,

$$a^\dagger = 1 + \tilde{a}, \quad (3.14)$$

where $\tilde{a}$ is known as the Doi-shifted creation operator [80]. Going forward, all creation operators will be replaced by their Doi-shifted counterpart as per Equation (3.14). The rigorous justification for this is beyond the scope of this brief overview. Essentially, the Doi-shift is introduced to simplify the calculations one encounters when deriving observables from the action (see Section 3.3). However, as the shift between $a^\dagger$ and $\tilde{a}$ is merely a constant, the actual *physics* of a system is agnostic to the Doi-shift. After applying the Doi shift, the differential equation describing the radioactive system, Equation (3.13), becomes

$$\frac{\partial |\psi(t)\rangle}{\partial t} = -r\tilde{a}a |\psi(t)\rangle. \quad (3.15)$$

More generally, the probability generating function for a reaction-diffusion system satisfies a Schrödinger-like equation of the form

$$\frac{\partial |\psi(t)\rangle}{\partial t} = \mathcal{H}(\tilde{a}, a) |\psi(t)\rangle, \quad (3.16)$$

which has the formal solution

$$|\psi(t)\rangle = e^{\mathcal{H}(\tilde{a}, a)t} |\psi(0)\rangle. \quad (3.17)$$

The operator $\mathcal{H}(\tilde{a}, a)$ encompasses the original reaction-diffusion processes described by the master equation (3.1). It can be thought of as a classical Hamiltonian operator and we will therefore refer to it as such.² The Hamiltonian is the generator of time translations

²Strictly speaking, $\mathcal{H}$ is a Liouvillian operator.

since $\mathcal{U}(t) = \exp(\mathcal{H}t)$ is the time-evolution operator, i.e. operating $\mathcal{U}(t)$ on any state at time t_0 evolves the system to a time $t + t_0$.

3.3 Action

Calculating the state of the system at time t after initialisation, i.e. $|\psi(t)\rangle$, requires an explicit form of the time-translation operator $\mathcal{U}(t) = \exp(\mathcal{H}t)$. Hence, we need to calculate the exponential of the Hamiltonian. Exponentiating the Hamiltonian is what ultimately produces the path integral in Doi-Peliti field theory. This is a complicated procedure, but ultimately amounts to promoting the bosonic operators to time-dependent (and possibly space-dependent) fields, i.e. $a \rightarrow \phi(t)$ and $\tilde{a} \rightarrow \tilde{\phi}(t)$.³ Then, after suitable coarse-graining, one recovers the action for a Doi-Peliti field theory. For a system with a single spatial dimension, the action is generally of the form

$$\mathcal{A}[\tilde{\phi}, \phi] = - \int_{-\infty}^{\infty} dt \int dx \left(\tilde{\phi}(x, t) \frac{\partial}{\partial t} \phi(x, t) - \mathcal{H}[\tilde{\phi}, \phi] \right), \quad (3.18)$$

which is a *functional* of the fields $\phi(t)$ and $\tilde{\phi}(t)$. The overall sign in front of the integral in Equation (3.18) is a matter of convention and depends on whether the action appears in the path integral as $\exp(-\mathcal{A})$ or $\exp(\mathcal{A})$. The sign in Equation (3.18) is consistent with the latter convention. Depending on the form of the Hamiltonian $\mathcal{H}$, the action $\mathcal{A}$ will contain bilinear terms (terms that are at most linear in both ϕ and $\tilde{\phi}$) and may also contain non-bilinear “interaction” terms, which are dealt with perturbatively. As a result, the action is typically split into two components, $\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_i$, where $\mathcal{A}_0$ is the bilinear part, containing only bilinear terms, and $\mathcal{A}_i$ is the perturbative part, encompassing the remaining non-bilinear terms.⁴

The interpretation of $\tilde{\phi}(x, t)$ creating a particle at position x and time t still holds at this level of description. However, $\phi(x, t)$ may now be better thought of as the act of *measuring* the system at a position x and time t . The reason for this will become clearer below, where we will also see that observables involving n copies of ϕ tend to represent n -point correlations.

If the system under consideration lacks spatial dependence then the integral over all space is simply omitted from Equation (3.18). For instance, by reading off its Hamiltonian from Equation (3.15), our example system undergoing radioactive decay has a corresponding action given by

$$\mathcal{A}[\tilde{\phi}, \phi] = - \int_{-\infty}^{\infty} dt \tilde{\phi}(t) \left(\frac{\partial}{\partial t} + r \right) \phi(t), \quad (3.19)$$

which contains only bilinear terms.

³The fields $\phi(t)$ and $\tilde{\phi}(t)$ arise from introducing coherent states $|\phi\rangle = \sum_n \phi^n |n\rangle / n! = \exp(\phi a^\dagger) |0\rangle$ and $\langle\phi^\dagger| = \sum_n \langle n| (\phi^\dagger)^n / n! = \langle 0| \exp(\phi^\dagger a)$. These coherent states are eigenfunctions of the bosonic operators and their eigenvalues are in fact the fields, i.e. $a|\phi\rangle = \phi|\phi\rangle$ and $\langle\phi^\dagger| \tilde{a} = \langle\phi^\dagger| (\phi^\dagger - 1) = \langle\phi^\dagger| \tilde{\phi}$. Derivations of the path integral can be found in Refs. [79, 107].

⁴Certain bilinear terms may be more easily treated perturbatively, such as those representing external potentials or a transmutation reaction [28, 42, 70]. These terms can also be absorbed into $\mathcal{A}_i$.

3.4 Bare propagator

Observables $\mathcal{O}$ in Doi-Peliti field theory are products of $\tilde{\phi}$ and ϕ , and are calculated from path integrals involving the action,

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi \mathcal{O} e^{\mathcal{A}}, \quad (3.20)$$

where $\mathcal{D}\tilde{\phi} \mathcal{D}\phi$ is a functional integration measure that also accounts for the overall normalisation of the path integral. The key ingredient to any field theory is a specific observable known as the “bare propagator”. The bare propagator is given by

$$\langle \phi(x, t) \tilde{\phi}(x_0, t_0) \rangle_0 = \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi \phi(x, t) \tilde{\phi}(x_0, t_0) e^{\mathcal{A}_0}, \quad (3.21)$$

where the subscript “0” on the expectation value in Equation (3.21) signifies that the path integral is being performed with respect to the bilinear part of the action $\mathcal{A}_0$. With the interpretation of the fields $\tilde{\phi}$ and ϕ as “creating a particle” and “measuring the system”, respectively, the interpretation of the propagator is that a single particle is created at position x_0 and time t_0 , and then the probability density for finding this particle at a position x is subsequently measured at time t . The bare propagator is thus, as its name suggests, the propagator for a stochastic system in the absence of non-linear interactions.

The diagrammatic representation of the bare propagator is a single line,

$$\langle \phi(x, t) \tilde{\phi}(x_0, t_0) \rangle_0 \equiv \begin{array}{c} x, t \\ \text{---} \\ x_0, t_0 \end{array}. \quad (3.22)$$

This highlights the centralness of the bare propagator to any field theory, since more complicated diagrams, representing higher-order interactions, are constructed only from these lines and vertices that join these lines together. As we will see later, the allowed vertices for the field theory of a particular system are determined by the terms contained in $\mathcal{A}_i$.

In Feynman diagrams, such as in Equation (3.22), time is read from right to left. While this peculiarity is often attributed to a matter of convention, it actually hints at a deeper connection. In particular, for systems involving multiple particle species, each Feynman diagram represents a matrix, and so the stitching together of two lines via a vertex can be viewed as matrix multiplication. To be consistent with the ordering of matrix multiplication going from right to left, each diagram similarly needs to be read from right to left.

An explicit expression for the bare propagator is obtained by first rewriting the path

integral in Equation (3.21) in terms of functional derivatives of source terms J and $\tilde{J}$ [79],⁵

$$\langle \phi(t) \tilde{\phi}(t_0) \rangle_0 = \frac{\delta}{\delta J(t)} \frac{\delta}{\delta \tilde{J}(t_0)} \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi e^{\mathcal{A}_0 + \int dt' (J(t')\phi(t') + \tilde{J}(t')\tilde{\phi}(t'))} \Big|_{J=0, \tilde{J}=0}, \quad (3.24)$$

where, for simplicity, any spatial degrees of freedom have been omitted. The equivalent derivation for a space-dependent system is analogous to the following. Since the action $\mathcal{A}_0$ in Equation (3.24) is bilinear, the path integral is simply a Gaussian integral over the fields $\tilde{\phi}$ and ϕ that can be readily evaluated [108], resulting in

$$\langle \phi(t) \tilde{\phi}(t_0) \rangle_0 = \frac{\delta}{\delta J(t)} \frac{\delta}{\delta \tilde{J}(t_0)} e^{\int dt' \tilde{J}(t') \mathbf{A}_t^{-1} J(t')} \Big|_{J=0, \tilde{J}=0}, \quad (3.25)$$

where $\mathbf{A}_t$ is the bilinear action operator, defined through

$$\mathcal{A}_0[\tilde{\phi}, \phi] = - \int_{-\infty}^{\infty} dt \tilde{\phi}(t) \mathbf{A}_t \phi(t). \quad (3.26)$$

In going from Equation (3.24) to Equation (3.25), we omitted any overall factors that may arise from the integration. This is because these factors can simply be absorbed into the normalisation of the path integral itself.

For systems involving multiple particle species, $\mathbf{A}_t$ is generally a matrix. Since $\mathbf{A}_t$ contains a time-derivative operation, its inverse is more easily determined by recasting the bare propagator in terms of Fourier-space variables. After performing a Fourier transform, the non-local time derivative in $\mathbf{A}_t$ becomes a local scalar in Fourier space.⁶ We then obtain the following expression for the bare propagator in Equation (3.25),

$$\langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle_0 = \frac{\delta}{\delta J(-\omega)} \frac{\delta}{\delta \tilde{J}(-\omega_0)} e^{\int d\omega' \tilde{J}(\omega') \mathbf{A}_{\omega'}^{-1} J(-\omega')} \Big|_{J=0, \tilde{J}=0}, \quad (3.28)$$

where I now introduce $d\omega = d\omega/(2\pi)$ and correspondingly $\delta(\omega + \omega_0) = 2\pi\delta(\omega + \omega_0)$. Then,

⁵Functional differentiation is mostly analogous to regular differentiation but with some subtleties. The key property that will be needed for the following derivation is

$$\frac{\delta J(t)}{\delta J(t')} = \delta(t - t'), \quad (3.23)$$

which can be seen more clearly by first writing $J(t) = \int dt' J(t')\delta(t - t')$.

⁶The convention used for the (inverse) Fourier transform over time and space is

$$\phi(x, t) = \int d\omega dk \phi(k, \omega) e^{ikx - i\omega t}. \quad (3.27)$$

performing the functional differentiation in Equation (3.28), we obtain

$$\begin{aligned}\langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle_0 &= \frac{\delta}{\delta J(-\omega)} \frac{\delta}{\delta \tilde{J}(-\omega_0)} \int \tilde{d}\omega' \tilde{J}(\omega') \mathbf{A}_{\omega'}^{-1} J(-\omega') \Big|_{J=0, \tilde{J}=0} \\ &= \int \tilde{d}\omega' \delta(\omega' + \omega_0) \mathbf{A}_{\omega'}^{-1} \delta(\omega - \omega') \\ &= \mathbf{A}_{\omega}^{-1} \delta(\omega + \omega_0),\end{aligned}\tag{3.29}$$

where we have used Equation (3.23) and that $\exp(\int \tilde{d}\omega' \tilde{J}(\omega') \mathbf{A}_{\omega'}^{-1} J(-\omega'))|_{J=0, \tilde{J}=0} = 1$. Thus, the bare propagator in Fourier space for any system is generally given by the inverse of its bilinear action operator.

The action operator for the system undergoing radioactive decay, Equation (3.19), is given by

$$\mathbf{A}_t = \frac{\partial}{\partial t} + r,\tag{3.30}$$

which, in Fourier space, is

$$\mathbf{A}_{\omega} = -i\omega + r.\tag{3.31}$$

Thus, its bare propagator in Fourier space is

$$\langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle_0 = \frac{\delta(\omega + \omega_0)}{-i\omega + r} \equiv \underline{\omega \quad \omega_0}.\tag{3.32}$$

Since the system undergoing radioactive decay does not have any higher-order terms in its action, Equation (3.19), there are in fact no corrections to the system’s “full propagator” $\langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle$, and so one can indeed write $\langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle = \langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle_0$.

To convert a bare propagator back to “real” spacetime variables, we take the inverse Fourier transform of Equation (3.29), explicitly,

$$\langle \phi(t) \tilde{\phi}(t_0) \rangle_0 = \int \tilde{d}\omega \tilde{d}\omega_0 \langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle_0 e^{-i\omega t - i\omega_0 t_0}.\tag{3.33}$$

Equation (3.33) can be evaluated via integration over appropriately oriented semi-circular contours in the upper- and lower-complex planes of ω and ω_0 . In the case of radioactive decay, the propagator in real space is found to be

$$\langle \phi(t) \tilde{\phi}(t_0) \rangle = \langle \phi(t) \tilde{\phi}(t_0) \rangle_0 = \Theta(t - t_0) e^{-r(t-t_0)}.\tag{3.34}$$

This is equal to the expected number of particles in the system at time t given a single particle is initialised at time t_0 . Here, the Heaviside step function $\Theta(t - t_0)$ represents this initialisation, but it more generally introduces causality into the field theory, i.e. the system does not evolve in time until it is initialised at time t_0 .

While the decay rate $r > 0$ for the example system of this chapter happened to have

an actual physical meaning, in general a similar “mass” term needs to be artificially added to the bilinear part of the Doi-Peliti action for *any* system. The reason for this is to regularise the infrared divergence one would otherwise obtain when performing the contour integration in Equation (3.33). This can be seen from taking $r \rightarrow 0$ *before* the contour integration is performed, which leads to a diverging erroneous result. However, we can safely remove the mass term by taking $r \rightarrow 0$ *after* the integration, as can be seen in Equation (3.34).

We have so far demonstrated the derivation of the bare propagator for a system starting from its microscopic master equation. However, if the dynamics of a system are already given in terms of a Fokker-Planck equation, then the route to deriving the bare propagator is more straightforward. In particular, if the probability density for a single-particle system satisfies a Fokker-Planck equation of the form

$$\frac{\partial P(x_1, x_2, \dots, t)}{\partial t} = \mathcal{L} P(x_1, x_2, \dots, t), \quad (3.35)$$

where $\mathcal{L}$ is the Fokker-Planck operator and $x_1, x_2, \dots$ are the particle degrees of freedom, then the corresponding Doi-Peliti action for the system is [106]

$$\mathcal{A}[\tilde{\phi}, \phi] = - \int dx_1 dx_2 \dots dt \tilde{\phi}(x_1, x_2, \dots, t) \left[\frac{\partial}{\partial t} - \mathcal{L} \right] \phi(x_1, x_2, \dots, t), \quad (3.36)$$

whence we readily identify the action operator as $\mathbf{A}_t = \partial_t - \mathcal{L}$. Hence, given a Fokker-Planck equation for a system, one can immediately read off the corresponding bare propagator using Equation (3.29) after writing $\mathcal{L}$ in terms of Fourier space variables.

3.5 Perturbative corrections

The effect of non-linear terms on an observable $\mathcal{O}$ are calculated by performing perturbative calculations around the bilinear part of the action, i.e.

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi \mathcal{O} e^{\mathcal{A}_0 + \mathcal{A}_i} = \sum_{k=0}^{\infty} \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi \mathcal{O} \frac{\mathcal{A}_i^k}{k!} e^{\mathcal{A}_0}, \quad (3.37)$$

where we have expanded $\exp(\mathcal{A}_i)$ as a power series in the interacting part of the action $\mathcal{A}_i$. Each term in the perturbation series of Equation (3.37) is represented by a unique Feynman diagram.

As an example, consider a generalisation of the radioactive decay system where each particle can now either branch into two particles with rate s , i.e. $A \xrightarrow{s} A + A$, or decay with rate r' , $A \xrightarrow{r'} \emptyset$. A more detailed discussion of the field theory for this system is given in Refs. [79, 97]. The master equation for this more general system is

$$\dot{p}(n; t) = s [(n-1)p(n-1; t) - np(n; t)] + r' [(n+1)p(n+1; t) - np(n; t)]. \quad (3.38)$$

Performing the second quantisation procedure along the lines described in Section 3.2,

we obtain the following differential equation for the corresponding probability generating function,

$$\frac{\partial |\psi(t)\rangle}{\partial t} = [s\tilde{a}^2 a - (r' - s)\tilde{a}a] |\psi(t)\rangle. \quad (3.39)$$

We can then read-off the action for this more general system as

$$\mathcal{A}[\tilde{\phi}, \phi] = - \int_{-\infty}^{\infty} dt \left[\tilde{\phi}(t) \left(\frac{\partial}{\partial t} + r' - s \right) \phi(t) - s\tilde{\phi}^2(t)\phi(t) \right], \quad (3.40)$$

whence we identify the bilinear part of the action as

$$\mathcal{A}_0[\tilde{\phi}, \phi] = - \int_{-\infty}^{\infty} dt \tilde{\phi}(t) \left(\frac{\partial}{\partial t} + r \right) \phi(t), \quad (3.41)$$

after redefining $r = r' - s$, and the interacting part of the action as

$$\mathcal{A}_i[\tilde{\phi}, \phi] = \int_{-\infty}^{\infty} dt s\tilde{\phi}^2(t)\phi(t). \quad (3.42)$$

The bare propagator for this branching-decay system is thus the same as that of the radioactive decay system and is given explicitly by Equation (3.32). This demonstrates the flexibility of the field theory, since we added a new interaction to the radioactive decay system without affecting the existing structure.

The interacting part of the action, Equation (3.42), tells us which vertices are allowed in the diagrammatic representation of the perturbation series in Equation (3.37). More specifically, each $\tilde{\phi}$ of $\mathcal{A}_i$ represents an outgoing leg of a vertex, while each ϕ represents an ingoing leg. In the case of the branching-decay system, there is thus a single vertex represented by

$$\text{Diagram: A red vertex with two outgoing legs and one ingoing leg, labeled } s \text{ above the vertex.} \quad (3.43)$$

where the legs of the vertex are deliberately shortened in the diagram to indicate that they have been “amputated”. The vertex in Equation (3.43) represents a particle branching into two particles both in appearance and in reality, which illustrates the ability of Feynman diagrams to visually represent the microscopic processes of a system in an intuitive way.

Once the bare propagator and vertices for a system have been identified, then the calculation of more general observables can be performed using Equation (3.37). First, we rewrite Equation (3.37) into the more useful form

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} e^{\mathcal{A}_i} \rangle_0 = \sum_{k=0}^{\infty} \frac{1}{k!} \langle \mathcal{O} \mathcal{A}_i^k \rangle_0, \quad (3.44)$$

where we have used the definition of $\langle \bullet \rangle_0$ from Equation (3.21). Equation (3.44) is now in a form where we can readily apply Wick’s theorem to simplify the calculations further.

Wick's Theorem allows one to reduce the expectation $\langle \bullet \rangle_0$ of an arbitrary product of $\tilde{\phi}$ and ϕ , as in Equation (3.44), to products of bare propagators $\langle \phi \tilde{\phi} \rangle_0$ by pairing off all $\tilde{\phi}$ and ϕ . If there is not an equal number of $\tilde{\phi}$ and ϕ in $\bullet$ then $\langle \bullet \rangle_0$ vanishes. These “Wick contractions” generalise in the case of multiple particle species. For instance, consider the following term one may encounter in the perturbative expansion for a system involving two particle species, where the additional species has associated fields $\tilde{\psi}$ and ψ ,

$$\langle \phi \psi \tilde{\phi} \phi \tilde{\psi} \tilde{\phi} \rangle_0 = 2 \langle \phi \tilde{\phi} \rangle_0 \langle \phi \tilde{\phi} \rangle_0 \langle \psi \tilde{\psi} \rangle_0. \quad (3.45)$$

In this case, the observable reduces to a product of bare propagators for *each* species. The factor 2 is a “symmetry factor” that accounts for the two possible ways of contracting the two pairs of $\tilde{\phi}$ and ϕ fields. There are no terms on the right-hand side of Equation (3.45) involving $\langle \phi \phi \rangle_0$ or $\langle \psi \tilde{\psi} \rangle_0$ etc. since these terms are usually chosen to vanish by construction. Each bare propagator on the right-hand side of Equation (3.45) corresponds to a single line in the corresponding Feynman diagram of this term.

To illustrate this further, consider the observable $\langle \phi(t_2) \phi(t_1) \tilde{\phi}(t_0) \rangle$ for the branching-decay system. This has the following diagrammatic representation,

$$\langle \phi(t_2) \phi(t_1) \tilde{\phi}(t_0) \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} \langle \phi(t_2) \phi(t_1) \tilde{\phi}(t_0) \mathcal{A}_i^k \rangle_0 = \langle \phi(t_2) \phi(t_1) \tilde{\phi}(t_0) \mathcal{A}_i \rangle_0 \equiv \begin{array}{c} t_1 \\ \text{ } \diagdown \text{ } s \\ \text{ } \diagup \text{ } t_2 \\ \text{ } \text{ } \text{ } t_0 \end{array}, \quad (3.46)$$

where, by Wick's Theorem, there are no other terms that contribute to this observable besides the first-order correction ($k = 1$), because there are always an unequal number of $\tilde{\phi}$ and ϕ for $k = 0$ and any $k \geq 2$. The Feynman diagram in Equation (3.46) has three lines. These originate from the full contraction of $\langle \phi(t_2) \phi(t_1) \tilde{\phi}(t_0) \mathcal{A}_i \rangle_0$, which produces a product of three bare propagators since $\mathcal{A}_i$ contributes a term $\tilde{\phi}^2 \phi$. Each of these lines, representing a bare propagator, are joined together by the only vertex of $\mathcal{A}_i$, given in Equation (3.43). An explicit calculation in Fourier space demonstrates this, i.e.

$$\begin{aligned} \langle \phi(\omega_2) \phi(\omega_1) \tilde{\phi}(\omega_0) \mathcal{A}_i \rangle_0 &= \langle \phi(\omega_2) \phi(\omega_1) \tilde{\phi}(\omega_0) \int d\omega_a d\omega_b d\omega_c \delta(\omega_a + \omega_b + \omega_c) s \tilde{\phi}(\omega_c) \tilde{\phi}(\omega_b) \phi(\omega_a) \rangle_0 \\ &= 2s \int d\omega_a d\omega_b d\omega_c \delta(\omega_a + \omega_b + \omega_c) \langle \phi(\omega_2) \tilde{\phi}(\omega_c) \rangle_0 \langle \phi(\omega_1) \tilde{\phi}(\omega_b) \rangle_0 \\ &\quad \times \langle \phi(\omega_a) \tilde{\phi}(\omega_0) \rangle_0 \\ &= 2s \int d\omega_a d\omega_b d\omega_c \delta(\omega_a + \omega_b + \omega_c) \frac{\delta(\omega_2 + \omega_c)}{-i\omega_2 + r} \frac{\delta(\omega_1 + \omega_b)}{-i\omega_1 + r} \frac{\delta(\omega_a + \omega_0)}{i\omega_0 + r} \\ &= 2s \frac{\delta(\omega_2 + \omega_1 + \omega_0)}{(-i\omega_2 + r)(-i\omega_1 + r)(i\omega_0 + r)}, \end{aligned} \quad (3.47)$$

where the factor 2 is once again a symmetry factor, and $\delta(\omega_2 + \omega_1 + \omega_0)$ represents overall frequency conservation. The real-space observable in Equation (3.46) can be calculated by taking the inverse Fourier transform of Equation (3.47), see Equation (3.33).

To conclude this chapter, I will list the so-called Feynman rules of Doi-Peliti field

theory that can be deduced from the examples given in this section.

1. Each line in a Feynman diagram represents a factor given by the explicit expression for the bare propagator. The bare propagator can be read-off from the bilinear part of the action $\mathcal{A}_0$ using Equation (3.29).
2. The vertices for a field theory are determined from each term in the interacting part of the action $\mathcal{A}_i$. If a term in $\mathcal{A}_i$ is of the form $\tilde{\phi}^N \phi^M$, then its corresponding vertex will have M ingoing amputated legs and N outgoing amputated legs.
3. For a system involving multiple particle species, each species is typically represented by a different symbol for its field and a different line style for the diagrammatic representation of its bare propagator.
4. Each term in the perturbative expansion of an observable has a corresponding unique Feynman diagram.
5. The number of times a vertex appears in a diagram is indicative of the “order” of the perturbative expansion. For instance, if $\mathcal{A}_{i_X}$ represents the perturbative part of the action for a particular interaction X , then the perturbative expansion at k^{th} order in Equation (3.37) will consist of all possible topologically inequivalent diagrams consisting of k vertices representing interaction X .
6. Lastly, in performing Wick contractions, “external” fields, i.e. those coming from $\mathcal{O}$, can be paired only with “internal” fields coming from $\mathcal{A}_i$. External fields cannot be paired with each other, whereas internal fields can.

~ Part 2 ~

Some minimal models of work
extraction

4

Fluctuation-enhanced work extraction from boundary-tumbling particles

This chapter is based on the following publication:

C. Roberts and G. Pruessner, Exact solution of a boundary tumbling particle system in one dimension, *Physical Review Research* **4**, 033234 (2022) [28].

The necessary permissions to reproduce this publication as part of my thesis are included in Appendices B.1.1 and B.2.7.

Author contributions to original manuscript: GP supervised the project, edited the manuscript, and derived the boundary tumbling length scale. I performed the bulk of the analytical derivations, performed all simulations, produced all figures, and wrote the bulk of the manuscript. GP and I interpreted the results.

Chapter summary

In this chapter, I consider a variant of the run-and-tumble particle model (see Chapter 2) where tumbling is restricted to the boundaries of a one-dimensional interval. To calculate the rate of work extraction from this system, I first derive the fully time-dependent solution to the probability density. The solution is obtained through a perturbative expansion in a Doi-Peliti field-theoretic framework, see Chapter 3. It transpires that the perturbative expansion has an elegant underlying structure which can be used to reduce its full calculation to a matter of linear algebra. The exact results—which are in agreement with Monte-Carlo simulations—show how the probability density is linked to the scale of diffusive fluctuations at the boundaries. A particular interesting feature is that only through the interplay of self-propulsion, diffusion, and boundary tumbling does the model admit a non-uniform probability density. In other words, in the absence of either self-propulsion or diffusion, the density is always uniform. Remarkably, this interplay also leads to a “boosted” rate of work extraction compared to the diffusionless case. By mapping the system to a periodic interval, it becomes clear that this is due to the rectification of thermal fluctuations in an apparent violation of The Second Law of Thermodynamics. However, by introducing an energetic cost associated with the boundary tumbling, it would appear that compliance with The Second Law is restored.

4.1 Introduction

For the first example of work extraction from active matter in Part 2, I will consider a model of confined run-and-tumble (RnT) motion for a particle which has tumbling

restricted to the boundaries of a one-dimensional interval. Studying such a “boundary tumbling” reaction is instrumental to understanding cellular locomotion, as experiments have shown *E. coli* adapt to the presence of confining walls by decreasing their tumble rate when within $20\ \mu\text{m}$, approximately a single run length, of a boundary [109]. This phenomenon can be studied through RnT models with differing tumble rates in the bulk and at the walls [19], as is the case here. However, the omission of bulk tumbling in this chapter means the particle must cross the full length of the system before a change in direction can occur. Though this is restrictive from a biological perspective, the upside is a technically tractable theory. Specifically, the fully time-dependent solution is brought within reach if bulk tumbling is neglected. On the other hand, this restriction actually makes the system under consideration closer in character to other real-life systems, such as someone swimming lengths of a swimming pool.

More generally, by studying this model, I develop techniques that are generally applicable to solving Fokker-Planck equations containing localised reaction terms. Deriving the solution to this model presents new challenges not encountered in models with spatially uniform tumbling, such as the standard confined RnT model [26, 27]. In particular, the incorporation of a localised reaction into a model of diffusive particles turns out to be one of the most significant challenges that is addressed in this chapter. Incorporating a localised boundary reaction is difficult because diffusive fluctuations result in infinitesimally small contact times between a particle and the boundary. This would suggest the probability to tumble at the boundaries vanishes if tumbling occurs with a finite rate. This also seemingly goes against what is typically observed at the macroscopic scale, where particles appear to get “stuck” at walls for finite periods of time, such as in bacterial ratchet motors [50]. This macroscopic perspective is equivalent to a lattice description where the lattice spacing exceeds the typical size of the fluctuations away from the boundary, allowing the particle to reside at an edge site for a finite time. This would suggest the reaction probability for a localised reaction does not vanish on a lattice, and thus a particle can still boundary tumble, in contrast with the continuum description. The derivation presented in this chapter provides a way to prevent the boundary tumbling reaction vanishing in the continuum description while still maintaining the correct *effective* rate. Accounting for the role of diffusion in a boundary reaction is necessary for correctly capturing the physics of finite reaction rates.

Based on the above, incorporating boundary tumbling simply by imposing boundary conditions can be fraught with ambiguity and difficult to implement mathematically. One method of incorporating diffusion-mediated surface reactions, such as boundary tumbling, is through the concept of boundary local time [110], where a reaction occurs when the time the particle spends in the boundary’s vicinity exceeds a certain value. The approach in this chapter is closely related, yet incorporates the relevant physics directly in the Fokker-Planck equation by defining a boundary length scale that is consistent with maintaining a finite reaction probability in the continuum limit, see Appendix 4.B.

Since the incorporation of boundary reactions in a Fokker-Planck equation draws on a

novel framework, I begin in Section 4.2 by solving the simpler Fokker-Planck equation for the reflecting boundaries drift-diffusion system without tumbling (see also Section 2.2.1 of Chapter 2). The derivation of the solution to this simpler Fokker-Planck equation sets the stage for subsequent perturbative calculations that introduce the boundary tumbling reaction. The framework used to perform the perturbative calculations is the path integral in the Doi-Peliti formalism [88, 90], see Chapter 3. Path integrals allow for the use of field-theoretic techniques, such as Feynman diagrams, that make the perturbative calculations more tractable. The Doi-Peliti formalism is chosen specifically because it respects the particle nature of the system, which is essential to capturing the phenomenology of active systems [105].

Section 4.3 discusses the boundary tumbling system and contains the main results of the chapter. The most important results are the derivation of closed-form expressions for the fully time-dependent probability density, Equations (4.28) and (4.29), and its steady-state limit, Equations (4.34) and (4.35), which are verified with Monte-Carlo simulations, Figure 4.4. Obtaining these exact results from a perturbative expansion is possible due to the Feynman diagrams of the field theory having a surprisingly elegant structure that is closed under multiplication. This significant result reduces the calculation of the full perturbation series to a matter of linear algebra, Appendix 4.C. The derivation of these solutions demonstrates it is possible to study other physically relevant localised reactions in a confined system, such as bacterial deposition [111], via a perturbative treatment of the corresponding terms in the Fokker-Planck equation.

In this chapter, I will use the terms “particle” and “particles” interchangeably since the probability density for a single particle is, up to a factor N , the same as that of an ensemble of N *non-interacting* particles.

4.2 Drift-diffusion with reflecting boundaries

4.2.1 Model

Consider a particle moving at position $x \in [0, L]$ on a one-dimensional interval with reflecting boundary conditions at $x = 0$ and $x = L$. Reflecting boundary conditions correspond to vanishing particle current at the boundaries and so ensure particle confinement. Confinement is an essential property of the boundary tumbling system and so is implemented at the level of the bare propagator so that it will be present at every subsequent order of the perturbation theory introduced in Section 4.3.

In the bulk of the interval $x \in (0, L)$ the stochastic motion of the particle is governed by the Langevin equation

$$\dot{x}(t) = v + \sqrt{2D}\xi(t), \quad (4.1)$$

where $\dot{x}$ is the instantaneous velocity of the particle, t is time, v is the particle’s constant self-propulsion speed, D is the diffusion constant and $\xi(t)$ is a Gaussian white noise defined by $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$. In Section 4.3, where boundary tumbling is introduced, the diffusive part of the motion will act as an additional variance on top of

the particle's ballistic movement. Therefore, the diffusion can be considered a result of thermal fluctuations which, in turn, quantify the frictional forces acting on the particle via Einstein's relation, see Chapter 2.

Alternatively, the probability density $P_0(x, t)$ evolves deterministically according to the drift-diffusion Fokker-Planck equation [62]

$$\frac{\partial P_0(x, t)}{\partial t} = \mathcal{L}P_0(x, t) = \left(D \frac{\partial^2}{\partial x^2} - v \frac{\partial}{\partial x} \right) P_0(x, t), \quad (4.2)$$

where $\mathcal{L}$ is the drift-diffusion Fokker-Planck operator. Equation (4.2) can be rewritten in the form of a continuity equation

$$\frac{\partial P_0(x, t)}{\partial t} + \frac{\partial J_0(x, t)}{\partial x} = 0, \quad (4.3)$$

where the particle current is given by

$$J_0(x, t) = vP_0(x, t) - D \frac{\partial P_0(x, t)}{\partial x}, \quad (4.4)$$

and the reflecting boundary conditions impose $J_0(0, t) = J_0(L, t) = 0$.

4.2.2 Solution and field theory

The system of equations governing the drift-diffusion system, Equations (4.2)–(4.4), is now cast as a Doi-Peliti field theory. In this formalism, Equation (4.2) is promoted to a bilinear action functional $\mathcal{A}_0$, see Equation (4.9), and its solution, i.e. the drift-diffusion probability density, assumes the role of a “bare propagator”, see Equation (4.11), which will be the essential component of the subsequent perturbative calculations that introduce the boundary tumbling in Section 4.3. Tutorials on the derivation of a Doi-Peliti field theory can be found in Refs. [79–81, 101] and, of course, Chapter 3.

I begin by defining the annihilator field

$$\phi(x, t) = \frac{1}{L} \sum_{n=0}^{\infty} \int \bar{d}\omega \, \phi_n(\omega) e^{-i\omega t} U_n(x), \quad (4.5a)$$

and the Doi-shifted creation field

$$\tilde{\phi}(x, t) = \frac{1}{L} \sum_{m=0}^{\infty} \int \bar{d}\omega_0 \, \tilde{\phi}_m(\omega_0) e^{-i\omega_0 t} \tilde{U}_m(x), \quad (4.5b)$$

where $\bar{d} := d/2\pi$, while $U_n(x)$ and $\tilde{U}_m(x)$ are, respectively, right and left eigenfunctions of $\mathcal{L}$ in Equation (4.2). Physical observables in Doi-Peliti field theory are constructed from products of the creation and annihilation fields, see Chapter 3. For instance, the propagator $\langle \phi(x, t) \tilde{\phi}(x_0, t_0) \rangle$ represents the probability density at position x and time t given a particle was created at position x_0 and time t_0 .

By solving Equations (4.2)–(4.4),¹ Appendix 4.A, the right eigenfunction for $n = 0$ is found to be a Boltzmann distribution,

$$U_0(x) = e^{\frac{v}{2D}x}, \quad (4.6a)$$

with eigenvalue $\lambda_0 = 0$, whilst the eigenfunctions for $n \in \mathbb{N}^+$ are given by

$$U_n(x) = 2e^{\frac{v}{2D}x} \cos(k_n x + \theta_n), \quad (4.6b)$$

where $k_n = n\pi/L$, the phases are given by $\theta_n = \arctan(-v/2Dk_n)$, and the eigenvalues associated with each $U_n(x)$ are $\lambda_n = -Dk_n^2 - v^2/4D < 0$, such that $\mathcal{L}U_n(x) = \lambda_n U_n(x)$.

The left and right eigenfunctions of $\mathcal{L}$ need to be orthogonal for the operator of the resulting action functional, Equation (4.9), to be rendered diagonal and thus local in n . This can be achieved by equipping the inner product with a suitable weight function $w(x)$ or, equivalently, by absorbing $w(x)$ into the left eigenfunctions to leave $\mathcal{L}$ in the desired self-adjoint form [117]. In the present case, the weight function is $w(x) = \exp(-vx/D)$ [115]. Hence, the (normalised) left eigenfunctions are given by

$$\tilde{U}_0(x) = \frac{vL/D}{\exp(vL/D) - 1}, \quad (4.7a)$$

$$\tilde{U}_m(x) = 2e^{-\frac{v}{2D}x} \cos(k_m x + \theta_m), \quad (4.7b)$$

where the specific choice of normalisation

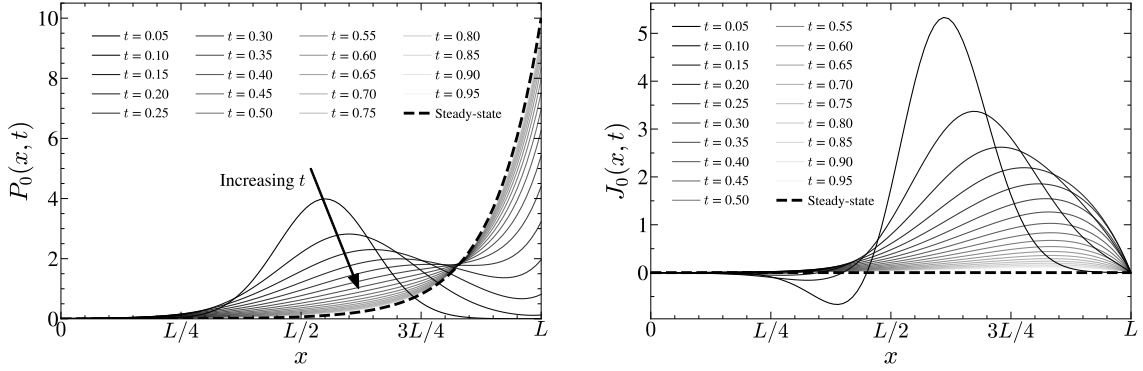
$$\int_0^L dx \tilde{U}_m(x) U_n(x) = \begin{cases} L, & n = m = 0, \\ 2L, & n = m > 0, \\ 0, & n \neq m, \end{cases} \quad (4.8)$$

results in a simple expression for the bare propagator, Equation (4.11).

By substituting the eigenfunctions, Equations (4.6a)–(4.7b), into the fields, Equations (4.5a) and (4.5b), the action functional for this system is found to be [22, 42, 70, 74]

$$\begin{aligned} \mathcal{A}_0 &= \int dt \int_0^L dx \tilde{\phi}(x, t) \left(\frac{\partial}{\partial t} - \mathcal{L} \right) \phi(x, t) \\ &= \frac{1}{L} \int d\omega \int d\omega_0 \delta(\omega + \omega_0) \left[\tilde{\phi}_0(\omega_0) (-i\omega + r) \phi_0(\omega) \right. \\ &\quad \left. + 2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_{nm} \tilde{\phi}_m(\omega_0) \left(-i\omega + Dk_n^2 + \frac{v^2}{4D} + r \right) \phi_n(\omega) \right], \end{aligned} \quad (4.9)$$

¹The solution to the reflecting boundaries drift-diffusion equations, Equations (4.2)–(4.4), first appears in Ref. [112] in Laplace space, and later in various other forms [113, 114]. The equivalent solution for absorbing boundary conditions is derived in Ref. [115]. Reference [116] contains derivations of Green's functions for the drift-diffusion equation for several different boundary conditions, the most relevant to the model presented in this chapter being for radiating and absorbing boundaries at opposite ends of a one-dimensional interval.



(a) Drift-diffusion probability density $P_0(x, t)$, Equation (4.13).

(b) Drift-diffusion particle current $J_0(x, t)$, Equation (4.4).

Figure 4.1: Probability density $P_0(x, t)$, Equation (4.13), and current $J_0(x, t)$, Equation (4.4), for the reflecting boundaries drift-diffusion system on an interval of length $L = 1$, initialised at position $x = L/2$ and time $t = 0$ with $v = 1$ and $D = 0.1$. In the numerical evaluation of $P_0(x, t)$ and $J_0(x, t)$, the infinite sum appearing in Equation (4.13) has been truncated at $n = 100$.

where $\delta(\omega + \omega_0) := 2\pi\delta(\omega + \omega_0)$, and $r > 0$ is a spontaneous extinction rate which is introduced to maintain causality and to regularise the infrared divergence at $\omega = 0$ when integrating back to direct time. After performing the path integral, see below, one can take $r \rightarrow 0^+$ to remove the extinction process.

An observable $\bullet$ is calculated at the bare level from the bare action via the path integral

$$\langle \bullet \rangle_0 := \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} \bullet e^{-\mathcal{A}_0}, \quad (4.10)$$

where the subscript “0” on the expectation value signifies that the integral is performed with respect to the non-perturbative bilinear part of the action $\mathcal{A}_0$ that will be perturbed about later, see Equation (4.20). The key path integral to perform is for the bare propagator $\langle \phi \tilde{\phi} \rangle_0$. The bare propagator can be calculated in closed form after the action has been made local by replacing semi-local derivative operators in $\mathcal{L}$, Equation (4.2), with their algebraic counterparts in Fourier space, Equation (4.9). Any non-linear terms in the action, and any further linear reaction terms, are incorporated perturbatively, Equation (4.20).

The result of the Gaussian integration in Equation (4.10) is that the bare propagator can simply be read off from the action $\mathcal{A}_0$, Equation (4.9), as

$$\langle \phi_n(\omega) \tilde{\phi}_m(\omega_0) \rangle_0 = \delta(\omega + \omega_0) \frac{\frac{L}{2} \delta_{nm} (1 + \delta_{n0})}{-i\omega + Dk_n^2 + (1 - \delta_{n0}) \frac{v^2}{4D} + r} \equiv \delta(\omega + \omega_0) \underline{n \quad m}, \quad (4.11)$$

where Feynman diagrams are read from right to left, as in Chapter 3. Feynman diagrams will be used extensively in Section 4.3.2 to make the perturbative calculations more tractable.

The probability density in real space and direct time, i.e. the Green’s function of

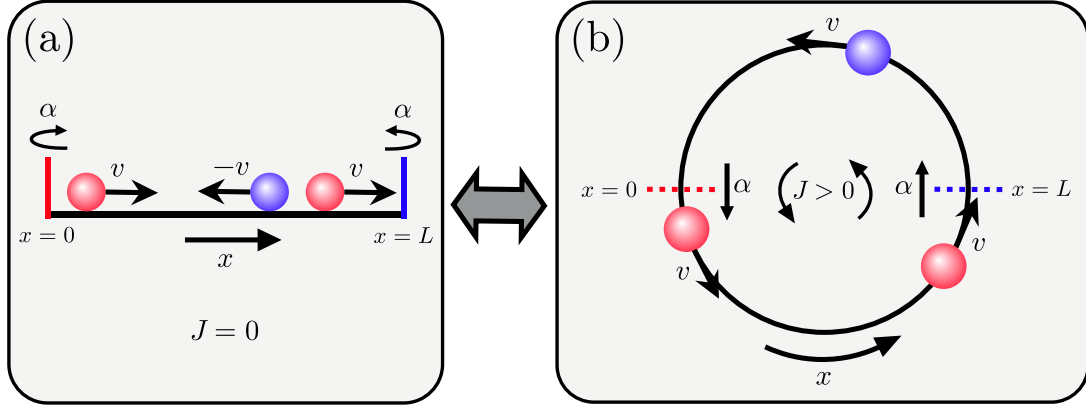


Figure 4.2: (a) Schematic representation of the boundary tumbling model on a finite interval of length L . Right-moving particles (red spheres) with self-propulsion speed $v > 0$ transmute with rate α into left-moving particles (blue spheres) with self-propulsion speed $-v$ at the right-hand boundary at $x = L$ (and vice versa at the left-hand boundary at $x = 0$). This system can be mapped to a model of a drift-diffusive particle on a spatially periodic domain of length $2L$ through Equation (4.16), as illustrated in (b). The transmutations at the boundaries of the interval in (a) are replaced by irreversible crossings of a semi-permeable membrane in (b). The reimagining of the system on a spatially periodic domain allows for a steady-state net current J to be generated, the implications of which are studied in Section 4.3.4.

Equation (4.2), is calculated from the inverse Fourier transform of the bare propagator,

$$P_0(x, t|x_0, t_0) \equiv \langle \phi(x, t) \tilde{\phi}(x_0, t_0) \rangle_0 = \frac{1}{L} \sum_{n=0}^{\infty} \frac{1}{L} \sum_{m=0}^{\infty} \int d\omega d\omega_0 \langle \phi_n(\omega) \tilde{\phi}_m(\omega_0) \rangle_0 \times U_n(x) \tilde{U}_m(x_0) e^{-i\omega t} e^{-i\omega_0 t_0}, \quad (4.12)$$

for a particle initialised at x_0 at time t_0 . By applying the residue theorem, and subsequently taking $r \rightarrow 0^+$, the probability density is found to be

$$P_0(x, t|x_0, t_0) = \frac{\Theta(t - t_0)}{L} \left[\frac{\text{Pe}}{\exp(\text{Pe}) - 1} e^{\frac{v}{D}x} + 2 \sum_{n=1}^{\infty} e^{-\left(Dk_n^2 + \frac{v^2}{4D}\right)(t-t_0)} e^{\frac{v}{2D}(x-x_0)} \cos(k_n x + \theta_n) \cos(k_n x_0 + \theta_n) \right], \quad (4.13)$$

where the Heaviside step function $\Theta(t - t_0)$ incorporates causality, i.e. there are no particles in the system until initialisation at time $t = t_0$, and the Péclet number $\text{Pe} = vL/D$ is the ratio of active to diffusive transport. The drift-diffusion probability density $P_0(x, t)$, Equation (4.13), and its corresponding current $J_0(x, t)$, Equation (4.4), are plotted in Figure 4.1 for a range of times.

4.3 Boundary tumbling

4.3.1 Model

The boundary tumbling system is now considered by allowing a particle with positive self-propulsion speed $v > 0$ (henceforth referred to as a “right-moving particle”) to transmute with rate α into a particle with negative self-propulsion speed $-v$ (a “left-moving particle”) at the right-hand boundary at $x = L$, and vice versa at the left-hand boundary at $x = 0$, whilst retaining all other properties of the system from Section 4.2. Figure 4.2(a) shows a schematic representation of the boundary tumbling model.

The boundary tumbling Fokker-Planck equation can be derived rigorously as a continuum limit of the master equation on a lattice—see Figure 4.3 for a schematic illustration of the lattice model. This is the normal route to deriving a Doi-Peliti field theory [74, 80, 101], specifically by applying the canonical quantisation procedure to rewrite, in terms of ladder operators, the evolution of the probability for a particular occupation number configuration. The continuum limit of the microscopic master equation ultimately recovers the Fokker-Planck equation [106], meaning the Doi-Peliti action functional is readily obtained from the Fokker-Planck operator, as in Equation (4.9). The only additional terms to the drift-diffusion Fokker-Planck equation, Equation (4.2), are the boundary tumbling for both states. As in a master equation, these additional terms are just the normal transmutation terms (see, for instance, Refs. [22, 42, 70]) supplemented with Kronecker-delta functions to restrict the reaction to the end lattice sites. In taking the continuum limit, the Kronecker-delta functions are promoted to Dirac-delta functions with an accompanying length scale ℓ to maintain dimensional consistency. This length scale is discussed in detail below and derived explicitly in Appendix 4.B. Hence, the boundary tumbling Fokker-Planck equation is

$$\frac{\partial P_R(x, t)}{\partial t} = D \frac{\partial^2 P_R(x, t)}{\partial x^2} - v \frac{\partial P_R(x, t)}{\partial x} + \ell \alpha \left[\delta(x) P_L(x, t) - \delta(x - L) P_R(x, t) \right], \quad (4.14a)$$

$$\frac{\partial P_L(x, t)}{\partial t} = D \frac{\partial^2 P_L(x, t)}{\partial x^2} + v \frac{\partial P_L(x, t)}{\partial x} - \ell \alpha \left[\delta(x) P_L(x, t) - \delta(x - L) P_R(x, t) \right], \quad (4.14b)$$

where $P_{R/L}(x, t)$ is the probability density for right/left-moving particles at position x and time t .²

As explained in the caption of Figure 4.3, the delta functions in Equation (4.14) enforce conversion between the different particle states to occur only at the boundaries of the system. For instance, the term proportional to $\delta(x)$ corresponds to conversion of a left-moving particle to a right-moving particle at the left-hand boundary at $x = 0$. The opposing signs of this term in the coupled equations represent gain and loss to each state respectively.

Another way of interpreting Equation (4.14) is through the lens of stochastic resetting. The terms proportional to delta functions in Equation (4.14) are analogous to those of a

²In Equation (4.14) and throughout, I use the convention $\int_0^L dx \delta(x) = \int_0^L dx \delta(x - L) = 1$.

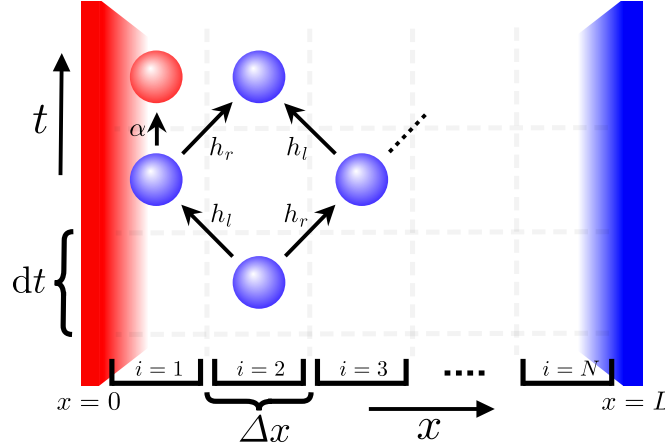


Figure 4.3: Schematic representation of the boundary tumbling model on a lattice of N sites. The arrows represent the possible paths a single particle could take. A left-moving particle (blue sphere) hops to the left or to the right in the bulk with respective rates $h_l = 2D/\Delta x^2 + v/\Delta x$ and $h_r = 2D/\Delta x^2 - v/\Delta x$ [56], where $v > 0$ implies a larger left-hopping rate. Upon reaching the left-most lattice site $i = 1$, facing the left-hand boundary at $x = 0$ (red wall), a left-moving particle converts to a right-moving particle (red sphere) with rate α . However, if α remains finite as the continuum limit is taken, the particle's reaction probability vanishes as $\Delta x \rightarrow 0$ because the time the particle spends in the left-most site decreases due to diffusive fluctuations. Thus, as the limit is taken, the reaction rate needs to increase while taking the size ℓ of the fluctuations into account. More specifically, α at the boundary needs to be replaced by $\ell\alpha/\Delta x$, or $\ell\alpha\delta(x)$ in the bulk, Equation (4.14). The length scale ℓ is given in Equation (4.15).

resetting model both in appearance and function, see Chapter 5. This is made explicit by rewriting $\ell\alpha[\delta(x)P_L(x,t) - \delta(x-L)P_R(x,t)]$ in Equation (4.14a), for instance, as $r_1(x,t)\delta(x) - r_2(x,t)P_R(x,t)$, where $r_1(x,t)$ and $r_2(x,t)$ are interpreted as space- and time-dependent resetting rates. This term now appears to represent the resetting of a right-moving particle to position $x = 0$. As the “resetting” takes place via space-dependent transmutations between species, it is in fact analogous to a finite-time resetting model. This analogy can also be extended to potential-mediated resetting [118, 119], as considered in Chapter 5, by reinterpreting the left-moving state as that of a diffusive particle subject to an intermittent potential $U(x) = vx$, which switches off only upon the particle's return to position $x = 0$. The above can equally be reformulated as resetting of a left-moving particle through suitable reinterpretation of the transmutation terms.

The standard RnT model with uniform tumble rate is recovered by replacing both $\ell\alpha\delta(x)$ and $\ell\alpha\delta(x-L)$ in Equation (4.14) with $\alpha/2$ [26, 27]. Thus, by comparing the boundary RnT model of this chapter with the standard RnT model, the need for the length scale ℓ is apparent on the grounds of dimensionality. The need for the factor ℓ on *physical* grounds, however, actually arises from the infinitesimally small contact time between a particle and a boundary due to diffusive fluctuations in a continuum model. This contact time does not vanish in the absence of diffusive fluctuations $D = 0$, or if the dynamics take place on a lattice where the lattice spacing Δx is much greater than the typical

size ℓ of these fluctuations. If the dynamics are scrutinised at finer spatial resolution, i.e. if $\Delta x \ll \ell$, then it becomes apparent that the particle makes an infinite number of microscopically small excursions away from the boundary, as in the continuum model. As D is increased, the size of these fluctuations increases and a more “coarse-grained” perspective (larger Δx) is required for a particle to appear to reside at a boundary—or, rather, in the end lattice site. Hence, to prevent the boundary tumbling probability from vanishing, ℓ in Equation (4.14) must increase with D to compensate for the increase in size of these fluctuations. More precisely, the length scale ℓ is defined such that a particle that resides at the boundary site with a probability according to the steady-state density of a drift-diffusive particle, as derived in Section 4.2, transmutes with average rate α . Leaving the details to Appendix 4.B, where ℓ is derived from the lattice description, the length scale that emerges in the continuum limit is

$$\ell = \frac{D}{v} \left(1 - e^{-\frac{vL}{D}} \right), \quad (4.15)$$

which is approximated by $\ell \approx D/v$ for $D/v \ll L$, and is restricted by the size of the system, i.e. $\ell \approx L$, for $D/v \gg L$.

To aid the interpretation of the results derived later in this chapter, it will be helpful to occasionally visualise the dynamics from the perspective of an analogous model. As illustrated in Figure 4.2, the model described in this section can be mapped to that of an analogous model on a spatially periodic domain—a “ring” of circumference $2L$. In the ring model, there are no right-moving or left-moving particle species, only a single drift-diffusive species with positive drift v (i.e. the particles favour motion in the anti-clockwise direction around the ring). Transmutation between species at the endpoints of the interval is replaced by irreversible crossings of semi-permeable membranes at $x = 0$ and $x = L$, as studied in Ref. [120]. These crossings occur with rate α , and thus $\alpha = 0$ confines particles to a half region of the ring, either $0 \leq x < L$ (if the particle was a right mover in the original finite-interval model) or $L \leq x < 2L$ (if the particle was a left mover in the finite-interval model). The mapping is made exact through the relation between the densities,

$$P_{\text{ring}}(x, t) = \begin{cases} P_R(x, t), & 0 \leq x < L, \\ P_L(2L - x, t), & L \leq x < 2L. \end{cases} \quad (4.16)$$

A key difference between the models is that the ring affords a non-zero steady-state net current J , whereas the finite interval does not. This will be crucial later on in this chapter when I consider viable ways of extracting work from this system. Unless explicitly stated, the remaining results of this chapter can be assumed to be for the finite-interval model illustrated in Figure 4.2(a). The ring model illustrated in Figure 4.2(b) will be considered mostly in Section 4.3.4, which deals with the extraction of work from this system.

4.3.2 Solution

The Fokker-Planck equation, Equation (4.14), couples two partial differential equations by terms proportional to delta functions. In the following, Doi-Peliti field theory is used to treat these boundary tumbling terms as perturbations to the bare propagator, Equation (4.11). Both the left-moving and right-moving states have the same bare propagator since Equation (4.11) is invariant under $v \rightarrow -v$. However, the eigensystem of the left-moving species differs from that of the right-moving species by the sign of v , as can be gleaned from Equations (4.2) and (4.14a) compared to (4.14b). With this in mind, I introduce left-moving eigenfunctions $V_n(x)$ and $\tilde{V}_n(x)$, defined as in Equations (4.6a)–(4.7b) by replacing v with $-v$. As a result, $U_n(x)$ and $\tilde{V}_n(x)$, and similarly $\tilde{U}_n(x)$ and $V_n(x)$, are generally not orthogonal for $v \neq 0$. Ordinarily, a reaction term would therefore pose a significant obstacle when calculating the perturbative corrections. As it turns out, the localisation of the transmutation reaction due to the delta functions is actually a blessing in disguise.

The perturbative treatment of the boundary tumbling begins with adding the following terms to the action of Equation (4.9), which can be derived from taking the continuum limit of the master equation describing the lattice model illustrated in Figure 4.3,

$$\begin{aligned} -\mathcal{A}_{R \rightarrow L} &= \ell\alpha \int dt \int_0^L dx \delta(x-L) \left(\tilde{\psi} - \tilde{\phi} \right) \phi \\ &= \int d\omega_a d\omega_b \delta(\omega_a + \omega_b) \sum_{ij} \left(\tilde{\psi}_i(\omega_a) \Delta_{\tilde{\psi}_i \phi_j} + \tilde{\phi}_i(\omega_a) \Delta_{\tilde{\phi}_i \phi_j} \right) \phi_j(\omega_b), \end{aligned} \quad (4.17a)$$

$$\begin{aligned} -\mathcal{A}_{L \rightarrow R} &= \ell\alpha \int dt \int_0^L dx \delta(x) \left(\tilde{\phi} - \tilde{\psi} \right) \psi \\ &= \int d\omega_a d\omega_b \delta(\omega_a + \omega_b) \sum_{ij} \left(\tilde{\phi}_i(\omega_a) \Delta_{\tilde{\phi}_i \psi_j} + \tilde{\psi}_i(\omega_a) \Delta_{\tilde{\psi}_i \psi_j} \right) \psi_j(\omega_b), \end{aligned} \quad (4.17b)$$

where $\psi = \psi(x, t)$ and $\tilde{\psi} = \tilde{\psi}(x, t)$ are, respectively, the annihilation and creation fields of the left-moving particle. The fields of the right-moving particle $\phi, \tilde{\phi}$ retain the same definitions from Equation (4.5). Equation (4.17a) is the action for the conversion that occurs at the right-hand boundary, qualitatively representing the creation of a left-moving particle $\tilde{\psi}\phi$ and the annihilation of a right-moving particle $-\tilde{\phi}\phi$. The integrals over eigenfunctions in the first line of both Equation (4.17b) and Equation (4.17a) become fully populated matrices Δ in Fourier space. For instance, the matrices

$$\Delta_{\tilde{\psi}_i \phi_j} = \frac{\ell\alpha}{L^2} \int_0^L dx \delta(x-L) \tilde{V}_i(x) U_j(x), \quad (4.18a)$$

$$\Delta_{\tilde{\phi}_i \phi_j} = -\frac{\ell\alpha}{L^2} \int_0^L dx \delta(x-L) \tilde{U}_i(x) U_j(x), \quad (4.18b)$$

arise from the $\tilde{\psi}\phi$ and $\tilde{\phi}\phi$ terms in Equation (4.17a) respectively. The first (respectively, second) index of the matrices Δ denotes their row (respectively, column) number. The

matrix elements are calculated explicitly in Appendix 4.C.a.

The full action is given by $\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_{R \rightarrow L} + \mathcal{A}_{L \rightarrow R}$, where the bilinear part of the action $\mathcal{A}_0$ now has an extra contribution for the ψ fields, i.e.

$$\begin{aligned} \mathcal{A}_0 = \frac{1}{L} \int \bar{d}\omega \, d\omega_0 \, \delta(\omega + \omega_0) & \left[\tilde{\phi}_0(\omega_0) (-i\omega + r) \phi_0(\omega) \right. \\ & + 2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_{nm} \tilde{\phi}_m(\omega_0) \left(-i\omega + Dk_n^2 + \frac{v^2}{4D} + r \right) \phi_n(\omega) \\ & + \tilde{\psi}_0(\omega_0) (-i\omega + r) \psi_0(\omega) \\ & \left. + 2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_{nm} \tilde{\psi}_m(\omega_0) \left(-i\omega + Dk_n^2 + \frac{v^2}{4D} + r \right) \psi_n(\omega) \right]. \end{aligned} \quad (4.19)$$

Perturbative corrections for $\mathcal{A}_{R \rightarrow L}$ and $\mathcal{A}_{L \rightarrow R}$ are performed by writing the path integral for $\mathcal{A}$ as

$$\begin{aligned} \langle \bullet \rangle &= \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} \mathcal{D}\psi \mathcal{D}\tilde{\psi} \bullet e^{-\mathcal{A}_0 - \mathcal{A}_{R \rightarrow L} - \mathcal{A}_{L \rightarrow R}} \\ &= \langle \bullet e^{-\mathcal{A}_{R \rightarrow L} - \mathcal{A}_{L \rightarrow R}} \rangle_0 \\ &= \sum_{N=0}^{\infty} \sum_{M=0}^{\infty} \frac{1}{N!} \frac{1}{M!} \langle \bullet (-\mathcal{A}_{R \rightarrow L})^N (-\mathcal{A}_{L \rightarrow R})^M \rangle_0, \end{aligned} \quad (4.20)$$

where the definition of the bilinear path integral, Equation (4.10), has been used in the second equality and, in the third equality, the exponential terms have been expanded as a power series of corrections. As explained in Chapter 3, Wick's theorem can be used to reduce the products of ϕ , $\tilde{\phi}$, ψ and $\tilde{\psi}$ on the right-hand side of the final line in Equation (4.20) to products of $\langle \phi \tilde{\phi} \rangle_0$ and $\langle \psi \tilde{\psi} \rangle_0$, given by Equation (4.11).

The goal is now to find a closed-form representation of the full perturbation series, Equation (4.20). Each term in the series corresponds to a unique Feynman diagram. For instance, the first-order corrections to the probability density for right-moving particles are represented by

$$\langle \phi_n(\omega) \tilde{\phi}_m(\omega_0) (-\mathcal{A}_{R \rightarrow L}) \rangle_0 \equiv \delta(\omega + \omega_0) \overset{n}{\text{---}} \bigcirc \overset{m}{\text{---}}, \quad (4.21a)$$

$$\langle \phi_n(\omega) \tilde{\psi}_m(\omega_0) (-\mathcal{A}_{L \rightarrow R}) \rangle_0 \equiv \delta(\omega + \omega_0) \overset{n}{\text{---}} \bigcirc \overset{m}{\text{---}}, \quad (4.21b)$$

depending on whether a right-moving or left-moving particle is initialised respectively. Equation (4.21) illustrates the Feynman rules of the field theory: the number of bare propagators $\langle \phi \tilde{\phi} \rangle_0$ (respectively, $\langle \psi \tilde{\psi} \rangle_0$) that arise on the left-hand sides of Equation (4.21) after Wick contraction corresponds to the number of straight red (respectively, wavy blue) lines in the corresponding Feynman diagrams on the right-hand side. Furthermore, the

exponents of $\mathcal{A}_{R \rightarrow L}$ and $\mathcal{A}_{L \rightarrow R}$ on the left-hand sides correspond to the number of times their corresponding vertices (white circles with a black outline) appear in the Feynman diagram. For instance, for the term where $N = 1$ and $M = 2$ in Equation (4.20), the corresponding Feynman diagram has one vertex where the incoming leg is a straight red line, and two vertices where the incoming leg is a wavy blue line.

The Fourier-space solutions to the boundary tumbling Fokker-Planck equation, Equation (4.14), will be referred to as full propagators. Dyson's equation relates the full propagators to a geometric series over the lower-order corrections in Equation (4.20) [81],

$$\begin{aligned}
 \mathbf{F} &= \begin{pmatrix} \langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle & \langle \phi(\omega) \tilde{\psi}(\omega_0) \rangle \\ \langle \psi(\omega) \tilde{\phi}(\omega_0) \rangle & \langle \psi(\omega) \tilde{\psi}(\omega_0) \rangle \end{pmatrix} \\
 &\equiv \delta(\omega + \omega_0) \begin{pmatrix} \text{---} \bullet \text{---} & \text{---} \bullet \text{---} \\ \text{---} \bullet \text{---} & \text{---} \bullet \text{---} \end{pmatrix} \\
 &= \delta(\omega + \omega_0) (\mathbf{G} + \mathbf{GTG} + \mathbf{GTGTG} + \dots) \\
 &= \delta(\omega + \omega_0) \mathbf{G} (\mathbb{1} + \mathbf{TG} + \mathbf{TGTG} + \dots) \\
 &= \delta(\omega + \omega_0) \mathbf{G} (\mathbb{1} - \mathbf{TG})^{-1},
 \end{aligned} \tag{4.22}$$

where the black circles represent sums over all possible corrections,

$$\mathbf{G} \equiv \begin{pmatrix} \text{---} & 0 \\ 0 & \text{---} \end{pmatrix} \tag{4.23}$$

is the matrix of bare propagators, Equation (4.11), and

$$\mathbf{T} := \begin{pmatrix} \Delta_{\tilde{\phi}\phi} & \Delta_{\tilde{\phi}\psi} \\ \Delta_{\tilde{\psi}\phi} & \Delta_{\tilde{\psi}\psi} \end{pmatrix} \equiv \begin{pmatrix} \text{---} \circ \text{---} & \text{---} \circ \text{---} \\ \text{---} \circ \text{---} & \text{---} \circ \text{---} \end{pmatrix} \tag{4.24}$$

is a transmutation matrix consisting of the four different matrices arising from the integrals over eigenfunctions in Equation (4.17).

It is convenient to define a new matrix

$$\mathbf{M} := \mathbf{TG} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \equiv \begin{pmatrix} \text{---} \circ \text{---} & \text{---} \circ \text{---} \\ \text{---} \circ \text{---} & \text{---} \circ \text{---} \end{pmatrix}, \tag{4.25}$$

where the explicit expressions for the infinite-dimensional submatrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$ are given in Appendix 4.C.b.

As the elements of $\mathbf{M}$ are infinite-dimensional matrices, the inverse of $(\mathbb{1} - \mathbf{M})$ in Equation (4.22) is not readily written in closed form. To make progress, I first calculate

the blockwise inverse of $(\mathbb{1} - \mathbf{M})$,³ which gives

$$\begin{aligned} \mathbf{F} = \delta(\omega + \omega_0) \mathbf{G} & \begin{pmatrix} (\mathbb{1} - \mathbf{B}(\mathbb{1} - \mathbf{D})^{-1}\mathbf{C} - \mathbf{A})^{-1} & 0 \\ 0 & (\mathbb{1} - \mathbf{C}(\mathbb{1} - \mathbf{A})^{-1}\mathbf{B} - \mathbf{D})^{-1} \end{pmatrix} \\ & \times \begin{pmatrix} \mathbb{1} & \mathbf{B}(\mathbb{1} - \mathbf{D})^{-1} \\ \mathbf{C}(\mathbb{1} - \mathbf{A})^{-1} & \mathbb{1} \end{pmatrix}. \end{aligned} \quad (4.26)$$

The full propagators can now be read off from Equation (4.26), for instance

$$\text{---} \bullet \text{---} = \text{---} (\mathbb{1} - \mathbf{B}(\mathbb{1} - \mathbf{D})^{-1}\mathbf{C} - \mathbf{A})^{-1}. \quad (4.27)$$

Obtaining a form for this propagator that can be readily transformed back to real space requires rewriting the remaining inverse matrices on the right-hand side of Equation (4.27) in closed form. The difficulty involved in calculating the inverse of these infinite-dimensional matrices is avoided by expanding the inverse matrices as a geometric series. The resulting matrix multiplications obey a group-like structure that can be used to reduce the series to a simpler expression. For instance, $\mathbf{D}^2 = f(\omega)\mathbf{D}$, where $f(\omega)$ is a scalar given in Appendix 4.C.c. For brevity, I will omit the explicit dependence on ω for scalars such as $f(\omega)$ in the following. Because of this group-like structure, $(\mathbb{1} - \mathbf{D})^{-1}$ in Equation (4.27) reduces to $\mathbb{1} + \mathbf{D} + \mathbf{D}^2 + \dots = \mathbb{1} + \mathbf{D} + f\mathbf{D} + \dots = \mathbb{1} + (1 - f)^{-1}\mathbf{D}$. Similarly useful identities between the other matrices can be used to replace the other matrix-inverse operations in Equation (4.27) with simpler expressions. The full details are left to Appendix 4.C. Ultimately, Equation (4.27) reduces to

$$\text{---} \bullet \text{---} = \text{---} \left(\mathbb{1} + \frac{(1 - f) \mathbf{A} + g \mathbf{A}'}{(1 - f)^2 - g^2} \right), \quad (4.28)$$

where the explicit expression for the scalar $g = g(\omega)$ is given in Appendix 4.C.c, and the explicit expressions for the matrix $\mathbf{A}'$, and the other “primed” matrices that I will introduce below, are given in Appendix 4.C.b. Similarly, for the propagator representing

³To obtain Equation (4.26) through blockwise inversion, I first define

$$(\mathbb{1} - \mathbf{M})^{-1} := \begin{pmatrix} \mathbf{W} & \mathbf{X} \\ \mathbf{Y} & \mathbf{Z} \end{pmatrix},$$

such that

$$\begin{aligned} \begin{pmatrix} \mathbb{1} - \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbb{1} - \mathbf{D} \end{pmatrix} \begin{pmatrix} \mathbf{W} & \mathbf{X} \\ \mathbf{Y} & \mathbf{Z} \end{pmatrix} &= \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}, \\ \begin{pmatrix} \mathbf{W} & \mathbf{X} \\ \mathbf{Y} & \mathbf{Z} \end{pmatrix} \begin{pmatrix} \mathbb{1} - \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbb{1} - \mathbf{D} \end{pmatrix} &= \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}. \end{aligned}$$

The 8 relations that can be extracted from these expressions, such as $(\mathbb{1} - \mathbf{A})\mathbf{W} + \mathbf{B}\mathbf{Y} = \mathbb{1}$, can then be used to solve for the four unknowns $\mathbf{W}$, $\mathbf{X}$, $\mathbf{Y}$ and $\mathbf{Z}$, by writing them in terms of $\mathbb{1}$, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$. The resulting expression for $(\mathbb{1} - \mathbf{M})^{-1}$ immediately gives Equation (4.26).

initialisation of a left-moving particle,

$$\text{---} \bullet \text{---} = \text{---} \frac{(1-f) B + g B'}{(1-f)^2 - g^2}. \quad (4.29)$$

The propagators involving the annihilator field ψ (those with an outgoing wavy blue leg representing a left-moving particle) can be obtained by symmetry from Equations (4.28) and (4.29), specifically by exchanging straight red lines and wavy blue lines of the Feynman diagrams. For $\langle \psi(\omega) \tilde{\psi}(\omega_0) \rangle$, this amounts to swapping the leading straight red line on the right-hand side of Equation (4.28) for a wavy blue line and replacing A and A' with D and D' respectively. Similarly, $\langle \psi(\omega) \tilde{\phi}(\omega_0) \rangle$ is obtained from Equation (4.29) by replacing the leading straight red line on the right-hand side with a wavy blue line whilst replacing B and B' with C and C' respectively.

The behaviour of the propagators in real space and direct time is obtained by evaluating the contour integral enclosing all of their poles along the negative imaginary axis. The characteristic timescale is determined by the pole with the largest non-zero imaginary part (i.e. the “least negative” pole). Defining this pole to occur at $\omega = \omega_c$, the long-time behaviour of the system $t \rightarrow \infty$ is determined by $P_R(x, t) - P_R(x) \propto \exp(-i\omega_c t)$, where $P_R(x)$ is the steady-state probability density. The steady-state density is obtained from the residue of the only vanishing pole $\omega = -ir \rightarrow 0^+$ of the full propagators. The explicit inverse Fourier transform of only one of Equation (4.28) or Equation (4.29) is required to obtain the full steady-state density of right-moving particles since the density is independent of initialisation provided $\alpha > 0$.⁴ Hence, the inverse Fourier transform is calculated by either replacing $\langle \phi_n(\omega) \tilde{\phi}_m(\omega_0) \rangle_0$ in Equation (4.12) with $\langle \phi_n(\omega) \tilde{\phi}_m(\omega_0) \rangle$, Equation (4.28), or by replacing $\langle \phi_n(\omega) \tilde{\phi}_m(\omega_0) \rangle_0$ with $\langle \phi_n(\omega) \tilde{\psi}_m(\omega_0) \rangle$, Equation (4.29), and $\tilde{U}_m(x_0)$ with $\tilde{V}_m(x_0)$. The stationary density that arises from either route is

$$P_R(x) = \frac{1}{2L} \left(\frac{\text{Pe}}{e^{\text{Pe}} - 1} e^{\frac{vx}{D}} + e^{\frac{vx}{2D}} C_{\text{Pe}} \frac{2v}{L} h(x) \right), \quad (4.30)$$

where

$$h(x) = \sum_{n=1}^{\infty} \frac{1 - (-1)^n e^{-\text{Pe}/2}}{\left(Dk_n^2 + \frac{v^2}{4D} \right) \sqrt{1 + \frac{v^2}{4D^2 k_n^2}}} \cos(k_n x + \theta_n), \quad (4.31)$$

and

$$C_{\text{Pe}} = \frac{\text{Pe}}{e^{-\text{Pe}} + \text{Pe} - 1 + \frac{v}{\ell\alpha} (1 - e^{-\text{Pe}})} = \frac{\text{Pe}}{e^{-\text{Pe}} + \text{Pe} - 1 + \frac{v^2}{D\alpha}}, \quad (4.32)$$

where the explicit form of ℓ from Equation (4.15) has been inserted into Equation (4.32) to afford a simpler expression. It turns out that Equation (4.31) is a Fourier series repre-

⁴The condition $\alpha > 0$ is necessary for the steady state to be independent of intialisation by allowing at least some transmutation between species. This can be seen in the invertibility of the propagators: setting $\alpha = 0$ leads to $\langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle = \langle \phi(\omega) \tilde{\phi}(\omega_0) \rangle_0$ in Equation (4.28) and $\langle \phi(\omega) \tilde{\psi}(\omega_0) \rangle = 0$ in Equation (4.29). In direct time, the former has the same steady state as Equation (4.13) but the latter vanishes. In short, ergodicity requires $\alpha > 0$.

sensation of

$$h(x) = \frac{L}{2v} \left(e^{-\frac{vx}{2D}} - \frac{\text{Pe}}{e^{\text{Pe}} - 1} e^{\frac{vx}{2D}} \right), \quad (4.33)$$

see Appendix 4.D. Hence, after inserting Equation (4.33) into Equation (4.30), the right-moving steady-state probability density has the closed form

$$P_R(x) = \frac{1}{2L} \left[(1 - C_{\text{Pe}}) \frac{\text{Pe}}{e^{\text{Pe}} - 1} e^{\frac{vx}{2D}} + C_{\text{Pe}} \right] = \frac{1}{2} (1 - C_{\text{Pe}}) P_0(x) + \frac{C_{\text{Pe}}}{2L}, \quad (4.34)$$

where the second equality shows $P_R(x)$ is, up to a constant shift, proportional to the steady-state density for a drift-diffusive particle without boundary tumbling $P_0(x)$, Equation (4.13). Both the shift and the proportionality factor are essentially determined by the constant C_{Pe} , Equation (4.32), which therefore captures the entire effect of the tumbling.

Equation (4.34) is the steady-state solution of the boundary tumbling Fokker-Planck equation, Equation (4.14), for the density of right-moving particles and is a key result of this chapter. The solution for the density of left-moving particles $P_L(x)$ can be found immediately by symmetry, since the steady-state density of left-moving particles is the same as that of right-moving particles after reflecting about $x = L/2$, i.e. $P_L(x) = P_R(L - x)$.

A physically relevant observable is the overall probability density $P(x)$, which is independent of whether particles are right-moving or left-moving, i.e.

$$P(x) = P_R(x) + P_L(x) = \frac{1}{L} \left[(1 - C_{\text{Pe}}) \frac{\text{Pe} \cosh \left[\text{Pe} \left(\frac{x}{L} - \frac{1}{2} \right) \right]}{2 \sinh \left(\frac{\text{Pe}}{2} \right)} + C_{\text{Pe}} \right], \quad (4.35)$$

which has the same functional form as the stationary density for confined RnT particles with uniform tumble rate [121]. Equations (4.34) and (4.35) are in good agreement with Monte-Carlo simulations, see Figure 4.4.

As a further check, I performed simulations to compare the average time it takes the particle to complete a length of the system and transmute between species for various α , finding the average times are all the same after subtracting $1/\alpha$. This confirms ℓ in Equation (4.15) correctly reproduces the desired waiting time $1/\alpha$ for a drift-diffusive particle to transmute at the boundaries. The simulations were performed on a lattice, as opposed to directly simulating the Langevin equation, Equation (4.1), to incorporate the reaction probability's dependence on lattice spacing Δx , Section 4.3.1.

As an aside, the transformation $v \rightarrow -v$ immediately obtains the solution to a system where a right-moving particle changes direction only at the left-hand boundary (and vice versa for the left-moving particle).

4.3.3 Discussion

The extent to which the boundary tumbling system's behaviour differs from that of the pure drift-diffusive system without tumbling, Section 4.2, is captured through the constant C_{Pe} . Vanishing tumble rate $\alpha \rightarrow 0$ results in $C_{\text{Pe}} = 0$, which recovers $P_R(x) \propto P_0(x)$, Equation (4.13). For $C_{\text{Pe}} = 1$, the right-moving probability density reduces to a uniform

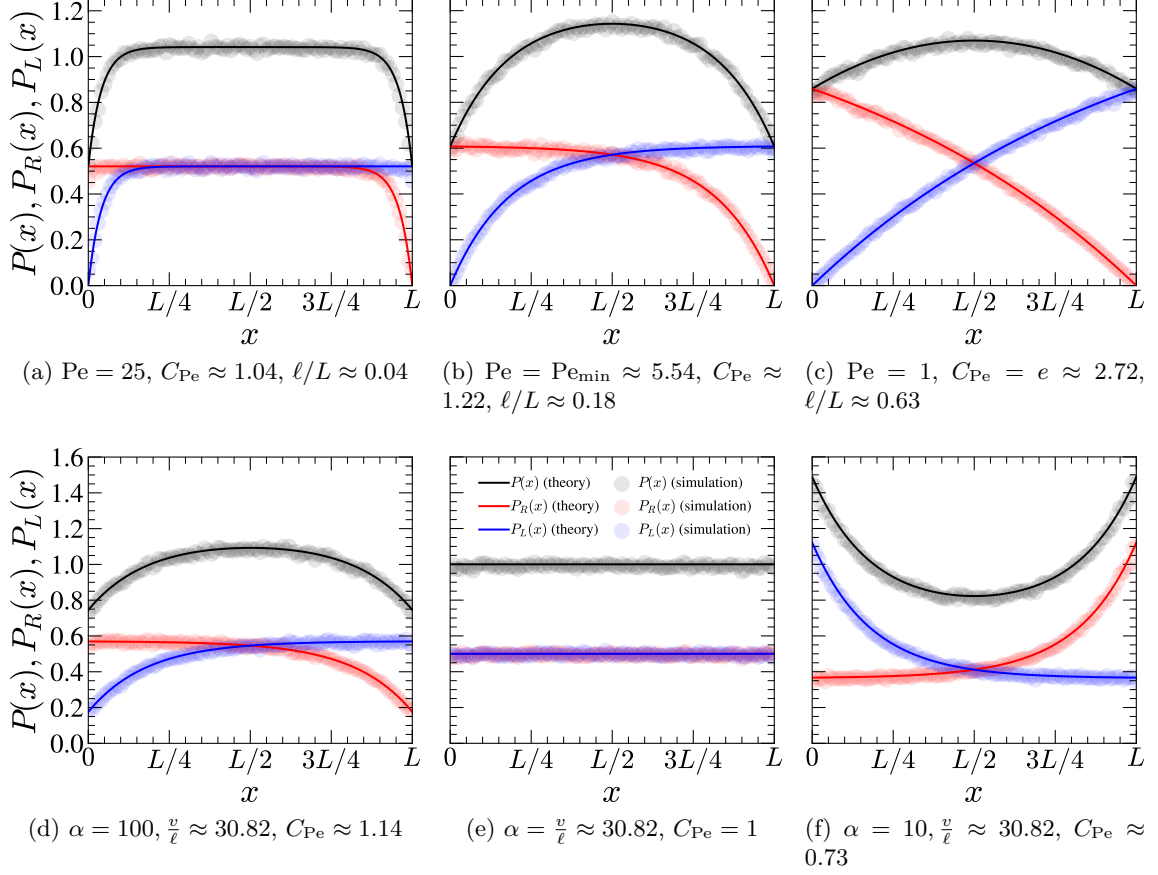


Figure 4.4: Comparison between the theoretical results (solid lines) for the stationary probability densities, $P_R(x)$, Equation (4.34), $P_L(x)$ and $P(x)$, Equation (4.35), and Monte-Carlo simulations (symbols) for varying Pe , (a)–(c), and varying α , (d)–(f). Simulation parameters were set as $D = 1$ and $L = 1$ such that the self-propulsion speed v fully determines the Péclet number, i.e. $Pe = v$. In (a)–(c), $\alpha \rightarrow \infty$ and in (d)–(f), $Pe = Pe_{\min} \approx 5.54$, see discussion after Equation (4.37). The interval is divided into a lattice with spacing $\Delta x = L/100$. In each of the 10^6 simulation runs, a particle is initialised at time $t = 0$ randomly in one of the two internal states and at a random site, before proceeding to hop between sites with rates $h_r = 2D/\Delta x^2 + v/\Delta x$ and $h_l = 2D/\Delta x^2 - v/\Delta x$ to the right and to the left respectively [56]. Upon reaching the right-most site, a right-moving particle converts to a left-moving particle with rate $\ell\alpha/\Delta x$, and vice versa for a left-moving particle at the left-most site. This conversion rate results in an effective waiting time $1/\alpha$ at the boundaries when diffusive fluctuations are taken into account. Estimates of the density were obtained from frequency histograms of the particle's final position by allowing a suitably long time ($t = 5$) to elapse for the simulations to converge to the theoretical steady state.

density $P_R(x) = 1/2L$. For $\alpha \rightarrow \infty$ and $\text{Pe} > 0$,

$$\lim_{\alpha \rightarrow \infty} C_{\text{Pe}} = \frac{\text{Pe}}{e^{-\text{Pe}} + \text{Pe} - 1} > 1, \text{ for } \text{Pe} > 0. \quad (4.36)$$

As seen in Equation (4.35), $C_{\text{Pe}} > 1$ results in a negative pre-factor of $\cosh[\text{Pe}(x/L - 1/2)]$, resulting in a unimodal distribution of particles that are mostly aggregated at the centre of the system, Figures 4.4a–4.4d. The typical bimodal distribution expected of confined RnT particles [26, 27] is obtained for $C_{\text{Pe}} < 1$, Figure 4.4f. Hence, the system undergoes a “shape transition” at $C_{\text{Pe}} = 1$ between distributions which resemble active-like, $C_{\text{Pe}} < 1$, and passive-like, $C_{\text{Pe}} > 1$, behaviour [68], see Figure 4.4e.

In parameter space, $C_{\text{Pe}} = 1$ corresponds to $\alpha = v/\ell$. For $\alpha < v/\ell$ there is a greater tendency for particles to accumulate at the boundaries because of the longer waiting time $1/\alpha$ to react, Figure 4.4f. This is otherwise known as the attracting boundaries case, whilst $\alpha > v/\ell$ corresponds to repelling boundaries [19]. For $\alpha = v/\ell$, the tendency of particles to aggregate at the centre or at the boundaries cancels exactly, which can be seen to result in uniform probability density $P(x) = 1/L$ in Equation (4.35) and Figure 4.4e.

The equality $\alpha = v/\ell$ itself represents a compromise between the time gained by reacting in the diffusive boundary layer of length ℓ and the time lost by waiting to react $1/\alpha$. Upon reaching the edge of a diffusive boundary layer at $x = \ell$ or $x = L - \ell$ from the bulk, the particle is in range of its diffusive fluctuations bringing it in contact with the boundary. Thus the particle *effectively* reacts within the boundary layer of length ℓ . In the case where $\alpha \rightarrow \infty$, a particle that enters the boundary layer can instantly jump to the boundary and then instantly convert to the opposite species. Hence, ℓ also takes on the role of a depletion region length, as can be seen by comparing $\ell/L = (1 - \exp(-\text{Pe}))/\text{Pe}$ in Figures 4.4a–4.4c. This shortens the particle’s journey between boundaries by the boundary layer length ℓ and hence the travel time shortens on average by ℓ/v . Uniform density is restored by introducing a finite reaction rate $\alpha = v/\ell$ that exactly compensates for the effective shortening of the system length by making particles wait an average time $1/\alpha = \ell/v$ in the boundary layer.

A more quantitative way to characterise the shape transition across $C_{\text{Pe}} = 1$ is through the variance $\sigma^2 := \overline{x^2} - \bar{x}^2$ of the probability density $P(x)$, where $\bar{x}^n = \int_0^L dx x^n P(x)$ is the n^{th} moment of the state-independent particle position. The variance, calculated using $P(x)$ from Equation (4.35), is

$$\sigma^2 = L^2 \left[\left(\frac{1}{2} + \frac{2}{\text{Pe}^2} - \frac{\coth(\frac{\text{Pe}}{2})}{\text{Pe}} \right) (1 - C_{\text{Pe}}) + \frac{C_{\text{Pe}}}{3} - \frac{1}{4} \right]. \quad (4.37)$$

When $\alpha = v/\ell$, corresponding to $C_{\text{Pe}} = 1$, $P(x)$ is uniform and so σ^2 , Equation (4.37), reduces to that of a uniform probability density, i.e. $\sigma^2 = L^2/12$. When $P(x)$ is unimodal, corresponding to $\alpha > v/\ell$ and $C_{\text{Pe}} > 1$, particles are aggregated mostly at the centre of the system and so $\sigma^2 < L^2/12$. For $\alpha < v/\ell$, there is some non-trivial function $\text{Pe}_{\text{min}}(\alpha)$ that minimises σ^2 as a function of Pe , Figure 4.5. In principle, this can be obtained from

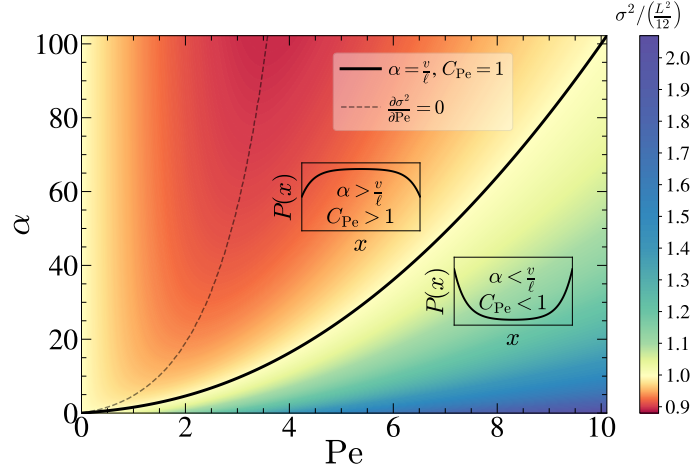


Figure 4.5: Variance σ^2 , Equation (4.37), of the probability density $P(x)$, Equation (4.35), as a function of α and Pe for parameters $D = 1$ and $L = 1$, such that $Pe = v$. The solid line $\alpha = v/\ell$, corresponding to $C_{Pe} = 1$, divides the plane into two halves. The top half corresponds to unimodal $P(x)$ and thus smaller variance than for a uniform probability density, i.e. $\sigma^2 < L^2/12$. The non-monotonic behaviour of σ^2 as a function of Pe means there is a curve (dashed line) at which σ^2 is minimised. For bimodal $P(x)$, depicted in the lower half of the plane, the variance is $\sigma^2 > L^2/12$ and monotonically increases with Pe .

$\partial_{Pe}\sigma^2 = 0$, but the resulting equation cannot be solved for Pe in closed form and so it must be solved numerically. Since σ^2 is a monotonically decreasing function of α , as seen in Figure 4.5, the minimum value of σ^2 occurs on this line at $\alpha \rightarrow \infty$. Through numerical evaluation, one finds $Pe_{\min} := Pe_{\min}(\alpha \rightarrow \infty) \approx 5.54$. Thus $(Pe, \alpha) = (5.54, \infty)$ is the point in parameter space where σ^2 is minimised. The corresponding probability density for $\alpha \rightarrow \infty$ and $Pe = Pe_{\min}$ is plotted in Figure 4.4b. Figures 4.4d–4.4f are also plotted for $Pe = Pe_{\min}$. For no activity, i.e. $Pe = 0$, the variance is $\sigma^2 = L^2/12$, consistent with the particles being purely diffusive. When the probability density is bimodal, corresponding to $\alpha < v/\ell$ and $C_{Pe} < 1$, the variance is $\sigma^2 > L^2/12$ since particles are mostly aggregated at the boundaries and are more spread out. In this regime, σ^2 monotonically increases with Pe as an increasing number of particles accumulate at the boundaries. In the limit $v \rightarrow \infty$, $\sigma^2 \rightarrow L^2/4$ as $P(x) \rightarrow \delta(x)/2 + \delta(x - L)/2$.

I will now consider the limiting behaviour of $P_R(x)$, Equation (4.34). The limiting behaviour of the other probability densities can be obtained immediately from the symmetry arguments $P_L(x) = P_R(L - x)$ and $P(x) = P_R(x) + P_R(L - x)$ and so will not be calculated explicitly. In the following, I pay particular attention to whether limits commute with $\alpha \rightarrow \infty$. As argued below, non-commuting limits reflect that the approach to a particular state can result in different physical features arising in the system.

Firstly, I consider the parameter limits equivalent to $Pe \rightarrow 0$. Though right-moving and left-moving particles are physically indistinguishable in the limit $v \rightarrow 0$, I assume they can still be identified by some other attribute (such as colour as in Figure 4.3). Taking

the $v \rightarrow 0$ limit first,

$$\lim_{v \rightarrow 0} P_R(x) = \frac{1}{L} \frac{D + \alpha L(L - x)}{2D + \alpha L^2}. \quad (4.38)$$

For $\alpha \rightarrow 0$ or $D \rightarrow \infty$ in Equation (4.38), $P_R(x) \rightarrow 1/(2L)$ as in the equilibrium case. For $\alpha \rightarrow \infty$ or $D \rightarrow 0$ in Equation (4.38), right-moving particles deplete linearly between the two boundaries, i.e. $P_R(x) \rightarrow (1 - x/L)/L$, as can be seen for small Pe in Figure 4.4c.

The limit $D \rightarrow \infty$ of the right-moving density $P_R(x)$ in Equation (4.34) does not commute with $\alpha \rightarrow \infty$. If $D \rightarrow \infty$ is taken first, then $P_R(x) \rightarrow 1/2L$, again in line with an equilibrium system. However, for $\alpha \rightarrow \infty$, the dimensionless parameter $v^2/D\alpha$ in C_{Pe} , Equation (4.32), vanishes and so $D \rightarrow \infty$ becomes equivalent to taking $\text{Pe} \rightarrow 0$ in C_{Pe} . Thus, first taking $\alpha \rightarrow \infty$ then $D \rightarrow \infty$ gives the same as the $v \rightarrow 0$ limit above, i.e. $P_R(x) \rightarrow (1 - x/L)/L$. Despite these limits not commuting, they retain the same overall probability density $P(x) \rightarrow 1/L$ when both $D \rightarrow \infty$ and $\alpha \rightarrow \infty$.

I now consider the $\text{Pe} \rightarrow \infty$ limits starting with $v \rightarrow \infty$. Treating the boundary as a separate case, $\lim_{v \rightarrow \infty} P_R(x < L) = 0$ and $\lim_{v \rightarrow \infty} P_R(x = L) = \infty$. Hence, one can assign

$$\lim_{v \rightarrow \infty} P_R(x) = \frac{1}{2} \delta(x - L), \quad (4.39)$$

for a correctly normalised density of right-moving particles. Equation (4.39) reflects that a particle with infinite self-propulsion speed v is not found in the bulk since it immediately jumps to the right-hand boundary where it waits to transmute for a finite time $1/\alpha$.

Similar care for boundary cases needs to be taken for $D \rightarrow 0$ in Equation (4.34), for which $\lim_{D \rightarrow 0} P_R(x < L) = (1 + v/L\alpha)^{-1}/2L$ and $\lim_{D \rightarrow 0} DP_R(x = L) = V[1 - (1 + v/L\alpha)^{-1}]/2$. In other words, $\lim_{D \rightarrow 0} P_R(x)$ diverges at $x = L$, but is finite in the bulk. Hence,

$$\lim_{D \rightarrow 0} P_R(x) = \frac{1}{2L} \frac{1}{1 + \frac{v}{L\alpha}} + \frac{1}{2} \delta(x - L) \left(1 - \frac{1}{1 + \frac{v}{L\alpha}} \right). \quad (4.40)$$

Equation (4.40) differs to Equation (4.39) because particles still have finite self-propulsion speed v and thus still spend a finite time travelling in the bulk. Taking $v \rightarrow \infty$ in Equation (4.40) recovers Equation (4.39). Taking $\alpha \rightarrow 0$ in Equation (4.40) also gives $P_R(x) \rightarrow \delta(x - L)/2$, since particles cannot transmute at the right-hand boundary and so get stuck there. Taking $\alpha \rightarrow \infty$ in Equation (4.40) gives $P_R(x) \rightarrow 1/2L$ since particles no longer wait to react at the boundary and so are uniformly distributed.

Different limiting behaviour is obtained from taking $\alpha \rightarrow \infty$ *before* the above $\text{Pe} \rightarrow \infty$ limits. As before, first taking $\alpha \rightarrow \infty$ restores the symmetry between $v \rightarrow \infty$ and $D \rightarrow 0$ as Pe becomes the only dimensionless parameter in C_{Pe} , Equation (4.36). Thus, taking either $v \rightarrow \infty$ or $D \rightarrow 0$ *after* $\alpha \rightarrow \infty$ results in

$$\lim_{\text{Pe} \rightarrow \infty} \lim_{\alpha \rightarrow \infty} P_R(x) = \begin{cases} \frac{1}{2L}, & 0 \leq x < L \\ 0, & x = L \end{cases}, \quad (4.41)$$

reflecting a right-moving particle can never be found at the right-hand boundary where it

transmutes instantly, but it should otherwise be uniformly distributed as it is not sensitive to any waiting time at the boundary. This is seen for large Pe in Figure 4.4a, where $P_R(x)$ approaches uniform density in the bulk but is still constrained to satisfy $P_R(L) = 0$.

Physically, the non-commuting limits $\alpha \rightarrow \infty$ and $Pe \rightarrow \infty$ demonstrate that different behaviour is obtained depending on whether C_{Pe} approaches 1 from above or below, i.e. $C_{Pe} \rightarrow 1^\pm$ in Equation (4.34). For instance, consider if the system first starts in the state where $\alpha \rightarrow \infty$ while D and v are both finite. This places the system state in the top half of the plane in Figure 4.5, above the curve $C_{Pe} = 1$, such that $P(x)$ is unimodal and resembles that of Figures 4.4a–4.4c. Then, evolving the system parameters so that $Pe \rightarrow \infty$, such as by cooling the surrounding particle bath so that $D \rightarrow 0$, shifts the system state in parameter space to the right till it meets the curve $C_{Pe} = 1$ from above, $C_{Pe} \rightarrow 1^+$. While the system is being evolved, $P_R(x)$ is restricted to $P_R(L) = 0$ and so retains this feature as the system approaches $C_{Pe} \rightarrow 1^+$, resulting in Equation (4.41). A similar argument applies to first taking $v \rightarrow \infty$ or $D \rightarrow 0$ followed by $\alpha \rightarrow \infty$, which places the system state in the lower half of the plane in Figure 4.5 such that $C_{Pe} \rightarrow 1^-$. In this case, the right-moving probability density $P_R(x)$ resembles that of Figure 4.4f and so does not have the feature $P_R(L) = 0$ as the system is evolved towards $C_{Pe} = 1$. Hence, the different approaches to $C_{Pe} = 1$ result in different probability densities in this limit.

To conclude the limiting behaviour of $P_R(x)$, for $L \rightarrow 0$, Equation (4.34) diverges since the particle is confined to a single point in space. In the limit of infinite system size $L \rightarrow \infty$, $P_R(x) \rightarrow 0$ because the particle is not confined and so does not have a non-trivial steady state.

I now consider how the current behaves under the same limits considered above. The steady-state current for right-moving particles is given by

$$J_R(x) = vP_R(x) - D \frac{\partial P_R(x)}{\partial x} = \frac{v}{2L} C_{Pe}. \quad (4.42)$$

The current for left-moving particles $J_L(x)$ is found by replacing $P_R(x)$ with $P_L(x)$ and v with $-v$ on the right-hand side of the first equality in Equation (4.42). This results in $J_L = -J_R$ and so both currents are constant across space, whilst the net current $J = J_R + J_L$ vanishes. The non-zero currents that arise when the internal state is known are a result of a given particle species appearing to continually enter the system at one boundary and then leave through the other. This is possible only if the particle can transmute between species and thus $\alpha > 0$ is necessary to obtain perpetual internal currents.

In contrast to the density, all limits of the current commute with $\alpha \rightarrow \infty$. First, taking $v \rightarrow 0$,

$$\lim_{v \rightarrow 0} J_R = \frac{\alpha D}{2D + \alpha L^2}, \quad (4.43)$$

which subsequently vanishes for $\alpha \rightarrow 0$ (no transmutation to generate a steady-state current) or $D = 0$ (particles do not move). Though the particle is no longer active for $v \rightarrow 0$, the transmutation effectively rectifies the motion of a single particle species and so a current is still observed if the species can be distinguished. Taking instead $v \rightarrow \infty$ or $D \rightarrow$

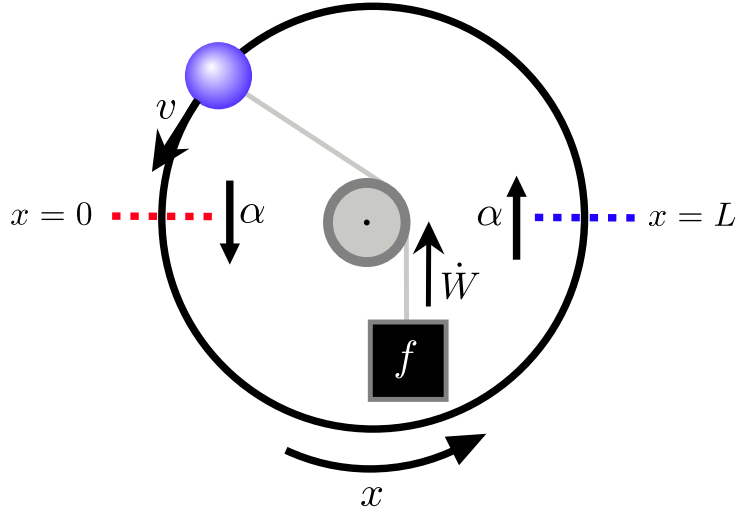


Figure 4.6: Schematic illustration of how the boundary tumbling system can be used to perform work against an external force f by harnessing the non-zero steady-state net current of the spatially periodic setup, see Figure 4.2(b) and Equation (4.45).

∞ in Equation (4.42) gives $J_R \rightarrow \alpha/2$ since particles traverse the system instantly and so the dynamics effectively reduce to a single point where a particle transmutes between species with rate α (the factor $1/2$ accounts for the probability to find the particle in the right-moving state). This is confirmed by taking $L \rightarrow 0$ in Equation (4.42), which gives the same result of $J_R \rightarrow \alpha/2$. In the opposite limit, $v \rightarrow -\infty$, the right-moving current $J_R \rightarrow 0$ since, in this case, particles are pinned against the boundary at which they came into existence by their own self-propulsion.

In the deterministic limit $D \rightarrow 0$, Equation (4.42) becomes

$$\lim_{D \rightarrow 0} J_R = \frac{\frac{1}{2}}{\frac{L}{v} + \frac{1}{\alpha}}, \quad (4.44)$$

reflecting a particle takes time $L/v + 1/\alpha$ to complete a length of the system since L/v time is spent moving between the boundaries and $1/\alpha$ time is spent waiting to react at the boundaries. Finally, taking $L \rightarrow \infty$ in Equation (4.42) gives $J_R \rightarrow 0$ due to the lack of a non-trivial steady-state density.

4.3.4 Fluctuation-enhanced work extraction

In this section, I present a way of extracting work from this system. Suppose now that an external counterforce of magnitude f is applied always against the particle's self-propelled motion, i.e. $v \rightarrow v - f$ in all v -dependent quantities of the system, e.g. $\text{Pe} \rightarrow (v - f)L/D$. The external counterforce is envisaged as playing the role of something like a mass on a pulley, such that the particle's self-propelled motion could theoretically be used to raise this mass and thus store gravitational potential energy. In other words, the system could be used to perform useful work. The requirement that the external counterforce is *always* directed against the particle's self-propelled motion naturally lends itself to the spatially

periodic “ring” variation of the model introduced at the end of Section 4.3.1, and illustrated in Figure 4.2(b). In Figure 4.6, I schematise how the non-zero net current of the ring model can be harnessed to do work against the external counterforce. Using the mapping between the finite interval and the spatially periodic domain originally presented in Figure 4.2 and Equation (4.16), it is easy to deduce that the net current on the ring is given by

$$J_{\text{ring}} = \frac{v - f}{2L} C_{\text{Pe}} = \begin{cases} J_R, & 0 \leq x < L, \\ -J_L, & L \leq x < 2L. \end{cases} \quad (4.45)$$

Hence, the average rate of work performed by the system is

$$\dot{W} = 2L J_{\text{ring}} f = (v - f) C_{\text{Pe}} f, \quad (4.46)$$

where $2L J_{\text{ring}}$ is the mean speed of the particle and recall that all $v \rightarrow v - f$ in the original expression for C_{Pe} , Equation (4.32). This expression for $\dot{W}$ should be immediately compared against that of the classic drift-diffusive particle (on a ring), which is $\dot{W} = (v - f)f$, see Section 2.6. Equation (4.36) demonstrates that $C_{\text{Pe}} > 1$ for $\alpha \rightarrow \infty$ and $\text{Pe} > 0$, and so the presence of the boundaries (or partially permeable membranes in the case of the ring) in the boundary tumbling model, as captured solely through C_{Pe} in Equation (4.46), results in more work being extracted per unit time than in their absence for the case of instantaneous transmutation/crossing.

Aside from the particle’s travel time between boundaries/membranes being shortened by ℓ/v , as described in Section 4.3.3, another reason for this “boosted” work extraction is that the crossing of the membranes (of the spatially periodic model) is irreversible, and so this has the effect of rectifying the particle’s thermal fluctuations. Essentially, the membranes act like a mechanical diode by preventing backwards motion of the particle beyond a maximum distance L . This could already be seen in Equation (4.43), where the absence of self-propulsion, which would normally correspond to an equilibrium system, still produces internal probability currents. The extent of this rectification is not limited in any way, and so the rate of work extraction can be made arbitrarily large by simply increasing the diffusion D . This can be seen in Figure (4.7), where it also becomes clear that optimal work extraction for large D eventually occurs for an external counterforce $f > v$, signifying that most of the work being performed by the system is not coming from the particle’s self-propelled motion, but rather from the membranes rectifying its thermal fluctuations. Said another way, it appears the net result of the system’s operation is that heat is extracted from a single heat bath (since there is only one diffusion parameter in this model) to perform useful work. This is seemingly in violation of The Second Law of Thermodynamics.

The resolution to this becomes clear after calculating the entropy production of the system. Since the crossing of the membranes is completely irreversible, the entropy production diverges. Another way of picturing this is that the particle’s internal state switches only at single points in space. The sharpness of these transitions signify that the system

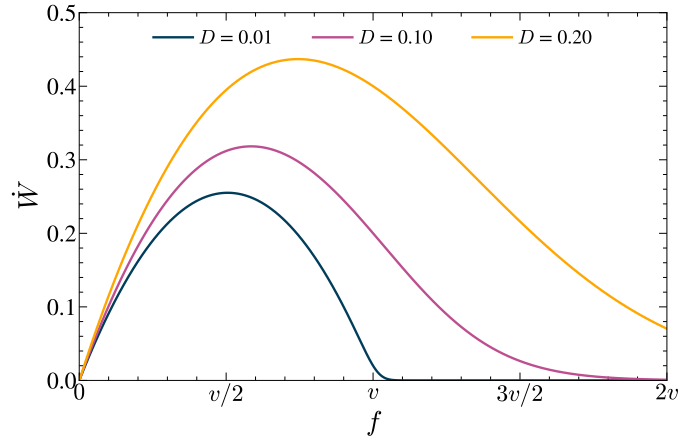


Figure 4.7: Rate of work extraction, Equation (4.46), for the boundary tumbling model. For small diffusion D , the rate of work extraction resembles that of a plain drift-diffusive particle, i.e. $\dot{W} = (v - f)f$, in the region $0 \leq f < v$. In contrast, for large f , the work extraction of the boundary tumbling model remains positive because the membranes prevent particles moving backwards beyond a maximum distance L . As D is increased, the rate of work extraction increases unbounded because of the rectification of thermal fluctuations by the membranes. This can also be seen in the value of f at which optimal work extraction occurs, which continually shifts to higher values as D is increased, since an increasingly larger proportion of the work being performed by the system comes from the rectification of thermal fluctuations rather than the particle's self-propulsion.

is making an infinitely precise measurement of the particle's position to know precisely when it has come into contact with a boundary/membrane. If the particle were able to switch states anywhere in space, even if the distribution of these switches was still highly localised at the membranes, then the crossing of the (smeared out) membranes would be reversible and the entropy production rendered finite. Diverging entropy production, however, tells us that the energetic cost associated with making these measurements is in fact (infinitely) greater than the work being extracted by rectification of the particle's thermal fluctuations. This restores consistency with The Second Law since the system cannot actually extract heat from the heat bath to perform useful work without a greater amount of work first being injected into the system itself.

If one desires work extraction from this system without a diverging operational cost, then additional terms need to be added to the model that allow the particle to transmute between both species at both boundaries, e.g. allow a right-moving particle to also transmute into a left-moving particle at the left-hand boundary. This would cancel the irreversibility mentioned above and hence result in finite entropy production. Yet, this could still never achieve work extraction exceeding the amount of energy that needs to be injected into the system for its operation. For instance, suppose β is introduced as the rate of these “reverse transmutations”. The rate of work extraction increases with the ratio α/β as this represents the ratio of forward to backward rectifications. However, so does the rate of entropy production, because the system becomes increasingly irreversible,

and this increasing rate of entropy production always exceeds the increasing rate of work extraction.

4.4 Conclusion

In this chapter, I derived the fully time-dependent, Equations (4.28) and (4.29), and steady-state, Equations (4.34) and (4.35), solutions to the probability density of a confined self-propelled particle that changes self-propulsion direction through interacting stochastically with boundaries. The results of this “boundary tumbling” RnT model were confirmed with lattice simulations, Figure 4.4. Localised reactions were handled within a perturbative framework, Section 4.3.2, and posed a significant technical challenge compared to a confined RnT system with uniform tumble rate [26, 27]. The derivation made use of field-theoretic techniques in the Doi-Peliti formalism [88, 90], thus making the developed framework easily extensible to including additional arbitrary interactions.

Of particular interest is the incorporation of diffusion in the model, which prevents particles from sticking to the boundaries in spite of their tendency to accumulate at the boundaries due to their self propulsion. While a Poissonian transmutation at the boundaries is trivial to implement and handle on a lattice, where particles can indeed appear to get stuck at a boundary, doing the same in the continuum posed physical and mathematical hurdles addressed in Section 4.3.1 and Appendix 4.B.

The results show that boundary RnT particles undergo a shape transition that depends on the size ℓ , Equation (4.15), of the diffusive fluctuations away from the boundaries. This transition is between particles mainly aggregating at the system centre for large transmutation rates $\alpha > v/\ell$, or at the boundaries for small transmutation rates $\alpha < v/\ell$, Figures 4.4d–4.4f. This transition is characterised by whether the variance σ^2 , Equation (4.37), of the overall probability density $P(x)$, Equation (4.35), is greater or smaller than that of a uniform probability density $L^2/12$.

The key part of this chapter is the study of work extraction in Section 4.3.4. There, I presented a viable way of extracting work from this boundary tumbling system, in particular finding that the particle’s interactions with the boundaries actually boost the rate of work extraction, as dictated by Equation (4.46). This arises from the rectification of thermal fluctuations at the boundaries in an irreversible reaction. As a result, these reactions also incur a diverging energetic cost that ensures compliance with The Second Law of Thermodynamics. If one wishes to have an “active engine” without diverging energy input, then additional terms need to be added to the model to make the reactions at the boundaries reversible. Including such terms would be an interesting extension to the work presented in this chapter.

CHAPTER 4 APPENDICES

4.A Right eigenfunctions of the reflecting boundaries drift-diffusion equation

A similar derivation to the following appears in Ref. [113]. The right eigenfunctions of the drift-diffusion equation with reflecting boundaries are derived in general by trialling

$$U_n(x) = Ae^{ax}. \quad (4.47)$$

Substituting Equation (4.47) into the eigenvalue equation

$$\mathcal{L}U_n(x) = \left(D\frac{\partial^2}{\partial x^2} - v\frac{\partial}{\partial x}\right)U_n(x) = \lambda_n U_n(x) \quad (4.48)$$

results in the characteristic equation

$$Da^2 - va - \lambda_n = 0. \quad (4.49)$$

Solving for the exponent a , I find

$$a_{\pm} = \frac{v}{2D} \pm \sqrt{\frac{v^2}{4D^2} + \frac{\lambda_n}{D}}. \quad (4.50)$$

Hence, the general solution is

$$U_n(x) = A_+e^{a_+x} + A_-e^{a_-x}. \quad (4.51)$$

The eigenvalues λ_n and one of the amplitudes $A_{\pm}$ are fixed by the boundary conditions, as demonstrated in the following. First, from substituting Equation (4.51) into the boundary condition $J(x=0, t) = 0$, Equation (4.4),

$$\left(D\frac{\partial}{\partial x} - v\right)U_n(x)\Big|_{x=0} = 0, \quad (4.52)$$

it follows that

$$A_- = A_+ \frac{\sqrt{v^2 + 4\lambda_n D} - v}{\sqrt{v^2 + 4\lambda_n D} + v}. \quad (4.53)$$

Similarly, applying the boundary condition at $x = L$,

$$\left(\sqrt{\frac{v^2}{4} + D\lambda_n} - \frac{v}{2}\right) \sinh\left(\sqrt{\frac{v^2}{4D^2} + \frac{\lambda_n}{D}}L\right) = 0, \quad (4.54)$$

implying the eigenvalues are given by $\lambda_0 = 0$ (from the first bracket) and $\lambda_n = -Dk_n^2 - v^2/4D$ (from the sinh function), as stated around Equations (4.6a) and (4.6b).

Beginning with $\lambda_0 = 0$, Equation (4.53) gives $A_- = 0$, while the exponent for the first

term in Equation (4.51) reduces to $a_+x = vx/D$, recovering the eigenfunction $U_0(x) = \exp(vx/D)$, Equation (4.6a).

Finally, I consider the eigenfunctions for $n > 0$, which have eigenvalues $\lambda_n = -Dk_n^2 - v^2/4D$. Substituting $\lambda_n = -Dk_n^2 - v^2/4D$ into Equation (4.53) and then substituting the resulting expression for A_- into Equation (4.51) yields

$$U_n(x) = A_+ e^{\frac{v}{2D}x} \left[e^{ik_n x} + \frac{2iDk_n - v}{2iDk_n + v} e^{-ik_n x} \right], \quad (4.55)$$

which reduces to Equation (4.6b) after rewriting in terms of trigonometric functions and with suitable normalisation determining A_+ .

4.B Derivation of boundary tumbling length scale

The boundary tumbling length scale ℓ , Equation (4.15), was introduced in Section 4.3.1 on dimensional grounds and as a way to account for fluctuations keeping a particle away from a boundary where it would otherwise transmute into the opposite species. In this section, the explicit form of the length scale is derived from a lattice model of N sites. I begin by demanding the effective transmutation rate is α for a particle that resides at the boundary site $i = N$ with a probability p_N according to the steady state of a non-transmuting drift-diffusion particle. The probability to reside at the boundary site decreases with the lattice spacing Δx due to fluctuations reducing the chances for the transmutation to take place at that site. To maintain a constant *effective* transmutation rate α , despite diminished residence probability, one needs to compensate for the decreasing residence probability at the transmutation site $i = N$ by increasing the rate with which transmutation takes place *conditional* to residence. I will consider only a right-moving particle, because the arguments readily translate to left-moving particles.

Denoting by p_i the steady-state probability to be located at site $i \in \{1, 2, \dots, N\}$ in a system with N sites, a right-moving particle therefore needs to transmute with effective rate α/p_N at the right-most site, captured in a master equation by adding a transmutation term with rate $\delta_{i,N}\alpha/p_N$. If the steady state were such that the particle resides at site $i = N$ almost surely, i.e. $p_N = 1$, the effective transmutation rate would simply be α and the dynamics a matter of the particle reaching the steady state and transmuting over and over. However, if the hopping rates are $h_r = 2D/\Delta x^2 + v/\Delta x$ and $h_l = 2D/\Delta x^2 - v/\Delta x$ to the right and to the left respectively [56], the solution to the steady-state equations $h_r p_{i-1} - (h_r + h_l)p_i + h_l p_{i+1} = 0$ is

$$p_i = \mathcal{N}^{-1} \left(\frac{h_r}{h_l} \right)^i, \quad (4.56)$$

with normalisation $\mathcal{N} = q(1 - q^N)/(1 - q)$, where

$$q = \frac{h_r}{h_l} = 1 + \frac{v\Delta x}{D} + \mathcal{O}(\Delta x^2). \quad (4.57)$$

After some algebra, it follows that p_N vanishes like Δx and so taking $\Delta x \rightarrow 0$ with $N\Delta x = L$ remaining constant gives

$$\lim_{\Delta x \rightarrow 0} \frac{p_N}{\Delta x} = \frac{v}{D} \left(1 - e^{-\frac{vL}{D}}\right)^{-1}. \quad (4.58)$$

In a master equation, the transmutation therefore needs to take place with rate

$$\lim_{\Delta x \rightarrow 0} \frac{\delta_{i,N}}{p_N} \alpha = \frac{D}{v} \left(1 - e^{-\frac{vL}{D}}\right) \alpha \delta(x - L) = \ell \alpha \delta(x - L), \quad (4.59)$$

using $\lim_{\Delta x \rightarrow 0} \delta_{i,N}/\Delta x = \delta(x - L)$ and the definition of the length scale ℓ of Equation (4.15).

Equation (4.59) remains valid even for $v < 0$, since $\ell \geq 0$ still. This would correspond to a system where particles have a bias towards the boundary where they came into existence by transmutation.

4.C Explicit expressions for integrals and matrices in Section 4.3.2

This appendix contains explicit expressions for some of the mathematical objects encountered in Section 4.3.2, namely the integrals over eigenfunctions arising from Equation (4.17), the perturbative matrices A, B, C and D defined in Equation (4.25), and their counterparts A', B', C' and D' that appear in Equations (4.28) and (4.29).

4.C.a Integrals of eigenfunctions

The integrals over eigenfunctions arising from the perturbative parts of the action, Equation (4.17), are

$$\begin{aligned} \Delta_{\tilde{\phi}_i \phi_j} &= -\frac{\ell \alpha}{L^2} \int_0^L dx \delta(x - L) \tilde{U}_i(x) U_j(x) \\ &= -\frac{\ell \alpha}{L^2} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} \delta_{i0} \delta_{j0} + \frac{2\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}/2} \frac{(-1)^j}{\sqrt{1 + v^2/4D^2 k_j^2}} \delta_{i0} (1 - \delta_{j0}) \right. \\ &\quad \left. + 2e^{\text{Pe}/2} \frac{(-1)^i}{\sqrt{1 + v^2/4D^2 k_i^2}} (1 - \delta_{i0}) \delta_{j0} \right. \\ &\quad \left. + \frac{4(-1)^{i+j}}{\sqrt{(1 + v^2/4D^2 k_i^2)(1 + v^2/4D^2 k_j^2)}} (1 - \delta_{i0})(1 - \delta_{j0}) \right), \end{aligned} \quad (4.60)$$

$$\begin{aligned} \Delta_{\tilde{\psi}_i \phi_j} &= \frac{\ell \alpha}{L^2} \int_0^L dx \delta(x - L) \tilde{V}_i(x) U_j(x) \\ &= -\Delta_{\tilde{\phi}_i \phi_j} e^{\text{Pe}}, \end{aligned} \quad (4.61)$$

$$\begin{aligned}
 \Delta_{\tilde{\psi}_i \psi_j} &= -\frac{\ell\alpha}{L^2} \int_0^L dx \delta(x) \tilde{V}_i(x) V_j(x) \\
 &= -\frac{\ell\alpha}{L^2} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} \delta_{i0} \delta_{j0} + \frac{2\text{Pe}}{1 - e^{-\text{Pe}}} \frac{1}{\sqrt{1 + v^2/4D^2 k_j^2}} \delta_{i0} (1 - \delta_{j0}) \right. \\
 &\quad \left. + \frac{2}{\sqrt{1 + v^2/4D^2 k_i^2}} (1 - \delta_{i0}) \delta_{j0} \right. \\
 &\quad \left. + \frac{4}{\sqrt{(1 + v^2/4D^2 k_i^2) (1 + v^2/4D^2 k_j^2)}} (1 - \delta_{i0}) (1 - \delta_{j0}) \right), \tag{4.62}
 \end{aligned}$$

$$\begin{aligned}
 \Delta_{\tilde{\phi}_i \psi_j} &= \frac{\ell\alpha}{L^2} \int_0^L dx \delta(x) \tilde{U}_i(x) V_j(x) \\
 &= \frac{\ell\alpha}{L^2} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}} \delta_{i0} \delta_{j0} + \frac{2\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}} \frac{1}{\sqrt{1 + v^2/4D^2 k_j^2}} \delta_{i0} (1 - \delta_{j0}) \right. \\
 &\quad \left. + \frac{2}{\sqrt{1 + v^2/4D^2 k_i^2}} (1 - \delta_{i0}) \delta_{j0} \right. \\
 &\quad \left. + \frac{4}{\sqrt{(1 + v^2/4D^2 k_i^2) (1 + v^2/4D^2 k_j^2)}} (1 - \delta_{i0}) (1 - \delta_{j0}) \right). \tag{4.63}
 \end{aligned}$$

4.C.b Perturbative matrices (amputated Feynman diagrams)

The perturbative matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$ in Equation (4.25), are calculated from the integrals in Equations (4.60)–(4.63), and the bare propagator, Equation (4.11), via $\mathbf{A}_{ij} = \sum_k \Delta_{\tilde{\phi}_i \phi_k} \langle \phi_k(\omega) \tilde{\phi}_j(\omega_0) \rangle$ and similarly for $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$. The primed counterparts to these matrices $\mathbf{A}'$, $\mathbf{B}'$, $\mathbf{C}'$, and $\mathbf{D}'$ that appear in Equations (4.28) and (4.29), arise as products of the unprimed matrices, see Appendix 4.C.c. The explicit forms of these matrices are

$$\begin{aligned}
 \mathbf{A}_{ij} = -\mathbf{C}_{ij} e^{-\text{Pe}} &= -\frac{\ell\alpha}{L} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{\delta_{i0} \delta_{j0}}{-i\omega + r} \right. \\
 &\quad + \frac{\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}/2} \frac{(-1)^j}{\sqrt{1 + v^2/4D^2 k_j^2}} \frac{\delta_{i0} (1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \\
 &\quad + 2e^{\text{Pe}/2} \frac{(-1)^i}{\sqrt{1 + v^2/4D^2 k_i^2}} \frac{(1 - \delta_{i0}) \delta_{j0}}{-i\omega + r} \\
 &\quad \left. + \frac{2(-1)^{i+j}}{\sqrt{(1 + v^2/4D^2 k_i^2) (1 + v^2/4D^2 k_j^2)}} \frac{(1 - \delta_{i0}) (1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right), \tag{4.64}
 \end{aligned}$$

$$\begin{aligned}
 D_{ij} = & -\frac{\ell\alpha}{L} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{\delta_{i0}\delta_{j0}}{-i\omega + r} + \frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{1}{\sqrt{1 + v^2/4D^2k_j^2}} \frac{\delta_{i0}(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right. \\
 & + \frac{2}{\sqrt{1 + v^2/4D^2k_i^2}} \frac{(1 - \delta_{i0})\delta_{j0}}{-i\omega + r} \\
 & \left. + \frac{2}{\sqrt{(1 + v^2/4D^2k_i^2)(1 + v^2/4D^2k_j^2)}} \frac{(1 - \delta_{i0})(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right), \tag{4.65}
 \end{aligned}$$

$$\begin{aligned}
 B_{ij} = & \frac{\ell\alpha}{L} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}} \frac{\delta_{i0}\delta_{j0}}{-i\omega + r} + \frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{e^{-\text{Pe}}}{\sqrt{1 + v^2/4D^2k_j^2}} \frac{\delta_{i0}(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right. \\
 & + \frac{2}{\sqrt{1 + v^2/4D^2k_i^2}} \frac{(1 - \delta_{i0})\delta_{j0}}{-i\omega + r} \\
 & \left. + \frac{2}{\sqrt{(1 + v^2/4D^2k_i^2)(1 + v^2/4D^2k_j^2)}} \frac{(1 - \delta_{i0})(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right), \tag{4.66}
 \end{aligned}$$

$$\begin{aligned}
 A'_{ij} = & -\frac{\ell\alpha}{L} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{\delta_{i0}\delta_{j0}}{-i\omega + r} + \frac{\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}/2} \frac{(-1)^j}{\sqrt{1 + v^2/4D^2k_j^2}} \frac{\delta_{i0}(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right. \\
 & + \frac{2e^{\text{Pe}}}{\sqrt{1 + v^2/4D^2k_i^2}} \frac{(1 - \delta_{i0})\delta_{j0}}{-i\omega + r} \\
 & \left. + \frac{2e^{\text{Pe}/2}(-1)^j}{\sqrt{(1 + v^2/4D^2k_i^2)(1 + v^2/4D^2k_j^2)}} \frac{(1 - \delta_{i0})(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right), \tag{4.67}
 \end{aligned}$$

$$\begin{aligned}
 B'_{ij} = & -D'_{ij}e^{-\text{Pe}} = \frac{\ell\alpha}{L} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} e^{-\text{Pe}} \frac{\delta_{i0}\delta_{j0}}{-i\omega + r} \right. \\
 & + \frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{e^{-\text{Pe}}}{\sqrt{1 + v^2/4D^2k_j^2}} \frac{\delta_{i0}(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \\
 & + \frac{2e^{-\text{Pe}/2}(-1)^i}{\sqrt{1 + v^2/4D^2k_i^2}} \frac{(1 - \delta_{i0})\delta_{j0}}{-i\omega + r} \\
 & \left. + \frac{2e^{-\text{Pe}/2}(-1)^i}{\sqrt{(1 + v^2/4D^2k_i^2)(1 + v^2/4D^2k_j^2)}} \frac{(1 - \delta_{i0})(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right), \tag{4.68}
 \end{aligned}$$

$$\begin{aligned}
 C'_{ij} = & \frac{\ell\alpha}{L} \left(\frac{\text{Pe}}{1 - e^{-\text{Pe}}} e^{\text{Pe}} \frac{\delta_{i0}\delta_{j0}}{-i\omega + r} + \frac{\text{Pe}}{1 - e^{-\text{Pe}}} \frac{e^{\text{Pe}/2}(-1)^j}{\sqrt{1 + v^2/4D^2k_j^2}} \frac{\delta_{i0}(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right. \\
 & + \frac{2e^{\text{Pe}}}{\sqrt{1 + v^2/4D^2k_i^2}} \frac{(1 - \delta_{i0})\delta_{j0}}{-i\omega + r} \\
 & \left. + \frac{2e^{\text{Pe}/2}(-1)^j}{\sqrt{(1 + v^2/4D^2k_i^2)(1 + v^2/4D^2k_j^2)}} \frac{(1 - \delta_{i0})(1 - \delta_{j0})}{-i\omega + Dk_j^2 + \frac{v^2}{4D} + r} \right). \tag{4.69}
 \end{aligned}$$

4.C.c Group structure of perturbative matrices

The perturbative matrices are, up to multiplicative factors $f(\omega)$ and $g(\omega)$, closed under the matrix multiplications that can feature in products of M , Equation (4.25). This is demonstrated in multiplication Table 4.1 below.

	A	B	C	D	A'	B'	C'	D'
A	fA	gB'			gA	fB'		
B			gA'	fB			fA'	gB
C	fC	gD'			gC	fD'		
D			gC'	fD			fC'	gD
A'	fA'	gB			gA'	fB		
B'			gA	fB'			fA	gB'
C'	fC'	gD			gC'	fD		
D'			gC	fD'			fC	gD'

Table 4.1: Multiplication table of the perturbative matrices defined in Appendix 4.C.b. Rows indicate the matrix multiplying from the left, e.g. row = A, column = B corresponds to $AB = gB'$. Blank entries indicate multiplications that never occur in practise, since the ordering of their corresponding Feynman diagrams prohibits it, see Equation (4.25).

The multiplicative factors resulting from the multiplications have the explicit form

$$\begin{aligned}
 f(\omega) = & -\frac{\ell\alpha}{L} \left(\frac{vL/D}{1 - \exp(-vL/D)} \frac{1}{-i\omega + r} + 2 \sum_{j=1}^{\infty} \frac{Dk_j^2}{(Dk_j^2 + \frac{v^2}{4D})(-i\omega + Dk_j^2 + \frac{v^2}{4D} + r)} \right) \\
 = & -\frac{\ell\alpha}{-i\omega + r} \left[\sqrt{\frac{-i\omega + \frac{v^2}{4D} + r}{D}} \coth \left(L \sqrt{\frac{-i\omega + \frac{v^2}{4D} + r}{D}} \right) + \frac{v}{2D} \right], \tag{4.70}
 \end{aligned}$$

$$\begin{aligned}
 g(\omega) &= -\frac{\ell\alpha}{L} \left(\frac{vL/D}{1 - \exp(-vL/D)} \frac{1}{-i\omega + r} + 2e^{\frac{vL}{2D}} \sum_{j=1}^{\infty} \frac{Dk_j^2(-1)^j}{(Dk_j^2 + \frac{v^2}{4D})(-i\omega + Dk_j^2 + \frac{v^2}{4D} + r)} \right) \\
 &= -\frac{\ell\alpha}{-i\omega + r} \sqrt{\frac{-i\omega + \frac{v^2}{4D} + r}{D}} \operatorname{csch} \left(L \sqrt{\frac{-i\omega + \frac{v^2}{4D} + r}{D}} \right) e^{\frac{vL}{2D}},
 \end{aligned} \tag{4.71}$$

where the closed-form representations of the infinite sums can be obtained using techniques for summing over Matsubara frequencies [122].

The highly ordered and symmetrical Table 4.1 suggests such mathematical structures may appear in more general models involving localised reactions. For instance, a similar structure would be found for a model that allows asymmetric self-propulsion speeds, $|v_L| \neq |v_R|$, and boundary tumbling rates, $\alpha_L \neq \alpha_R$, for each species. In this case, the multiplicative factors given in Equations (4.70)–(4.71) would split into non-degenerate values for each of the species, i.e. $f \rightarrow f_L, f_R$ and $g \rightarrow g_L, g_R$.

4.C.d Derivation of full propagators

Using Table 4.1, the full propagator in Equation (4.27) can be reduced to a closed-form expression by expanding the inverse matrices it contains as geometric series. Firstly, according to Table 4.1, $DD = fD$ and therefore $(\mathbb{1} - D)^{-1} = \mathbb{1} + (1 - f)^{-1}D$. This can be used to rewrite Equation (4.27) as

$$\text{---} \bullet \text{---} = \text{---} \left(\mathbb{1} - BC - \frac{1}{1-f} BDC - A \right)^{-1}. \tag{4.72}$$

Next, the products $BC = gA'$, $DC = gC'$, and subsequently $BC' = fA'$, give

$$\text{---} \bullet \text{---} = \text{---} \left(\mathbb{1} - \left(A + \frac{g}{1-f} A' \right) \right)^{-1}. \tag{4.73}$$

Finally, using Table 4.1 to replace products involving only A and A' ,

$$\left(A + \frac{g}{1-f} A' \right)^n = \left(f + \frac{g^2}{1-f} \right)^{n-1} \left(A + \frac{g}{1-f} A' \right), \tag{4.74}$$

such that expanding the right-hand side of Equation (4.73) as a geometric series obtains Equation (4.28). Equation (4.29), and the propagators to observe a left-moving particle, can be obtained by a similar procedure.

4.D Derivation of closed-form expression for $h(x)$

Here, I show how to go from the series representation of $h(x)$, Equation (4.31), to its closed-form expression in Equation (4.33).

First, it can be verified numerically (before its explicit calculation in Equation (4.42)) that the steady-state current for the right-moving particle J_R is constant across space.

Hence,

$$\int_0^L dx J_R(x) = LJ_R. \quad (4.75)$$

Next, the integrand on the left-hand side of Equation (4.75) can be rewritten using the general expression for the current of a right-moving particle, Equation (4.4). This relates the current to $P_R(x)$ and, in turn, $h(x)$ via Equation (4.30). After inserting the series representation of $h(x)$, Equation (4.31), the left-hand side of Equation (4.75) can be written in closed form after exchanging integration and summation. This gives $vC_{\text{Pe}}/2 = LJ_R$, recovering the result of Equation (4.42) without needing to first calculate C_{Pe} in closed form.

The expression $J_R = vC_{\text{Pe}}/2L$, in combination with Equations (4.4) and (4.30), can be used to derive the differential equation

$$\frac{dh(x)}{dx} - \frac{v}{2D}h(x) = -\frac{L}{2D}e^{-\frac{v}{2D}x}, \quad (4.76)$$

which has solution

$$h(x) = \frac{L}{2v} \left(e^{-\frac{v}{2D}x} + k(\text{Pe})e^{\frac{v}{2D}x} \right), \quad (4.77)$$

where $k(\text{Pe})$ is a constant to be determined. To find the explicit form of $k(\text{Pe})$, Equation (4.77) can be rearranged to give

$$k(\text{Pe}) = \frac{2v}{L}h(x)e^{-\frac{v}{2D}x} - e^{-\frac{v}{D}x} = \text{const}. \quad (4.78)$$

Then, after inserting the series representation of $h(x)$, Equation (4.31), into Equation (4.78), one can verify numerically $k(1) \approx -1/(e-1)$ and $k(2) \approx -2/(e^2-1)$ etc. This suggests $k(\text{Pe}) = -\text{Pe}/(\exp(\text{Pe})-1)$, which results in Equation (4.77) reducing to Equation (4.33) and implies $h(x)$ in Equation (4.33) is the closed-form representation of Equation (4.31).

To verify this conjecture, I calculated the coefficients $a_n = 2 \int_0^L dx h(x) \cos(k_n x + \theta_n)/L$ in the basis expansion $h(x) = \sum_{n=1}^{\infty} a_n \cos(k_n x + \theta_n)$, using the conjectured form of $h(x)$, Equation (4.33). The calculated coefficients a_n did indeed match those in Equation (4.31), verifying that $h(x)$ in Equations (4.31) and (4.33) are the same function.

5

Ratcheting through supervised resetting

This chapter is based on the following publication:

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The necessary permissions to reproduce this publication as part of my thesis are included in Appendices B.1.2, B.2.6, and B.2.9.

Author contributions to original manuscript: I conceived and supervised the project. ES derived the bulk of the analytical results. EL performed the numerical simulations. EL and I produced all figures. ES and I wrote the bulk of the manuscript. All authors interpreted the results and edited the manuscript.

Chapter summary

In this chapter, we will briefly move away from active systems and instead consider a non-equilibrium system sustained by external forcing. *External* forcing implies that any resulting work extraction is not autonomous, due to the need for a hypothetical controller to implement the forcing. This chapter’s purpose is to highlight this key distinction between active matter and externally forced systems. The model in question is of a Brownian particle subject to stochastic resetting facilitated by an asymmetric “ratchet” potential. The ratchet potential switches on with a constant rate, but switches off only upon the particle’s first passage to a resetting point at the minimum of the potential. On a spatially periodic domain, repeating this cycle sustains a non-equilibrium steady-state, as well as a directed steady-state current, which can be harnessed to perform useful work. I derive exact analytic expressions for the probability densities of the free-diffusion and resetting phases, the associated currents for each phase, and an efficiency parameter that quantifies the return in current for given power input. I also show in what limits optimal current and efficiency are obtained. The analytical results are corroborated by simulations, and have implications for experimentally viable finite-time-resetting protocols.

5.1 Introduction

The field of stochastic resetting has received much attention since its inception over a decade ago [123–125]. In stochastic resetting, the recurrent restarting of a process from its initial state establishes internal probability currents and, remarkably, a non-equilibrium steady-state even if the underlying dynamics otherwise satisfy detailed balance. One of

the most striking properties of stochastic resetting is that it can render the mean first-passage time of a diffusive search process finite [126–128], thus offering an attractive way of improving transport properties [129, 130]. On top of its myriad variations and applications, such as to biology [131, 132], computer science [133], and finance [134], resetting has most recently been shown to improve the efficiency of Brownian heat engines [135].

The prototypical model of stochastic resetting involves a Brownian particle subject to instantaneous resets to its initial position at a constant rate. This is in stark contrast to experimental implementations of stochastic resetting, where it takes a finite time to reset a particle back to its initial position [136–139]. Given these recent experimental advances, others have sought to devise theoretical models that emulate this finite-time resetting [75, 140–149]. Unlike instantaneous resetting, finite-time resetting can be mediated by a physical mechanism, such as an external potential [118, 119, 150, 151]. Aside from being more physically realistic, it was recently shown that potential-mediated resetting can actually expedite diffusive search processes compared to instantaneous resetting [150, 152].

The probability currents generated through stochastic resetting naturally lead to questions about work extraction and the efficiency of resetting [153–156]. For instance, resetting models could be modified to generate useful work by introducing an underlying asymmetry into the resetting mechanism. Harnessing the asymmetry of an autonomous engine to generate work is an idea dating back to Feynman’s “ratchet and pawl” machine [47], see Chapter 1. In a similar vein, models of molecular motors provide a mechanism for Brownian particles to exhibit a net drift [157, 158], akin to the movement of motor proteins along filaments [159, 160]. This directed motion can be brought about by the asymmetry of a ratchet potential, in combination with either external forces or states that fluctuate in time [161–163]. Alternatively, the particles themselves can self-propel, in which case their motion in an asymmetric potential readily breaks time-reversal symmetry, as has been the study of so-called “active ratchets” in recent times [20–22, 164], see also Chapter 6. Active ratchets are essentially autonomous engines that can be exploited to extract useful thermodynamic work [21, 51].

There has been a recent surge of numerical studies investigating resetting in combination with asymmetric potentials [143, 165, 166]. However, analytical studies are comparatively lacking, especially for experimentally relevant models. In this chapter, I study the motion of an overdamped Brownian particle subject to finite-time resetting facilitated by a piecewise-linear ratchet potential on a spatially periodic domain. The potential switches on with a constant rate, but switches off only upon the particle’s first passage to a resetting point at the minimum of the potential, at which point the particle returns to freely diffusive motion and restarts the cycle. This is similar to the fluctuating ratchets used to model molecular motors [157, 158, 162, 163], where a time-varying potential switches between two or more states (such as “on” and “off”). However, in these “non-resetting” ratchet models, the switching is controlled by some other form of systematic driving, e.g. with a constant rate. In the model presented in this chapter, the resetting of the particle to the potential minimum means it fully exploits the potential’s height to further bias

its motion through the ratchet’s asymmetry, paving the way for an optimised current. This chapter brings together stochastic resetting and fluctuating potentials to provide a minimal *experimentally motivated* finite-time-resetting model that exhibits a net current.

The remainder of this chapter is organised as follows. After introducing the model in Section 5.2, I derive the system’s steady-state probability density in Section 5.3. This is supplemented by a derivation of the time-dependent probability densities in Appendix 5.B. In Section 5.4, we turn our attention to the current, which, to the best of my knowledge, constitutes the first systematic analytic study of a steady-state net current generated through finite-time resetting. The fact that a net current can be generated motivates study of the energetic cost of this resetting in Section 5.5, and to measure the efficiency of the current generation for given power input [167, 168]. Throughout this chapter, the analytical results are supported by extensive numerical simulations. Finally, I conclude and summarise the results in Section 5.6.

5.2 Model

I consider an overdamped Brownian particle in one dimension which has two phases to its motion. In the “diffusion phase”, the particle freely diffuses and so its stochastic motion is governed by the following Langevin equation,

$$\dot{x}_D(t) = \sqrt{2D_0}\xi(t), \quad (5.1)$$

where t is time, D_0 is the diffusion constant, $\xi(t)$ is a Gaussian white noise with zero mean $\xi(t) = 0$ and correlation $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$, and the subscript D indicates that motion is in the diffusion phase.

While in the diffusion phase, a potential $V(x)$ with period L is switched on with a Poissonian rate r , upon which the particle enters the “resetting phase”. The potential is switched off again only upon the particle reaching a resetting point located at $x = nL$ for $n \in \mathbb{Z}$, which coincide with the potential minima. To obtain a model with non-vanishing steady-state density and current, the position x is wrapped onto a periodic domain, i.e. positions $x + nL$ are identified with x , thus constraining the particle’s motion to the interval $x \in [0, L)$. Due to these periodic boundary conditions, any reference henceforth to $x = 0$ can be assumed to equally refer to $x = L$, and vice versa.

By iterating the cycle of diffusion and resetting phases, a non-equilibrium steady-state is sustained from the constant injection of energy at the beginning of each resetting phase to increase the particle’s potential energy. Denoting the period where the potential $V(x)$ is switched on with a subscript R , the Langevin equation for the particle while in the resetting phase is

$$\dot{x}_R(t) = -V'(x_R) + \sqrt{2D_0}\xi(t), \quad (5.2)$$

where the friction coefficient that would normally appear in Equation (5.2) has been set to unity without loss of generality. We are interested in using the resetting potential $V(x)$ to rectify the particle’s motion in order to generate a steady-state current, in which case the

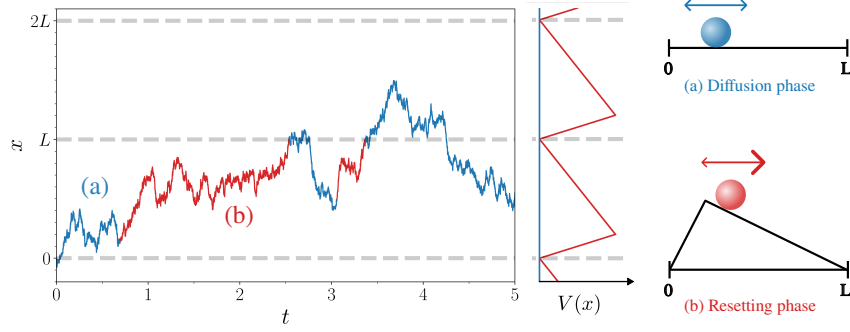


Figure 5.1: Example simulated trajectory from numerically integrating Equations (5.1) and (5.2) for parameters $L = 1$, $a = 0.2$, $h = 0.1$, $D_0 = 0.1$, and $r = 2$, see Appendix 5.A for simulation details. Here, the trajectory is plotted on an extended domain for visualisation purposes; however, all results in the main text are calculated for a position x wrapped back onto a periodic domain $x \in [0, L)$. The blue (respectively, red) sections of the line indicate when the particle is in the diffusion (respectively, resetting) phase. The ratchet potential $V(x)$, Equation (5.3), is visualised alongside the particle trajectory. The horizontal dashed lines indicate the resetting positions at $x = nL$ for $n \in \mathbb{Z}$. Resetting phases can start at any position x , but must end at these resetting points. [Figure credit: Eloise Lardet].

potential needs to impart a bias on the particle’s motion. To render the system exactly solvable, $V(x)$ is chosen to be a piecewise-linear asymmetric potential with an apex at $x = a$ [21, 162], i.e. a “ratchet potential” defined by

$$V(x) = \begin{cases} V^{[1]}(x) = \frac{h}{a}x, & 0 \leq x < a, \\ V^{[2]}(x) = \frac{h}{L-a}(L-x), & a \leq x < L, \end{cases} \quad (5.3)$$

where h is the maximum height of the potential, occurring at $x = a$. Notably, this setup generalises instantaneous stochastic resetting, since the limit $h \rightarrow \infty$ corresponds to the particle being instantaneously reset to the origin $x = 0$ when the potential is switched on. In the instantaneous resetting case, the parameter a controls whether the particle instantaneously jumps a distance x to the left, if $0 \leq x < a$, or a distance $L - x$ to the right, if $a \leq x < L$. The full model for finite h is illustrated by an example stochastic trajectory in Figure 5.1.

To demonstrate the rectification mechanism, consider the case where $a < L/2$. When the potential is switched on, the particle is more likely to be found in the larger $a \leq x < L$ region of the resetting potential, which imparts a positive drift velocity $-V^{[2]'}(x) = h/(L-a)$ on the particle towards the origin $x = L^-$. Hence, on average, the particle experiences a positive drift while in the resetting phase. Since motion in the diffusion phase is symmetric, the particle’s overall motion is rectified in the positive direction, corresponding to a positive net current. A negative current of equal magnitude is obtained for a ratchet potential where the position of the apex is reflected across $x = L/2$, i.e. $a \rightarrow L - a$.

Using a periodic asymmetric potential in combination with resetting to generate a net

current was recently investigated in Ref. [143]. However, in that work, the current was not induced by recurrent activation of the potential, as in the model studied in this chapter. Instead, the authors of Ref. [143] obtained numerical results for a system in which a Brownian particle moves in a static asymmetric potential. The particle switches off its diffusion with a constant rate, leading to a deterministic return to the potential minimum proceeded by the particle restarting its diffusion. The model considered in this chapter is arguably more experimentally accessible than this “stop-and-start” model, as diffusion is typically not an internal degree of freedom that can be autonomously switched on or off, whereas an external potential can be readily modulated by an external controller. Furthermore, the exact results for the model considered in this chapter can be used to *analytically* study experimentally relevant observables, such as the probability densities and currents for each phase, as well as the efficiency of the current generation. For completeness, I derive the analytic solution for the stop-and-start model in Appendix 5.C.

5.3 Probability densities

The dynamics of the system can be equivalently encoded in the probability densities $P_{D/R}(x, t)$ to observe the particle in the diffusion/resetting phase at a position x at time t . Since the ratchet potential, Equation (5.3), is piecewise linear, it is convenient to separate the probability density for the resetting phase into separate components for each region. Here and throughout the rest of this chapter, these separate components are distinguished by a superscript $[i]$, where $i \in \{1, 2\}$, i.e.

$$P_R(x, t) = \begin{cases} P_R^{[1]}(x, t), & 0 \leq x < a \\ P_R^{[2]}(x, t), & a \leq x < L \end{cases}. \quad (5.4)$$

The probability densities obey the following coupled Fokker-Planck equations,

$$\frac{\partial P_D(x, t)}{\partial t} = -\frac{\partial J_D(x, t)}{\partial x} - rP_D(x, t) + \left(J_R^{[2]}(L^-, t) - J_R^{[1]}(0^+, t) \right) \delta(x), \quad (5.5a)$$

$$\frac{\partial P_R^{[1]}(x, t)}{\partial t} = -\frac{\partial J_R^{[1]}(x, t)}{\partial x} + rP_D(x, t) + J_R^{[1]}(0^+, t)\delta(x), \quad (5.5b)$$

$$\frac{\partial P_R^{[2]}(x, t)}{\partial t} = -\frac{\partial J_R^{[2]}(x, t)}{\partial x} + rP_D(x, t) - J_R^{[2]}(L^-, t)\delta(x), \quad (5.5c)$$

where L^- (respectively, 0^+) is the limit of x approaching L (respectively, 0) from below (respectively, above), and the currents for each phase are given by

$$J_D(x, t) = -D_0 \frac{\partial P_D(x, t)}{\partial x}, \quad (5.6a)$$

$$J_R^{[i]}(x, t) = -D_0 \frac{\partial P_R^{[i]}(x, t)}{\partial x} - V'^{[i]} P_R^{[i]}(x, t), \quad (5.6b)$$

where each $V'^{[i]}$ is spatially independent, and $J_R^{[2]}(L^-, t) - J_R^{[1]}(0^+, t)$ is the net flux directed into the origin $x = 0$ in the resetting phase, which quantifies the rate at which the particle

arrives at the resetting point. One always has $J_R^{[2]}(L^-, t) \geq 0$ and $J_R^{[1]}(0^+, t) \leq 0$, regardless of the system parameters, since the individual terms of Equation (5.6b) are both positive for $i = 2$, and both negative for $i = 1$, as will become clear once $P_R(x, t)$ is derived later. Hence, the term $(J_R^{[2]}(L^-, t) - J_R^{[1]}(0^+, t))\delta(x)$ in Equation (5.5) always represents a source term for the diffusion phase, while the terms $-J_R^{[2]}(L^-, t)\delta(x)$ and $J_R^{[1]}(0^+, t)\delta(x)$ always represent sink terms for each region in the resetting phase.

Upon summing the probabilities in Equation (5.5), one recovers the continuity equation

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial J(x, t)}{\partial x}, \quad (5.7)$$

where $P(x, t) = P_D(x, t) + P_R(x, t)$ is the overall probability density, $J(x, t) = J_D(x, t) + J_R(x, t)$ is the net current, and recall that $P_R(x, t)$ is composed of components $P_R^{[i]}(x, t)$ that are valid only for specific regions of space as per Equation (5.4). Hence, the sink term $-rP_D(x, t)$ from Equation (5.5a) is cancelled in Equation (5.7) by the source terms $rP_D(x, t)$ from Equations (5.5b) and (5.5c) in a piecewise manner, first by that of Equation (5.5b) in the region $x \in [0, a)$, and then by that of Equation (5.5c) in the region $x \in [a, L)$.

This setup generalises the mod-linear resetting model of Ref. [119] by allowing the resetting potential to be asymmetric and periodic in order to generate a non-zero net current $J(x, t)$. The model of Ref. [119] can be recovered from the model considered in this chapter by setting $a = L/2$ while taking $L \rightarrow \infty$ and $h \rightarrow \infty$ in such a way that the gradients $V'^{[i]}$ remain constant. The periodicity of the potential imposes the following periodic boundary conditions,

$$P_D(0, t) = P_D(L, t), \quad (5.8a)$$

$$P_R^{[1]}(0, t) = P_R^{[2]}(L, t) = 0, \quad (5.8b)$$

where Equation (5.8b) also imposes that a particle in the resetting phase can never be found at the origin because it would instantly transmute to the diffusion phase.

We are interested in the steady-state behaviour of the system, for which the left-hand sides of Equation (5.5) vanish, i.e. $\lim_{t \rightarrow \infty} \partial_t P_{D,R}(x, t) = 0$. Henceforth, I will represent all steady-state quantities by dropping the ‘ t ’ from their arguments, e.g. $P_D(x) \equiv \lim_{t \rightarrow \infty} P_D(x, t)$. The steady-state net current J is independent of position as a result of the steady-state condition $\partial_t P(x) = -\partial_x J = 0$, where $P(x) = P_D(x) + P_R(x)$ is the overall probability density at stationarity.

I now recast the dynamics in dimensionless form. This will allow more efficient exploration of the full parameter space later in this chapter by reducing the description of the system from five dimensional parameters h, a, L, r, D_0 , to three dimensionless parameters, to be specified below. Defining the typical diffusion length scale between resets $\sigma := \sqrt{D_0/r}$ and the average time for the potential to switch on $\tau := 1/r$ as the units of distance and time, respectively, the dimensionless Fokker-Planck equation at stationarity

is

$$0 = \frac{\partial^2 \tilde{P}_D(\tilde{x})}{\partial \tilde{x}^2} - \tilde{P}_D(\tilde{x}) + \left(\tilde{J}_R^{[2]}(\ell^-) - \tilde{J}_R^{[1]}(0^+) \right) \delta(\tilde{x}), \quad (5.9a)$$

$$0 = \frac{\partial^2 \tilde{P}_R^{[1]}(\tilde{x})}{\partial \tilde{x}^2} + \tilde{V}'^{[1]} \frac{\partial \tilde{P}_R^{[1]}(\tilde{x})}{\partial \tilde{x}} + \tilde{P}_D(\tilde{x}) + \tilde{J}_R^{[1]}(0^+) \delta(\tilde{x}), \quad (5.9b)$$

$$0 = \frac{\partial^2 \tilde{P}_R^{[2]}(\tilde{x})}{\partial \tilde{x}^2} + \tilde{V}'^{[2]} \frac{\partial \tilde{P}_R^{[2]}(\tilde{x})}{\partial \tilde{x}} + \tilde{P}_D(\tilde{x}) - \tilde{J}_R^{[2]}(\ell^-) \delta(\tilde{x}), \quad (5.9c)$$

where I have represented non-dimensionalised quantities with a tilde, e.g. $\tilde{x} = x/\sigma$, $\tilde{P}_{D,R} = \sigma P_{D,R}$, and $\tilde{J}_R = \tau J_R$. The gradients of the potential in dimensionless form are given by

$$\tilde{V}'(\tilde{x}) = \begin{cases} \tilde{V}'^{[1]} = \frac{\kappa}{\delta \ell}, & 0 \leq \tilde{x} < \delta \ell \\ \tilde{V}'^{[2]} = -\frac{\kappa}{(1-\delta)\ell}, & \delta \ell \leq \tilde{x} < \ell \end{cases}, \quad (5.10)$$

where $\ell := L/\sigma$ is the rescaled system length, and I have introduced relevant dimensionless parameters, namely the coupling strength $\kappa := h/D_0$ of the particle to the potential, and the potential asymmetry parameter $\delta := a/L \in [0, 1]$, i.e. the position of the ratchet apex for an interval normalised to unit length. In dimensionless form, the periodic boundary conditions (5.8) become

$$\tilde{P}_D(0, t) = \tilde{P}_D(\ell, t), \quad (5.11a)$$

$$\tilde{P}_R^{[1]}(0, t) = \tilde{P}_R^{[2]}(\ell, t) = 0. \quad (5.11b)$$

To obtain the steady-state probability density for the diffusion phase $\tilde{P}_D(\tilde{x})$, I first solve Equation (5.9a) away from the resetting point, i.e. in the region $\tilde{x} \in (0, \ell)$, where the term proportional to the Dirac delta function vanishes. This results in

$$\tilde{P}_D(\tilde{x}) = A_D e^{\tilde{x}} + B_D e^{-\tilde{x}}. \quad (5.12)$$

By integrating Equation (5.9a) over the region $\tilde{x} \in [-\epsilon, \epsilon]$, recalling that $-\epsilon$ is identified with $\ell - \epsilon$, and then taking $\epsilon \rightarrow 0^+$, one obtains the following jump condition at the origin

$$\left. \frac{\partial \tilde{P}_D(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow 0^+} - \left. \frac{\partial \tilde{P}_D(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow \ell^-} = - \left(\tilde{J}_R^{[2]}(\ell^-) - \tilde{J}_R^{[1]}(0^+) \right). \quad (5.13)$$

Using this jump condition (5.13) in combination with the periodic boundary condition (5.11a), one can fix the constants A_D and B_D in Equation (5.12), eventually obtaining

$$\tilde{P}_D(\tilde{x}) = \frac{p_D}{2} \frac{\cosh(\tilde{x} - \frac{\ell}{2})}{\sinh(\frac{\ell}{2})}, \quad (5.14)$$

where I have integrated Equation (5.14) over the entire interval $\tilde{x} \in [0, \ell]$ to yield $\tilde{J}_R^{[2]}(\ell^-) -$

$\tilde{J}_R^{[1]}(0^+) = p_D$, where

$$p_D = \int_0^\ell d\tilde{x} \tilde{P}_D(\tilde{x}) \quad (5.15)$$

is the probability to be in the diffusion phase at stationarity. I similarly define $p_R = p_R^{[1]} + p_R^{[2]}$ as the probability to be in the resetting phase at stationarity, where

$$p_R^{[1]} = \int_0^{\delta\ell} d\tilde{x} \tilde{P}_R^{[1]}(\tilde{x}), \quad (5.16a)$$

$$p_R^{[2]} = \int_{\delta\ell}^\ell d\tilde{x} \tilde{P}_R^{[2]}(\tilde{x}), \quad (5.16b)$$

are the probabilities for the particle to be found in the different regions of the ratchet and in the resetting phase.

I now proceed to obtain the steady-state probability density for the resetting phase $\tilde{P}_R(\tilde{x})$. Due to the discontinuity in the potential at the apex $\tilde{x} = \delta\ell$, we also have continuity of the probability density and current for the resetting phase at this position, i.e.

$$\tilde{P}_R^{[1]}(\delta\ell) = \tilde{P}_R^{[2]}(\delta\ell), \quad (5.17a)$$

$$\tilde{J}_R^{[1]}(\delta\ell) = \tilde{J}_R^{[2]}(\delta\ell), \quad (5.17b)$$

where the current for the resetting phase is defined in Equation (5.6b). We also have the jump condition at the origin,

$$\left. \frac{\partial \tilde{P}_R^{[1]}(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow 0^+} - \left. \frac{\partial \tilde{P}_R^{[2]}(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow \ell^-} = \tilde{J}_R^{[2]}(\ell^-) - \tilde{J}_R^{[1]}(0^+) = p_D. \quad (5.18)$$

As above, I first solve Equations (5.9b)–(5.9c) in the region $\tilde{x} \in (0, \ell)$, where the terms proportional to the Dirac delta function vanish. After inserting the solution for $\tilde{P}_D(\tilde{x})$, Equation (5.14), into Equations (5.9b)–(5.9c) and then solving, one eventually obtains

$$\tilde{P}_R(\tilde{x}) = \begin{cases} \frac{p_D}{2} \frac{\delta\ell}{e^\ell - 1} \left(\frac{e^{\ell-\tilde{x}}}{\lambda_-^{[1]}} - \frac{e^{\tilde{x}}}{\lambda_+^{[1]}} \right) + A_R^{[1]} e^{-\frac{\kappa\tilde{x}}{\delta\ell}} + B_R^{[1]}, & 0 \leq \tilde{x} < \delta\ell \\ \frac{p_D}{2} \frac{(1-\delta)\ell}{e^\ell - 1} \left(\frac{e^{\tilde{x}}}{\lambda_-^{[2]}} - \frac{e^{\ell-\tilde{x}}}{\lambda_+^{[2]}} \right) + A_R^{[2]} e^{\frac{\kappa\tilde{x}}{(1-\delta)\ell}} + B_R^{[2]}, & \delta\ell \leq \tilde{x} < \ell \end{cases}, \quad (5.19)$$

where I have written the solution in terms of the compact notation $\lambda_\pm^{[1]} = \kappa \pm \delta\ell$, $\lambda_\pm^{[2]} = \kappa \pm (1-\delta)\ell$. Equation (5.19) is valid only when both $\lambda_-^{[1]} \neq 0$ and $\lambda_-^{[2]} \neq 0$. I provide the solutions for the edge cases (i) $\lambda_-^{[1]} = 0 \neq \lambda_-^{[2]}$, (ii) $\lambda_-^{[2]} = 0 \neq \lambda_-^{[1]}$, and (iii) $\lambda_-^{[1]} = \lambda_-^{[2]} = 0$ at the end of Appendix 5.B. The constants $A_R^{[1]}, A_R^{[2]}, B_R^{[1]}, B_R^{[2]}$ in Equation (5.19) are fixed by the periodic boundary condition (5.11b), continuity conditions (5.17), and the jump condition (5.18). The diffusion-phase probability p_D can be fixed in terms of the system parameters ℓ, κ, δ through the normalisation condition,

$$p_D + p_R^{[1]} + p_R^{[2]} = 1, \quad (5.20)$$

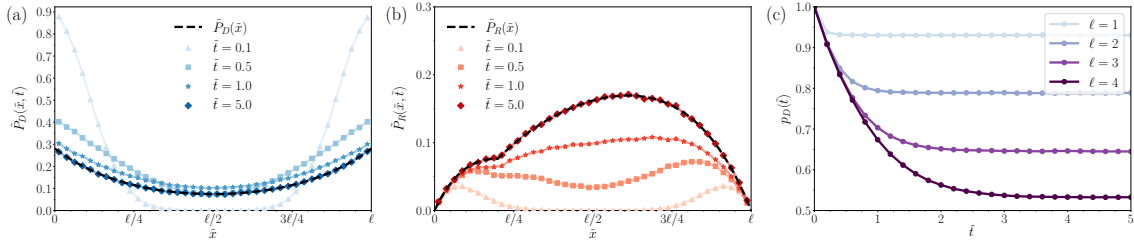


Figure 5.2: (a)–(b) Time evolution of the probability densities for each phase $\tilde{P}_{D,R}(\tilde{x}, \tilde{t})$, as determined from simulations. Simulation parameters are $\ell = 4$, $\kappa = 1$, $\delta = 0.2$ for a particle initialised at the origin $\tilde{x} = 0$ at time $\tilde{t} = 0$, i.e. $\tilde{P}_D(\tilde{x}, 0) = \delta(\tilde{x})$. Full simulation details are given in Appendix 5.A. The time-dependent densities converge to the theoretical steady-state densities, $\tilde{P}_D(\tilde{x})$ and $\tilde{P}_R(\tilde{x})$, given in Equations (5.14) and (5.19), respectively. (c) Probability of being in the diffusion phase $p_D(\tilde{t})$ as a function of time for various values of ℓ , as obtained from simulations for a single particle initialised at the origin $\tilde{x} = 0$ in the diffusion phase at time $\tilde{t} = 0$, with $\kappa = 1$ and $\delta = 0.2$.

where the probabilities for the particle to be found in each phase $p_{D,R}$ are defined in Equations (5.15)–(5.16). In principle, applying all of the aforementioned conditions yields closed-form solutions for the densities $\tilde{P}_D(\tilde{x})$, Equation (5.14), and $\tilde{P}_R(\tilde{x})$, Equation (5.19). However, the full expressions are too cumbersome to write down here, in particular that of the overall normalisation p_D . Nevertheless, it turns out that in certain (relevant) limits, other observables such as the net current $\tilde{J}$ are compact enough to display explicitly in terms of the system parameters. I demonstrate this in Section 5.4.

As noted in Refs. [118, 119], an alternative way to fix p_D is to relate the probability of being in either phase to the mean first-passage time $T_R(x_0)$ for the particle to reach the origin $x = 0$ (or $x = L$) from a position x_0 in the resetting phase. Specifically,

$$p_D = \frac{\tau}{\tau + \int_0^L dx_0 T_R(x_0) P(x_0|D)}, \quad (5.21)$$

where $\tau = 1/r$ is the average time spent in the diffusion phase in a single cycle, and $P(x_0|D) = P_D(x_0)/p_D$ (the conditional steady-state probability density to be at position x_0 given the particle is in the diffusion phase) provides the weighting for initially being found at position x_0 at the start of the resetting phase, such that $\int_0^L dx_0 T_R(x_0) P(x_0|D)$ is the average time spent in the resetting phase each cycle. However, Equations (5.20) and (5.21) are not independent conditions, since I show in Appendix 5.D that Equation (5.21) can be derived from Equation (5.20) using only the definition of the mean first-passage time. For completeness, I derive the mean first-passage time $T_R(x_0)$ in Appendix 5.E. The time-dependent behaviour of $p_D(t)$ is plotted in Figure 5.2(c), where it can be seen that $p_D(t)$ saturates to a steady-state value p_D determined by Equation (5.20) or, equivalently, Equation (5.21).

In addition to the steady-state solutions derived in this section, I demonstrate how to derive the fully time-dependent Laplace-space solutions in Appendix 5.B. The time-

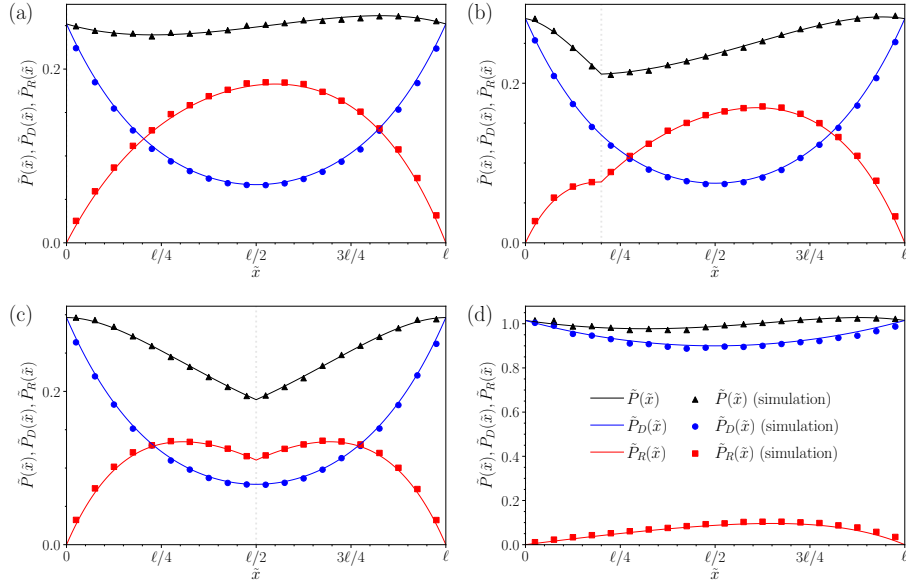


Figure 5.3: Steady-state probability densities $\tilde{P}_D(\tilde{x})$, Equation (5.14), $\tilde{P}_R(\tilde{x})$, Equation (5.19), and $\tilde{P}(\tilde{x}) = \tilde{P}_D(\tilde{x}) + \tilde{P}_R(\tilde{x})$, as a function of particle position $\tilde{x}$ for parameters (a) $\delta = 0$, $\ell = 4$, $\kappa = 1$, (b) $\delta = 0.2$, $\ell = 4$, $\kappa = 1$, (c) $\delta = 0.5$, $\ell = 4$, $\kappa = 1$, and (d) $\delta = 0$, $\ell = 1$, $\kappa = 4$. Vertical dotted lines indicate the position of the ratchet apex $\tilde{x} = \delta\ell$ (equivalent to $x = a$) for the cases where $\delta > 0$. Simulation data are plotted as symbols and are in excellent agreement with the theoretical results. Full simulation details are given in Appendix 5.A.

dependent densities, $\tilde{P}_D(\tilde{x}, \tilde{t})$ and $\tilde{P}_R(\tilde{x}, \tilde{t})$, are plotted in Figures 5.2(a) and 5.2(b), respectively. It can be seen that the time-dependent densities converge to the expressions for the theoretical steady-state densities, $\tilde{P}_D(\tilde{x})$ and $\tilde{P}_R(\tilde{x})$, given in Equations (5.14) and (5.19), respectively.

The solutions for the steady-state densities $\tilde{P}_D(\tilde{x})$, Equation (5.14), and $\tilde{P}_R(\tilde{x})$, Equation (5.19), are plotted in Figure 5.3 alongside simulation results for a few different sets of parameters. Data from the simulations are in excellent agreement with the theoretical results. The figure shows that the probability density in the diffusion phase $\tilde{P}_D(\tilde{x})$ has a symmetric exponential form about the origin $x = 0$, as is typical for a resetting model. The diffusion-phase density is also periodic, as required by the boundary conditions, with a minimum at the centre of the interval $\tilde{x} = \ell/2$, such that it is also symmetric about $\tilde{x} = \ell/2$. The shape of the probability density in the resetting phase $\tilde{P}_R(\tilde{x})$ heavily depends on the position of the ratchet potential's apex $\delta\ell$. In particular, the resetting density is symmetric if the potential is symmetric, i.e. $\delta = 1/2$, see Figure 5.3(c), but is otherwise asymmetric and generally has a prominent corner at the apex as a result of the different potential gradients either side of $\tilde{x} = \delta\ell$.

Figure 5.4 shows the probability of the particle being in the diffusion phase at stationarity, Equation (5.15). This captures the competition between the relevant timescales of the system, namely the average times spent in the diffusion and resetting phases, as illustrated by Equation (5.21). The particle has a greater chance of being in the diffusion

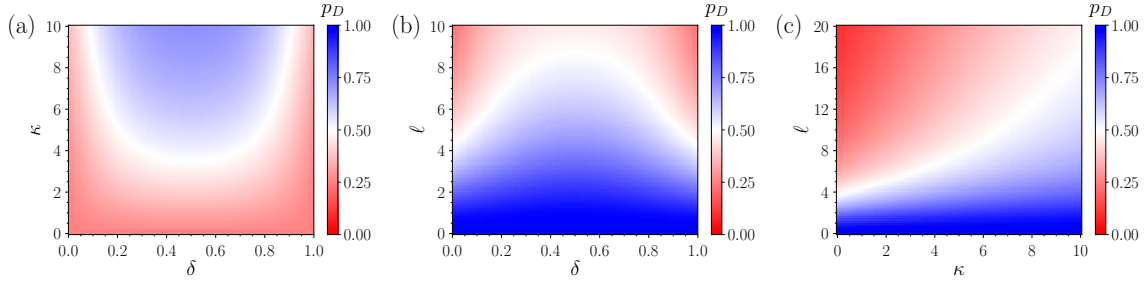


Figure 5.4: Steady-state probability to be in the diffusion phase p_D , Equation (5.15), as a function of the dimensionless parameters ℓ , κ , and δ . The constant parameter in each subfigure is (a) $\ell = 8$, (b) $\kappa = 4$, and (c) $\delta = 0.2$.

phase for larger κ and smaller ℓ . Larger κ indicates a stronger coupling to the potential, and therefore the potential resets the particle to the diffusion phase quicker, thus spending less time in the resetting phase and more time in the diffusion phase. In fact, $p_D \rightarrow 1$ as $\kappa \rightarrow \infty$. Similarly, smaller ℓ indicates the particle has been able to explore more of the interval between resetting phases, i.e. the density is more equilibrated between resets, and so the particle spends a greater proportion of its time in the diffusion phase. As above, $p_D \rightarrow 1$ as $\ell \rightarrow 0$.

In Figure 5.4, it can be seen that the particle spends more time in the resetting phase for a fully asymmetric ratchet, i.e. $\delta = 0$ or $\delta = 1$. As this is not immediately clear from intuition alone, I attempt to explain this behaviour with the following heuristic argument. Consider the case where the particle has had sufficient time between resetting phases to spread out uniformly across the interval as this allows one to make several simplifying assumptions about the dynamics. In this case, the probability of being found in either region upon entering the resetting phase is given by the fraction of the interval the region covers, i.e. δ for $i = 1$ and $1 - \delta$ for $i = 2$. For a sufficiently strong potential, one can further approximate the particle as being returned to the origin deterministically by the force from the ratchet. In other words, the average time spent in region $i = 1$ or region $i = 2$ during the resetting phase is simply the average distance the particle travels to the origin (half the length of the region) divided by the force in that region, resulting in $\delta^2 \ell^2 / 2\kappa$ for $i = 1$ and $(1 - \delta)^2 \ell^2 / 2\kappa$ for $i = 2$. Weighting these times by the probability to be found in either region, the average time spent in the resetting phase each cycle under these approximations is $(3\delta^2 - 3\delta + 1)\ell^2 / 2\kappa$, which is minimised for a symmetric ratchet, $\delta = 1/2$, and maximised for a fully asymmetric ratchet, $\delta = 0$ or $\delta = 1$.

5.4 Current

The currents for the diffusion $\tilde{J}_D(\tilde{x})$ and resetting $\tilde{J}_R(\tilde{x})$ phases are related to the probability densities calculated in Section 5.3 through Equations (5.6a) and (5.6b), respectively.

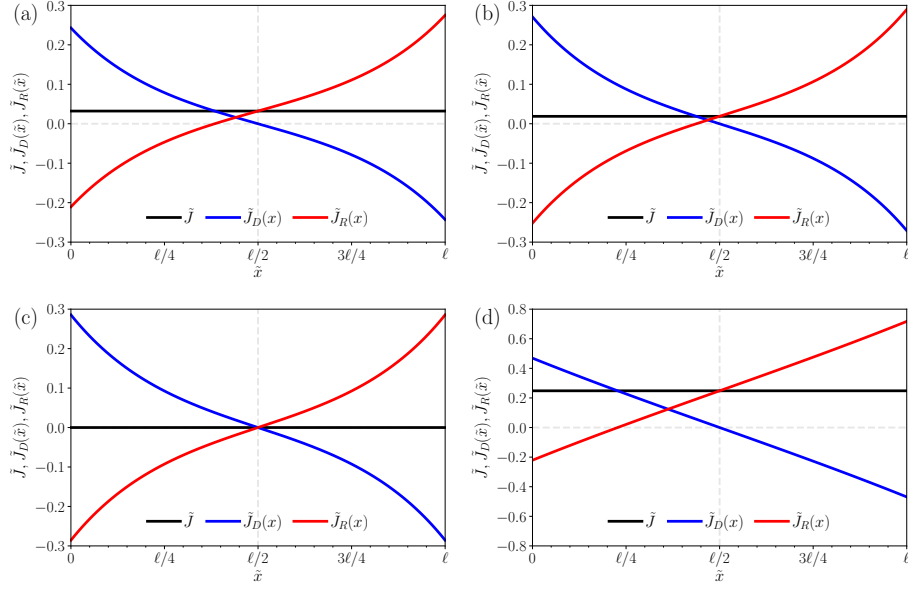


Figure 5.5: Steady-state currents $\tilde{J}_D(x)$, Equation (5.6a), $\tilde{J}_R(x)$, Equation (5.6b), and $\tilde{J} = \tilde{J}_D(x) + \tilde{J}_R(x)$, Equation (5.22), plotted for the same sets of parameters used in Figure 5.3, i.e. (a) $\delta = 0$, $\ell = 4$, $\kappa = 1$, (b) $\delta = 0.2$, $\ell = 4$, $\kappa = 1$, (c) $\delta = 0.5$, $\ell = 4$, $\kappa = 1$, and (d) $\delta = 0$, $\ell = 1$, $\kappa = 4$. Dashed grey lines are shown for $\tilde{J} = 0$ and $\tilde{x} = \ell/2$, and act as a guide for the eye.

The net current is then given by $\tilde{J} = \tilde{J}_D(x) + \tilde{J}_R(x)$, yielding

$$\tilde{J} = \frac{p_D}{2} \frac{\kappa^2}{(e^\ell - 1)(1 - e^\kappa) \lambda_+^{[1]} \lambda_-^{[1]} \lambda_+^{[2]} \lambda_-^{[2]}} \left(\lambda_-^{[1]} \lambda_+^{[2]} e^{\lambda_+^{[1]}} + (2\delta - 1) \left(\lambda_+^{[1]} \lambda_+^{[2]} e^\ell - \lambda_-^{[1]} \lambda_-^{[2]} \right) - \lambda_+^{[1]} \lambda_-^{[2]} e^{\lambda_+^{[2]}} \right), \quad (5.22)$$

where p_D is fixed from either Equation (5.20) or Equation (5.21), and I have reused the same compact notation $\lambda_\pm^{[1]} = \kappa \pm \delta\ell$, $\lambda_\pm^{[2]} = \kappa \pm (1 - \delta)\ell$ introduced in Equation (5.19). In the present section, I explore the parameter space of the net current $\tilde{J}$. Given that Equation (5.22) is rather opaque, I focus on exploring its more relevant limiting behaviour and general properties, as well as that of the currents associated with each phase, $\tilde{J}_D(x)$ and $\tilde{J}_R(x)$.

The net current $\tilde{J}$, Equation (5.22), and currents for each phase $\tilde{J}_{D,R}(x)$, are plotted in Figure 5.5 for the same sets of parameters used to plot the corresponding probability densities in Figure 5.3. The diffusion-phase current is always zero at the halfway point of the interval, i.e. $\tilde{J}_D(\ell/2) = 0$, and the spatially averaged diffusion-phase current vanishes, i.e. $\int_0^\ell d\tilde{x} \tilde{J}_D(\tilde{x})/\ell = 0$. More generally, the diffusion-phase current is antisymmetric about the origin $\tilde{x} = 0$, i.e. $\tilde{J}_D(\tilde{x}) = -\tilde{J}_D(\ell - \tilde{x})$. This immediately implies the diffusion-phase current is also antisymmetric about the halfway point $\tilde{x} = \ell/2$, which can be easily seen by redefining $\tilde{x} = \tilde{x}' - \ell/2$ in the above relation. These symmetry properties arise because

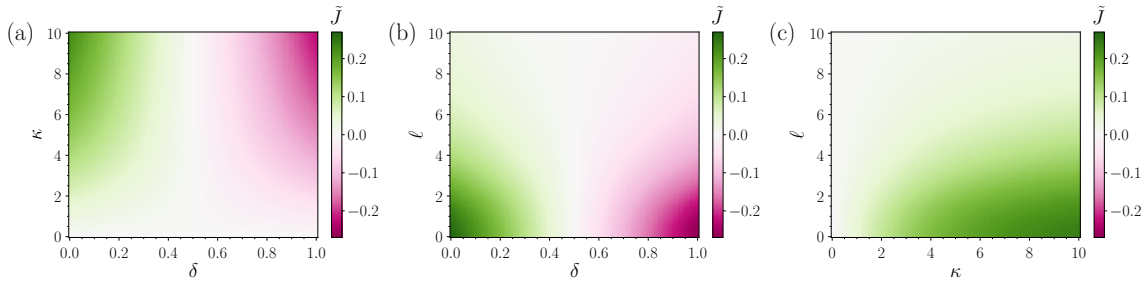


Figure 5.6: Steady-state current $\tilde{J}$, Equation (5.22), as a function of the dimensionless parameters ℓ , κ , and δ . The constant parameter in each subfigure is (a) $\ell = 4$, (b) $\kappa = 4$, and (c) $\delta = 0.2$.

the diffusion phase is not biased by any potential, and so every time the particle is reset to the origin $\tilde{x} = 0$, its density proceeds to diffuse away symmetrically, see Figure 5.2(a). Unlike the diffusion phase, the resetting-phase current $\tilde{J}_R(\tilde{x})$ is generally antisymmetric about the halfway point $\tilde{x} = \ell/2$ and the origin $\tilde{x} = 0$ *only* after adjusting by a constant shift (of the net current $\tilde{J}$), i.e. $\tilde{J}_R(\tilde{x}) - \tilde{J} = -(\tilde{J}_R(\ell - \tilde{x}) - \tilde{J})$. This is expected from the antisymmetry properties of $\tilde{J}_D(\tilde{x})$, since $\tilde{J}_D(\tilde{x}) = \tilde{J} - \tilde{J}_R(\tilde{x})$ by definition. As a result of this antisymmetry, the spatially averaged resetting-phase current is simply the net current, i.e. $\int_0^\ell d\tilde{x} \tilde{J}_R(\tilde{x})/\ell = \tilde{J}$, indicating that the resetting-phase current is solely responsible for the non-zero net current that is generated by an asymmetric ratchet, $\delta \neq 1/2$, see Figures 5.5(a), 5.5(b), and 5.5(d). On the other hand, for a symmetric ratchet, $\delta = 1/2$, the resetting-phase current has the same antisymmetry properties as the diffusion-phase current and so the net current $\tilde{J}$ vanishes, see Figure 5.5(c).

The role of the ratchet's symmetry is more clearly elucidated from inserting the explicit expression for the resetting-phase current $\tilde{J}_R^{[i]}(\tilde{x}) = -\partial_{\tilde{x}} \tilde{P}_R^{[i]}(\tilde{x}) - \tilde{V}'^{[i]} \tilde{P}_R^{[i]}(\tilde{x})$ into the relation $\tilde{J} = \int_0^\ell d\tilde{x} \tilde{J}_R(\tilde{x})/\ell$ found above, whence

$$\tilde{J} = -\frac{1}{\ell} \int_0^\ell d\tilde{x} \tilde{V}'(\tilde{x}) \tilde{P}_R(\tilde{x}) = \frac{\kappa}{\ell^2} \left(\frac{p_R^{[2]}}{1-\delta} - \frac{p_R^{[1]}}{\delta} \right), \quad (5.23)$$

where I have used $\tilde{P}_R(0) = \tilde{P}_R(\ell) = 0$, Equation (5.11b), the definitions for each $p_R^{[i]}$, Equation (5.16), and have inserted the explicit expressions for each $\tilde{V}'^{[i]}$, Equation (5.10). Equation (5.23) relates the current $\tilde{J}$ to the probabilities of being found in either region of the ratchet and shows, in particular, that the current vanishes when there is an equal chance of being found in either region, $p_R^{[1]} = p_R^{[2]}$, i.e. when the ratchet is symmetric $\delta = 1/2$.

The net current $\tilde{J}$, Equation (5.22), is plotted in Figure 5.6 as a function of the three dimensionless parameters ℓ, κ, δ . Figure 5.6 shows that maximum positive current is obtained for a fully asymmetric ratchet $\delta = 0$, since this removes the region of the ratchet that imparts an unfavourable negative drift. Figure 5.6 also shows that a stronger coupling to the potential κ leads to a larger current. This is because larger κ reduces the time it

takes to reset the particle and reduces the chance of unfavourable trajectories where the particle diffuses up the gradient of the potential. Larger ℓ , indicating a relatively small diffusion distance $\sigma = \sqrt{D_0/r}$ between resetting phases, is seen to decrease the current. If ℓ satisfies either $1/\ell < \delta < 1/2$ or $1/\ell < 1 - \delta < 1/2$, equivalent to $\sigma < a < L/2$ and $\sigma < L - a < L/2$, respectively, then the majority of resetting cycles will result in the particle being reset without “completing a lap” of the system (on an extended periodic landscape, this would be equivalent to the particle being reset to the same resetting point each time). This results in an effective confinement of the particle close to the origin $\tilde{x} = 0$, reducing any current generated to rare noise-induced escapes from this effective confinement.

I now consider several relevant limiting cases of the net current $\tilde{J}$, Equation (5.22). First, I consider instantaneous stochastic resetting $\kappa \rightarrow \infty$. In this limit, the force from the potential is infinitely strong and so the particle is instantaneously reset to the origin $\tilde{x} = 0$ every time the potential is switched on. The current in the instantaneous resetting limit $\kappa \rightarrow \infty$ is given by

$$\lim_{\kappa \rightarrow \infty} \tilde{J} = \frac{\sinh\left(\frac{(1-2\delta)\ell}{2}\right)}{2 \sinh\left(\frac{\ell}{2}\right)}, \quad (5.24)$$

which is bounded by $1/2 - \delta$ from above or below depending on whether $\delta < 1/2$ or $\delta > 1/2$, respectively, and decays monotonically to zero as $\ell \rightarrow \infty$. Equation (5.24) could have equally been derived from the diffusion-phase density, Equation (5.14), alone using the following argument. For instantaneous resetting $\kappa \rightarrow \infty$, the net current depends solely on where the particle enters the resetting phase, as this determines the distance the particle travels upon being reset. Hence, one can deduce that the current will be given by

$$\lim_{\kappa \rightarrow \infty} \tilde{J} = \frac{1}{\ell} \int_{\delta\ell}^{\ell} dy (\ell - y) \tilde{P}_D(y|D) - \frac{1}{\ell} \int_0^{\delta\ell} dy y \tilde{P}_D(y|D), \quad (5.25)$$

where the first term arises from trajectories where the particle ends its diffusion phase in the $i = 2$ region of the ratchet at position y , resulting in a jump forward by a distance $\ell - y$ upon being reset. The second term comes from the particle ending its diffusion phase in the $i = 1$ region, in which case it jumps backwards a distance y upon being reset. By using that $\tilde{P}_D(y|D) = \tilde{P}_D(y)$ for $\kappa \rightarrow \infty$, since $p_D = 1$ in this case, then inserting the explicit expression for $\tilde{P}_D(y)$ from Equation (5.14) into Equation (5.25), and finally evaluating the integrals, the instantaneous resetting limit, Equation (5.24), is recovered. In the limit $\kappa \rightarrow 0$, the current vanishes because there is no potential to rectify the particle’s motion, and so its dynamics reduce to purely diffusive motion on an unbiased interval.

As illustrated in Figure 5.6, the net current $\tilde{J}$, Equation (5.22), is larger for a fully asymmetric ratchet, $\delta \rightarrow 0$, since the drift imparted by the potential is always positive in

this case. In this “ideal ratchet” limit $\delta \rightarrow 0$, one obtains the more compact expression

$$\begin{aligned} \lim_{\delta \rightarrow 0} \tilde{J} &= \frac{p_D}{2} \frac{\kappa^2(e^\ell - 1)(e^\kappa + 1) - \kappa\ell(e^\ell + 1)(e^\kappa - 1)}{(\kappa^2 - \ell^2)(e^\kappa - 1)(e^\ell - 1)} \\ &= \frac{\kappa^2(e^\ell - 1)(e^\kappa + 1) - \kappa\ell(e^\ell + 1)(e^\kappa - 1)}{2\kappa^2(e^\kappa - 1)(e^\ell - 1) + \kappa\ell^2(e^\kappa + 1)(e^\ell - 1) - \ell^2(e^\kappa - 1)(\ell - 2 + e^\ell(\ell + 2))}, \end{aligned} \quad (5.26)$$

while the opposite limit $\delta \rightarrow 1$ simply returns the above expression with an overall minus sign.

Figure 5.6(a) suggests the maximum possible current is obtained for a ratchet that is both fully asymmetric $\delta \rightarrow 0$, and infinitely strong $\kappa \rightarrow \infty$. This corresponds to an instantaneous resetting model in which a particle jumps forward every resetting event. Taking both $\kappa \rightarrow \infty$ and $\delta \rightarrow 0$ in Equation (5.22) leads to $\tilde{J} \rightarrow 1/2$, which also establishes an upper bound on the current that can be generated. This could have equally been derived through the following physical argument. Suppose the diffusion phase ends with the particle located a distance y from the origin $\tilde{x} = 0$. Then, upon being reset, the particle will jump forward by either y or $\ell - y$, i.e. an average distance $\ell/2$. Given the diffusion-phase dynamics are symmetric and hence do not contribute to the net current, the average number of times the particle passes a point in the interval of length ℓ is therefore $\tilde{J} = 1/2$. In dimensionful units, this equates to $J = r/2$, and so the physical current can be made arbitrarily large by increasing the resetting rate r , since this corresponds to an infinitely frequent series of instantaneous jumps forward.

As seen in Figure 5.6, the current’s dependence on the system parameters is monotonic. However, the average drift speed of the particle’s rectified motion, given by

$$\langle \tilde{v} \rangle = \tilde{J}\ell \quad (5.27)$$

in dimensionless units, has non-monotonic dependence on the system length ℓ for finite κ or δ , as shown in Figure 5.7. For $\kappa \rightarrow \infty$ and $\delta \rightarrow 0$, however, $\langle \tilde{v} \rangle \rightarrow \ell/2$, suggesting the particle’s drift speed diverges as $\ell \rightarrow \infty$. In this case, it is advantageous to have a larger system length ℓ for obtaining greater drift speed, as the particle always jumps forward upon being reset and the distance it jumps is greater for larger ℓ .

5.5 Energetic cost and efficiency of resetting

In the previous section, it was found that the dimensionless current $\tilde{J}$ is trivially maximised by taking $\delta \rightarrow 0$ and $\kappa \rightarrow \infty$, the latter being equivalent to an infinitely strong potential. The physical current $J = r\tilde{J}$ is then maximised by an infinite resetting rate $r \rightarrow \infty$. While maximising the current is a physically relevant objective, it does not take into account the cost associated with using the potential to reset the particle. In particular, we expect a potential of greater amplitude to incur a greater energetic cost. A larger resetting rate r would similarly represent a larger rate with which energy needs to be supplied to the system.

To quantify the energetic cost associated with producing a current in this system,

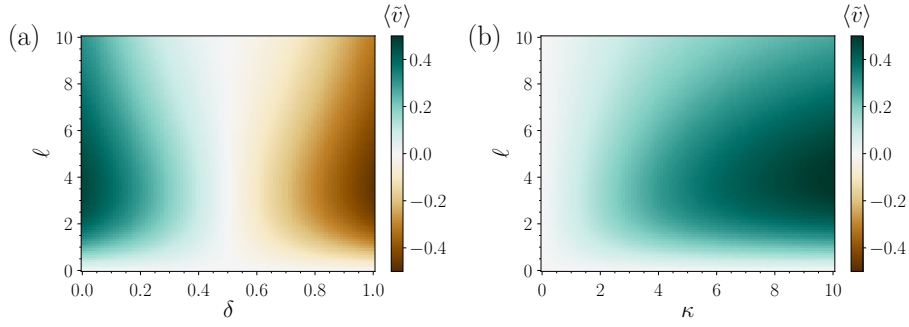


Figure 5.7: Steady-state average drift speed $\langle \tilde{v} \rangle$, Equation (5.27), as a function of the dimensionless parameters ℓ , κ , and δ . The constant parameter in each subfigure is (a) $\kappa = 4$ and (b) $\delta = 0.2$.

we are motivated to study a suitable efficiency parameter. For non-equilibrium systems, the thermodynamic efficiency $\eta_{\text{th}} = \dot{W}/(\dot{W} + D_0\dot{S})$ is typically studied [21, 51], where $\dot{W}$ is the useful power that can be extracted from the system (such as by doing work against an external force [21, 24, 51, 54, 169]) and $\dot{S}$ is the entropy production rate [38], which quantifies the irreversibility of the dynamics. As for many resetting models, the entropy production of the model considered in this chapter diverges due to the resetting process being unidirectional [170]. Hence, the thermodynamic efficiency vanishes and therefore cannot be used to distinguish between different parameters. This is avoided in approximate resetting schemes, such as motion in a fluctuating confining potential [75, 171], or resetting to a distribution [120, 172], for which the corresponding entropy production rates are finite. However, for resetting to a single point, an alternative way of quantifying the energetic cost must be sought.

One recent proposal for an appropriate cost function associated with resetting is based on the distance the particle travels upon being reset [173]. A drawback of this is that it does not take into account the nature of the mechanism by which the particle is reset. A different proposal that is more grounded in thermodynamics is based on an experimental implementation of stochastic resetting, where the cost of a reset is defined as the total energy supplied to an experimental trapping device, such as an optical trap, over the duration of the resetting phase [136]. In the same vein, I define an experimentally motivated, yet analytically tractable, cost function given by the average rate of work done by the potential in order to repeatedly return the particle to the origin. The work done over the course of a single resetting phase is equal to the difference in potential energy of the particle at the beginning and end of the phase [75, 154, 171]. Since every stochastic trajectory in the resetting phase ends at $x = 0$, where $V(0) = 0$, then the net work done in a resetting phase starting at position $x = x_s$ is simply $V(x_s)$. Said another way, the average rate of work done is equal to the power supplied to the system to sustain the repeated jumps in the particle's potential energy from switching on the resetting potential, see Figure 5.8(a). Therefore, the average work done over a complete cycle of diffusion and resetting phases is $\int_0^L dx V(x)P(x|D)$, where $P(x|D) = P_D(x)/p_D$ is the conditional probability density for

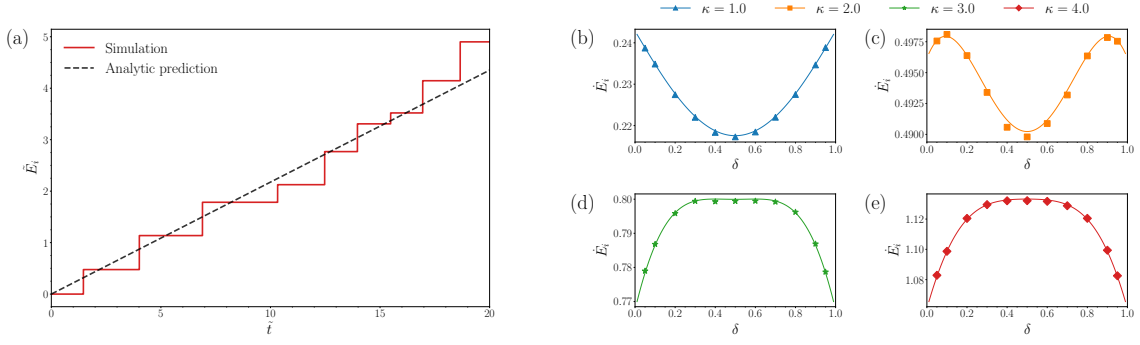


Figure 5.8: Energetic cost of resetting compared to simulations. (a) Cumulative energy input for a single simulated particle against time. The analytical prediction for the cumulative energy input is obtained by multiplying the exact analytic expression for energy input rate, Equation (5.29), by the elapsed time, and is plotted as a dashed line. In the simulation, the cumulative energy input experiences discontinuous jumps of $\tilde{V}(\tilde{x})$ each time the potential is switched on, i.e. when the particle goes from the diffusion phase to the resetting phase. The simulation parameters are $\ell = 4$, $\kappa = 1$, $\delta = 0.5$. (b)–(e) Rate of energy input $\dot{E}_i$ compared to simulations. The theoretical results from Equation (5.29) are shown as solid lines. The simulation data are plotted as symbols for $\kappa = 1, 2, 3, 4$, against various values of $\delta \in (0, 1)$, with $\ell = 4$. The simulations show very good agreement with the analytical results. The simulated energy input rates were calculated by averaging 10^4 particle realisations up to a total time $\tilde{t} = 500$. The simulations of the energetic cost were performed with a smaller timestep $\delta\tilde{t} = 10^{-5}$ than the other simulations in this chapter due to the small variation in energetic cost (see, in particular, subfigure (c)) necessitating a higher degree of accuracy.

the particle to be found at position x *given* it is in the diffusion phase. Meanwhile, the average time for a resetting cycle is $\tau + \int_0^L dx T_R(x)P(x|D) = 1/(rp_D)$, see Equation (5.21). Hence, by dividing the average work done over a cycle by the average time for a cycle, the steady-state rate of energy input/work done is

$$\dot{E}_i = r \int_0^L dx V(x)P_D(x). \quad (5.28)$$

Equation (5.28) vanishes for either $h \rightarrow 0$ or $r \rightarrow 0$, and diverges in the instantaneous resetting limit $h \rightarrow \infty$, as expected for a physically meaningful measure of the energetic cost associated with resetting.

By evaluating the integral in Equation (5.28), the following expression for the energy input rate in terms of the dimensionless parameters and p_D is obtained,

$$\dot{E}_i = p_D \frac{\kappa \sinh\left(\frac{\delta\ell}{2}\right) \sinh\left(\frac{(1-\delta)\ell}{2}\right)}{\delta\ell(1-\delta) \sinh\left(\frac{\ell}{2}\right)}. \quad (5.29)$$

Figure 5.8 shows that Equation (5.29) is in good agreement with simulations. Figure 5.9 shows that the energy input rate generally increases with κ and decreases with ℓ . The

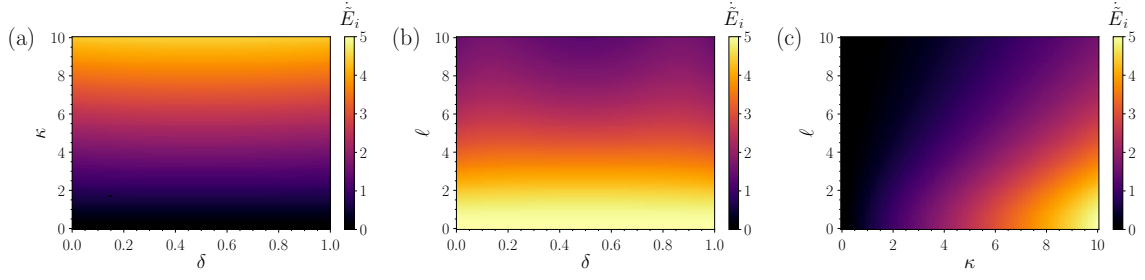


Figure 5.9: Steady-state energy input rate $\dot{E}_i$, Equation (5.29), as a function of the dimensionless parameters ℓ , κ , and δ . The constant parameter in each subfigure is (a) $\ell = 2$, (b) $\kappa = 10$, and (c) $\delta = 0.2$.

energy input rate decreases with ℓ because larger ℓ represents a relatively smaller diffusion distance $\sigma = \sqrt{D_0/r}$ between resets, meaning the particle is effectively confined closer to the origin $\tilde{x} = 0$ between resets, and so the potential does relatively little work to reset the particle each cycle. Varying the asymmetry parameter δ has comparatively little effect on the energy input rate, but there is an interesting non-monotonic dependence on δ nonetheless, as can be seen in Figures 5.8(b)–(e).

In the fully asymmetric limit $\delta \rightarrow 0$, the energy input rate can be written out exactly in terms of the dimensionless parameters, i.e.

$$\lim_{\delta \rightarrow 0} \dot{E}_i = p_D \frac{\kappa}{2} = \frac{\kappa(\kappa^2 - \ell^2)(e^\kappa - 1)(e^\ell - 1)}{2\kappa^2(e^\kappa - 1)(e^\ell - 1) + \kappa\ell^2(e^\kappa + 1)(e^\ell - 1) - \ell^2(e^\kappa - 1)(\ell - 2 + e^\ell(\ell + 2))}, \quad (5.30)$$

and so, in this case, the rate that energy is supplied to the system is simply equal to the average height of the potential, $\kappa/2$, divided by the total time for a complete cycle ($1/p_D$ in dimensionless units).

We now wish to compare the energetic cost of resetting against the return in current, similarly to the cost-weighted efficacy [174] and payoff [175] functions recently defined for diffusive search processes with stochastic resetting. I define the efficiency parameter as

$$\eta = \frac{\langle \tilde{v} \rangle^2}{\dot{E}_i}, \quad (5.31)$$

where, in the units used in this chapter, $\langle \tilde{v} \rangle^2$ is the energy per unit time associated with the current flow. Equation (5.31) is also known as the “Stokes” efficiency and is bounded from above by 1 [168]. It is thus a meaningful measure of useful power output $\langle v \rangle^2$ to power input $\dot{E}_i$. The efficiency can be expressed compactly in terms of the probabilities to be in either phase and the dimensionless parameters,

$$\eta = \frac{1}{p_D} \left(\frac{p_R^{[2]}}{1 - \delta} - \frac{p_R^{[1]}}{\delta} \right)^2 \frac{\kappa\delta(1 - \delta) \sinh\left(\frac{\ell}{2}\right)}{\ell \sinh\left(\frac{\delta\ell}{2}\right) \sinh\left(\frac{(1 - \delta)\ell}{2}\right)}, \quad (5.32)$$

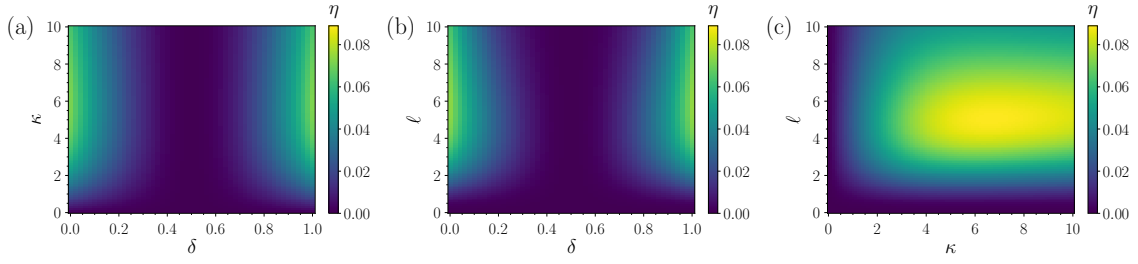


Figure 5.10: Efficiency η , Equation (5.32), as a function of the dimensionless parameters ℓ , κ , and δ . The constant parameter in each subfigure is (a) $\ell = 4$, (b) $\kappa = 4$, and (c) $\delta = 0.2$. The maximum efficiency in each subfigure is achieved at (a) $\delta = 0$, $\kappa = 5.9$; (b) $\delta = 0$, $\ell = 5.7$; and (c) $\kappa = 6.7$, $\ell = 5.1$.

where it should be stressed again that p_D and p_R have closed-form expressions, determined from Equation (5.20), but they are too complicated to write out explicitly here. Equation (5.32) is plotted in Figure 5.10, which shows that the efficiency has a non-monotonic dependence on κ and ℓ due to a compromise between larger κ and smaller ℓ resulting in greater current, but also incurring a greater energetic cost. The efficiency is generally greater for a fully asymmetric ratchet, $\delta \rightarrow 0$ or $\delta \rightarrow 1$, due to the magnitude of the particle's average drift speed $\langle \tilde{v} \rangle$ increasing faster than the energetic cost $\dot{\tilde{E}}_i$ as $\delta \rightarrow 0$ or $\delta \rightarrow 1$. In the limit $\delta \rightarrow 0$, the efficiency reduces to the exact expression,

$$\lim_{\delta \rightarrow 0} \eta = \frac{\kappa \ell^2 (\ell \coth(\ell/2) - \kappa \coth(\kappa/2))^2}{(\ell^2 - \kappa^2)(2(\ell^2 - \kappa^2) + \ell^3 \coth(\ell/2) - \ell^2 \kappa \coth(\kappa/2))}, \quad (5.33)$$

which is plotted in Figure 5.11, and could have equally been obtained by taking $\delta \rightarrow 1$ in Equation (5.32). One can now find values for the remaining parameters that optimise the efficiency. For instance, the optimal $\kappa = \kappa^*$ for a given ℓ that maximises the efficiency is found by solving $\partial_\kappa \eta|_{\kappa=\kappa^*} = 0$.

Figure 5.11 demonstrates that asymptotically perfect efficiency can be achieved for a region of parameter space where both $\kappa \rightarrow \infty$ and $\ell \rightarrow \infty$. However, naïvely taking $\kappa \rightarrow \infty$ or $\ell \rightarrow \infty$ in Equation (5.33) returns $\eta \rightarrow 0$. Extra care needs to be taken when taking these limits in order to recover $\eta \rightarrow 1^-$. Physically, $D_0 \rightarrow 0$ is expected to be optimal as it removes the possibility of unfavourable trajectories where the particle diffuses up the potential gradient. To take $D_0 \rightarrow 0$, one can take $\kappa \rightarrow \infty$ and $\ell \rightarrow \infty$ while keeping $\kappa/\ell^2 = c = h/(L^2 r)$ a finite constant. This yields a finite efficiency $\eta = 1/(1 + 2c)$, implying that decreasing c will result in better efficiency. One may then be tempted to set $c = 0$ to yield perfect efficiency, but recall that this breaks the previous requirement of c being a finite constant. Strictly speaking, to recover $\eta \rightarrow 1^-$, one needs to ensure $D_0 \rightarrow 0$ much faster than $c \rightarrow 0$. While these limits are somewhat academic, they still provide useful insight into how the efficiency of potential-mediated resetting could be optimised in an experiment.

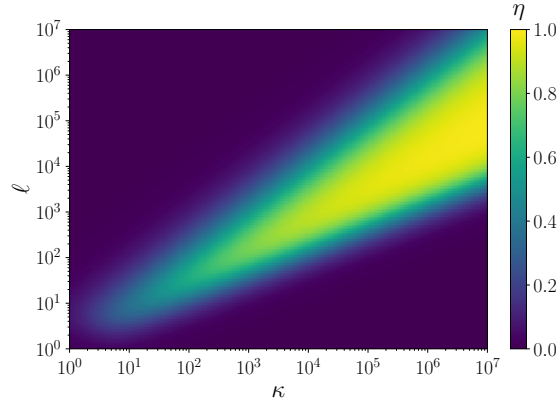


Figure 5.11: Efficiency η in the limit $\delta \rightarrow 0$, Equation (5.33), as a function of κ and ℓ on a log-log scale.

5.6 Conclusion

In this chapter, I introduced an experimentally motivated resetting model, whereby the resetting of a particle to its initial position is mediated by a periodic ratchet potential, Equation (5.3), allowing a steady-state net current to be generated. In particular, the ratchet potential switches on with a constant rate, but switches off only upon the particle’s first passage to the minimum of the potential. Not only does this constitute an optimised variation of the fluctuating potential ratchet model [158], it also generalises other well-known resetting models [119, 123], which can be recovered in certain limits.

I derived the exact solutions for the steady-state phase-dependent probability densities, Equations (5.12) and (5.19), which were analysed in detail in Section 5.3 and corroborated by particle-based Monte Carlo simulations, see Figures 5.2 and 5.3. This was supplemented by a derivation of the time-dependent densities in Appendix 5.B, as well as a derivation of the steady-state densities for a similar “stop-and-start” resetting model in Appendix 5.C. From the densities I derived an exact expression for the steady-state net current, Equation (5.22), in Section 5.4. I showed the net current is tightly bound from above by $r/2$, where r is the rate the potential is switched on, by considering the optimal limits of an infinitely strong $\kappa \rightarrow \infty$, Equation (5.24), and fully asymmetric $\delta \rightarrow 0$, Equation (5.26), potential. As far as I am aware, this is the first analytic study of a steady-state net current generated through finite-time resetting. I made connection with experiments and work extraction in Section 5.5, where I calculated the power input that would be required to sustain this system, Equation (5.28), and compared it with simulations, see Figure 5.8. I then went further by studying an efficiency parameter that quantifies the useful power output—in the form of current—for given power input, Equation (5.31), before finding the parameters that yield (asymptotically) perfect efficiency.

The model presented in this chapter can be extended in several ways. Firstly, the model is formulated for overdamped dynamics, and so it could be generalised to underdamped dynamics by incorporating inertia. In particular, it would be interesting to see in what

parameter regimes inertia improves the current. One may expect inertia to enhance the current for a fully asymmetric ratchet where the force from the ratchet is always in the desired direction, but hindered for finite apex positions as then the ratchet has a region of much larger force in the reverse direction. Another possible avenue for further research is to allow the resetting phase to end at a position determined by a distribution, such as a Gaussian of finite width centred at the minimum of the potential. Allowing the resetting phase to potentially end at any position renders the entropy production finite, which would then pave the way for a study of the thermodynamic efficiency. An alternative approach could be to associate some inherent precision error with determining when the particle has reached the potential minimum in the resetting phase. As the error is made smaller, the associated cost of measurement increases [169], and so this becomes an additional consideration for finite-time-resetting schemes where the resetting potential is modulated by a hypothetical external controller. If the potential is considered to be periodic on an extended domain, then the present model becomes exactly a finite-time-resetting variation of the local-resetting model studied in Ref. [130]. One could then investigate how the addition of a finite resetting time affects the boost in late-time diffusion seen in the local-resetting model. Finally, an interesting analogue to the stop-and-start model considered in Appendix 5.C could be an active particle whose self-propulsion stochastically switches off with a constant rate, and switches back on again only upon the particle reaching the potential minimum. Active particles in static ratchets generally prefer to move up the shallower slope of the potential [21, 22], whereas the stop-and-start resetting scheme tends to rectify particles down the shallower slope. An active stop-and-start resetting model may then have non-monotonic dependence on the system parameters to reflect this competition, as well as the possibility of displaying current reversals.

CHAPTER 5 APPENDICES

5.A Simulation details

By rescaling space and time by $\sigma = \sqrt{D_0/r}$ and $\tau = 1/r$, respectively, the Langevin equations (5.1)–(5.2) can be rewritten in terms of the nondimensional parameters ℓ, κ, δ defined in the main text, i.e.

$$\dot{\tilde{x}}_D(\tilde{t}) = \sqrt{2}\xi(\tilde{t}), \quad (5.34a)$$

$$\dot{\tilde{x}}_R(\tilde{t}) = -\tilde{V}'(\tilde{x}_R) + \sqrt{2}\xi(\tilde{t}), \quad (5.34b)$$

where the gradient of the ratchet potential $\tilde{V}'(\tilde{x})$ is given by Equation (5.10). The probability at each timestep to go from the diffusion phase (5.34a) to the resetting phase (5.34b) is $\Delta\tilde{t}$, i.e. the timestep duration, and the particle returns to the diffusion phase from the resetting phase with probability 1 upon crossing either $\tilde{x} = 0$ or $\tilde{x} = \ell$. Equation (5.34) is solved numerically using the Euler-Maruyama method (see Chapter 2) with timestep $\Delta\tilde{t} = 10^{-4}$. Simulations were run up till a final time $\tilde{t} = 20$ for the numerical estimates of the steady-state probability densities in Figure 5.3, and were averaged over 10^6 realisations.

5.B Time-dependent solutions for probability densities

In this appendix, I demonstrate how to derive the time-dependent probability densities for each phase, $P_{D,R}(x, t)$. For clarity, the derivation is performed in terms of the dimensionful variables h, a, L, D_0 , and r , whose definitions can be found in the main text. An analogous derivation for a similar model appears in Ref. [119]. The time-dependent probability densities obey the coupled Fokker-Planck equations (5.5) which, for convenience, I repeat here:

$$\frac{\partial P_D(x, t)}{\partial t} = D_0 \frac{\partial^2 P_D(x, t)}{\partial x^2} - r P_D(x, t) + \left(J_R^{[2]}(L^-, t) - J_R^{[1]}(0^+, t) \right) \delta(x), \quad (5.35a)$$

$$\frac{\partial P_R^{[1]}(x, t)}{\partial t} = D_0 \frac{\partial^2 P_R^{[1]}(x, t)}{\partial x^2} + V'^{[1]} \frac{\partial P_R^{[1]}(x, t)}{\partial x} + r P_D(x) + J_R^{[1]}(0^+, t) \delta(x), \quad (5.35b)$$

$$\frac{\partial P_R^{[2]}(x, t)}{\partial t} = D_0 \frac{\partial^2 P_R^{[2]}(x, t)}{\partial x^2} + V'^{[2]} \frac{\partial P_R^{[2]}(x, t)}{\partial x} + r P_D(x) - J_R^{[2]}(L^-, t) \delta(x). \quad (5.35c)$$

As in the main text, the solution for the resetting-phase density is separated into two components

$$P_R(x, t) = \begin{cases} P_R^{[1]}(x, t), & 0 \leq x < a, \\ P_R^{[2]}(x, t), & a \leq x < L, \end{cases} \quad (5.36)$$

to align with the different regions of the potential, which have gradients given by

$$V'(x) = \begin{cases} V'^{[1]} = \frac{h}{a}, & 0 \leq x < a, \\ V'^{[2]} = -\frac{h}{L-a}, & a \leq x < L. \end{cases} \quad (5.37)$$

I begin with the time-dependent solution for the diffusion-phase probability density $P_D(x, t)$, described by Equation (5.35a). In addition to the periodic boundary conditions,

$$P_D(0, t) = P_D(L, t), \quad (5.38a)$$

$$P_R(0, t) = P_R(L, t) = 0, \quad (5.38b)$$

the initial conditions are defined as

$$P_D(x, 0) = \delta(x), \quad (5.39a)$$

$$P_R(x, 0) = 0, \quad (5.39b)$$

i.e. the particle is initialised at the origin in the diffusion phase. From the definition of the Laplace transform,

$$\hat{P}_{D,R}(x, s) = \int_0^\infty dt e^{-st} P_{D,R}(x, t), \quad (5.40)$$

the Laplace-transformed diffusion-phase density satisfies

$$D_0 \frac{\partial^2 \hat{P}_D(x, s)}{\partial x^2} - (s + r) \hat{P}_D(x, s) + \left(1 + \hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)\right) \delta(x) = 0, \quad (5.41)$$

where I have used that

$$\int_0^\infty dt e^{-st} \frac{\partial P_D(x, t)}{\partial t} = s \hat{P}_D(x, s) - \delta(x) \quad (5.42)$$

after integrating by parts, recalling the initial condition $P_D(x, 0) = \delta(x)$, Equation (5.39a).

Integrating Equation (5.41) over the region $[-\epsilon, \epsilon]$, recalling $-\epsilon \sim L - \epsilon$, and taking $\epsilon \rightarrow 0^+$, results in the following jump condition at the origin,

$$D_0 \left(\left. \frac{\partial \hat{P}_D(x, s)}{\partial x} \right|_{x \rightarrow 0^+} - \left. \frac{\partial \hat{P}_D(x, s)}{\partial x} \right|_{x \rightarrow L^-} \right) = - \left(1 + \hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)\right), \quad (5.43)$$

where $\hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)$ will be fixed in terms of the parameters later by Equation (5.57).

Now consider Equation (5.41) in the region $x \in (0, L)$, where the term proportional to the Dirac delta function vanishes. Solving in this region, I obtain

$$\hat{P}_D(x, s) = \hat{B}_D(s) e^{\sqrt{\frac{s+r}{D_0}} x} + \hat{C}_D(s) e^{-\sqrt{\frac{s+r}{D_0}} x}, \quad (5.44)$$

where $\hat{B}_D(s)$ and $\hat{C}_D(s)$ are constants to be determined. The periodic boundary condition (5.38a) implies

$$\hat{C}_D(s) = \frac{\exp(\sqrt{\frac{s+r}{D_0}} L) - 1}{1 - \exp(-\sqrt{\frac{s+r}{D_0}} L)} \hat{B}_D(s). \quad (5.45)$$

Then, inserting the expression for $\hat{C}_D(s)$, Equation (5.45), into Equation (5.44) and applying the jump condition (5.43), gives

$$\hat{B}_D(s) = \frac{1 + \hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)}{2\sqrt{D_0(r+s)} \left(\exp\left(\sqrt{\frac{s+r}{D_0}} L\right) - 1 \right)}, \quad (5.46a)$$

$$\hat{C}_D(s) = e^{-\sqrt{\frac{s+r}{D_0}} L} \frac{1 + \hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)}{2\sqrt{D_0(r+s)} \left(\exp\left(\sqrt{\frac{s+r}{D_0}} L\right) - 1 \right)}. \quad (5.46b)$$

Then, by defining

$$\hat{A}_D(s) = \frac{1 + \hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)}{2\sqrt{D_0(r+s)}}, \quad (5.47)$$

the Laplace-transformed diffusion-phase density can be written as

$$\hat{P}_D(x, s) = \hat{A}_D(s) \frac{\cosh\left(\sqrt{\frac{s+r}{D_0}} \left(x - \frac{L}{2}\right)\right)}{\sinh\left(\sqrt{\frac{s+r}{D_0}} \frac{L}{2}\right)}. \quad (5.48)$$

I will now proceed to obtain the time-dependent solution for the resetting-phase probability density $P_R(x, t)$, described by Equations (5.35b)–(5.35c). Taking the Laplace transform of Equations (5.35b)–(5.35c) gives

$$D_0 \frac{\partial^2 \hat{P}_R^{[1]}(x, s)}{\partial x^2} + V^{[1]} \frac{\partial \hat{P}_R^{[1]}(x, s)}{\partial x} - s \hat{P}_R^{[1]}(x, s) + r \hat{P}_D(x, s) + \hat{J}_R^{[1]}(0^+, s) \delta(x) = 0, \quad (5.49a)$$

$$D_0 \frac{\partial^2 \hat{P}_R^{[2]}(x, s)}{\partial x^2} + V^{[2]} \frac{\partial \hat{P}_R^{[2]}(x, s)}{\partial x} - s \hat{P}_R^{[2]}(x, s) + r \hat{P}_D(x, s) - \hat{J}_R^{[2]}(L^-, s) \delta(x) = 0. \quad (5.49b)$$

As for the diffusion-phase density, Equation (5.49) is considered in the region $x \in (0, L)$ such that inserting the solution for $\hat{P}_D(x, s)$, Equation (5.48), results in the following partial differential equations for each component of the Laplace-transformed resetting-phase density,

$$D_0 \frac{\partial^2 \hat{P}_R^{[1]}(x, s)}{\partial x^2} + \frac{h}{a} \frac{\partial \hat{P}_R^{[1]}(x, s)}{\partial x} - s \hat{P}_R^{[1]}(x, s) + r \hat{A}_D(s) \frac{\cosh\left(\sqrt{\frac{s+r}{D_0}} \left(x - \frac{L}{2}\right)\right)}{\sinh\left(\sqrt{\frac{s+r}{D_0}} \frac{L}{2}\right)} = 0, \quad (5.50a)$$

$$D_0 \frac{\partial^2 \hat{P}_R^{[2]}(x, s)}{\partial x^2} - \frac{h}{L-a} \frac{\partial \hat{P}_R^{[2]}(x, s)}{\partial x} - s \hat{P}_R^{[2]}(x, s) + r \hat{A}_D(s) \frac{\cosh\left(\sqrt{\frac{s+r}{D_0}} \left(x - \frac{L}{2}\right)\right)}{\sinh\left(\sqrt{\frac{s+r}{D_0}} \frac{L}{2}\right)} = 0. \quad (5.50b)$$

The solutions for each component of the resetting-phase density are then given by

$$\hat{P}_R^{[1]}(x, s) = \hat{g}^{[1]}(x, s) + \hat{A}_R^{[1]}(s)\hat{h}_{a_1}(x, s) + \hat{B}_R^{[1]}(s)\hat{h}_{b_1}(x, s), \quad (5.51a)$$

$$\hat{P}_R^{[2]}(x, s) = \hat{g}^{[2]}(x, s) + \hat{A}_R^{[2]}(s)\hat{h}_{a_2}(x, s) + \hat{B}_R^{[2]}(s)\hat{h}_{b_2}(x, s), \quad (5.51b)$$

where the $\hat{g}^{[i]}(x, s)$ are the particular solutions of Equation (5.50), $(\hat{h}_{a_i}, \hat{h}_{b_i})$ are the homogeneous solutions, and $(\hat{A}_R^{[i]}, \hat{B}_R^{[i]})$ are constants to be fixed. The homogeneous solutions are given by

$$\hat{h}_{a_1}(x, s) = \exp\left(-\frac{x}{2D_0a}\left(h + \sqrt{h^2 + 4D_0a^2s}\right)\right), \quad (5.52a)$$

$$\hat{h}_{b_1}(x, s) = \exp\left(-\frac{x}{2D_0a}\left(h - \sqrt{h^2 + 4D_0a^2s}\right)\right), \quad (5.52b)$$

$$\hat{h}_{a_2}(x, s) = \exp\left(\frac{x}{2D_0(L-a)}\left(h + \sqrt{h^2 + 4D_0a^2s}\right)\right), \quad (5.52c)$$

$$\hat{h}_{b_2}(x, s) = \exp\left(\frac{x}{2D_0(L-a)}\left(h - \sqrt{h^2 + 4D_0a^2s}\right)\right), \quad (5.52d)$$

while the particular solutions (for the case when both $h/a \neq \sqrt{Dr}$ and $h/(L-a) \neq \sqrt{Dr}$) are given by

$$\begin{aligned} \hat{g}^{[1]}(x, s) = & \hat{A}_D(s) \frac{D_0ra^2}{(r+s)h^2 - D_0ra^2} \\ & \times \frac{r \cosh\left(\sqrt{\frac{r+s}{D_0}}\left(x - \frac{L}{2}\right)\right) - \sqrt{\frac{r+s}{D_0}} \frac{h}{a} \sinh\left(\sqrt{\frac{r+s}{D_0}}\left(x - \frac{L}{2}\right)\right)}{\sinh\left(\sqrt{\frac{r+s}{D_0}} \frac{L}{2}\right)}, \end{aligned} \quad (5.53a)$$

$$\begin{aligned} \hat{g}^{[2]}(x, s) = & \hat{A}_D(s) \frac{D_0r(L-a)^2}{(r+s)h^2 - D_0r(L-a)^2} \\ & \times \frac{r \cosh\left(\sqrt{\frac{r+s}{D_0}}\left(x - \frac{L}{2}\right)\right) + \sqrt{\frac{r+s}{D_0}} \frac{h}{L-a} \sinh\left(\sqrt{\frac{r+s}{D_0}}\left(x - \frac{L}{2}\right)\right)}{\sinh\left(\sqrt{\frac{r+s}{D_0}} \frac{L}{2}\right)}. \end{aligned} \quad (5.53b)$$

Next, I fix the constants $\hat{A}_R^{[1]}(s), \hat{A}_R^{[2]}(s), \hat{B}_R^{[1]}(s), \hat{B}_R^{[2]}(s)$ in Equation (5.51). In addition to the periodic boundary condition, Equation (5.38b), we also have the following continuity conditions at the apex $x = a$,

$$P_R^{[1]}(a, t) = P_R^{[2]}(a, t), \quad (5.54a)$$

$$J_R^{[1]}(a, t) = J_R^{[2]}(a, t), \quad (5.54b)$$

where the latter condition (5.54b) can be expressed explicitly as the jump condition

$$D_0 \left(\left. \frac{\partial P_R^{[2]}(x, t)}{\partial x} \right|_{x \rightarrow a^+} - \left. \frac{\partial P_R^{[1]}(x, t)}{\partial x} \right|_{x \rightarrow a^-} \right) = \left(V'^{[1]}(x \rightarrow a^-) - V'^{[2]}(x \rightarrow a^+) \right) P_R^{[1]}(a, t). \quad (5.55)$$

The boundary conditions for the resetting-phase density $\hat{P}_R^{[i]}(x, s)$ can be summarised by the matrix equation $\mathbf{M}(s) \cdot \left(A_R^{[1]}(s), B_R^{[1]}(s), A_R^{[2]}(s), B_R^{[2]}(s) \right) = \mathbf{u}(s)$, explicitly

$$\begin{bmatrix} \hat{h}_{a_1}(0, s) & \hat{h}_{b_1}(0, s) & 0 & 0 \\ 0 & 0 & \hat{h}_{a_2}(L, s) & \hat{h}_{b_2}(L, s) \\ \hat{h}_{a_1}(a, s) & \hat{h}_{b_1}(a, s) & \hat{h}_{a_2}(a, s) & \hat{h}_{b_2}(a, s) \\ \frac{\frac{h}{a} + \frac{h}{L-a}}{D_0} \hat{h}_{a_1}(a, s) + \partial_x \hat{h}_{a_1}(a, s) & \frac{\frac{h}{a} + \frac{h}{L-a}}{D_0} \hat{h}_{b_1}(a, s) + \partial_x \hat{h}_{b_1}(a, s) & -\partial_x \hat{h}_{a_2}(a, s) & -\partial_x \hat{h}_{b_2}(a, s) \end{bmatrix} \cdot \begin{bmatrix} \hat{A}_R^{[1]}(s) \\ \hat{B}_R^{[1]}(s) \\ \hat{A}_R^{[2]}(s) \\ \hat{B}_R^{[2]}(s) \end{bmatrix} = \begin{bmatrix} -\hat{g}^{[1]}(0, s) \\ -\hat{g}^{[2]}(L, s) \\ -(\hat{g}^{[1]}(a, s) - \hat{g}^{[2]}(a, s)) \\ -\left(\partial_x \hat{g}^{[1]}(a, s) - \partial_x \hat{g}^{[2]}(a, s) + \frac{\frac{h}{a} + \frac{h}{L-a}}{D_0} \hat{g}^{[1]}(a, s) \right) \end{bmatrix}, \quad (5.56)$$

where the expressions arising from the first two rows of Equation (5.56) enforce the periodic boundary condition (5.38b), the third row enforces Equation (5.54a), and the final row enforces Equation (5.54b). Explicit expressions for the constants $\hat{A}_R^{[1]}(s), \hat{A}_R^{[2]}(s), \hat{B}_R^{[1]}(s), \hat{B}_R^{[2]}(s)$ in terms of the system parameters are obtained by multiplying the matrix inverse with the vector on the right-hand side of Equation (5.56), i.e. $\left(\hat{A}_R^{[1]}(s), \hat{B}_R^{[1]}(s), \hat{A}_R^{[2]}(s), \hat{B}_R^{[2]}(s) \right) = \mathbf{M}^{-1}(s) \cdot \mathbf{u}(s)$. It then remains to find an explicit expression for $\hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s)$ in terms of the system parameters. This can be achieved using the jump condition of the resetting-phase density at the origin, obtained by integrating Equation (5.49) over the region $[-\epsilon, \epsilon]$, recalling $-\epsilon \sim L - \epsilon$, and then taking $\epsilon \rightarrow 0^+$, i.e.

$$D_0 \left(\left. \frac{\partial \hat{P}_R^{[1]}(x, s)}{\partial x} \right|_{x \rightarrow 0^+} - \left. \frac{\partial \hat{P}_R^{[2]}(x, s)}{\partial x} \right|_{x \rightarrow L^-} \right) = \hat{J}_R^{[2]}(L^-, s) - \hat{J}_R^{[1]}(0^+, s), \quad (5.57)$$

which concludes the derivation of the solutions for the densities in Laplace space.

In principle, exact expressions for the time-dependent probability densities in real space, i.e. $P_{D,R}(x, t)$, can be obtained by taking the inverse Laplace transform of Equations (5.48) and (5.51), though the resulting expressions are too complicated to write down here explicitly. The steady-state limits of the probability densities $P_{D,R}(x)$, Equations (5.14) and (5.19), are recovered using the final value theorem, i.e.

$$\lim_{t \rightarrow \infty} P_{D,R}(x, t) = \lim_{s \rightarrow 0} s P_{D,R}(x, s). \quad (5.58)$$

It turns out that $\lim_{s \rightarrow 0} s \hat{A}_D(s) = p_D/2$, where $\hat{A}_D(s)$ is given by Equation (5.47) and p_D is the normalisation of the diffusion-phase probability density, defined by Equation (5.15) in the main text. For the case when both $h/a \neq \sqrt{Dr}$ and $h/(L-a) \neq \sqrt{Dr}$, the final value theorem recovers the steady-state solutions of the main text, Equations (5.14) and

(5.19), namely (in dimensionless form)

$$\tilde{P}_D(\tilde{x}) = \frac{p_D}{2} \frac{\cosh(\tilde{x} - \frac{\ell}{2})}{\sinh(\frac{\ell}{2})}, \quad (5.59a)$$

$$\tilde{P}_R(\tilde{x}) = \begin{cases} \frac{p_D}{2} \frac{\delta \ell}{e^\ell - 1} \left(\frac{e^{\ell - \tilde{x}}}{\lambda_-^{[1]}} - \frac{e^{\tilde{x}}}{\lambda_+^{[1]}} \right) + A_R^{[1]} e^{-\frac{\kappa \tilde{x}}{\delta \ell}} + B_R^{[1]}, & 0 \leq \tilde{x} < \delta \ell, \\ \frac{p_D}{2} \frac{(1 - \delta) \ell}{e^\ell - 1} \left(\frac{e^{\tilde{x}}}{\lambda_-^{[2]}} - \frac{e^{\ell - \tilde{x}}}{\lambda_+^{[2]}} \right) + A_R^{[2]} e^{\frac{\kappa \tilde{x}}{(1 - \delta) \ell}} + B_R^{[2]}, & \delta \ell \leq \tilde{x} < \ell. \end{cases} \quad (5.59b)$$

For completeness, the edge-case solutions for the resetting-phase probability density are given by

- Case (i): $h/a = \sqrt{Dr} \neq h/(L - a)$, $(\lambda_-^{[1]} = 0 \neq \lambda_-^{[2]})$

$$\tilde{P}_R(\tilde{x}) = \begin{cases} \frac{p_D}{2} \frac{2e^{\ell - \tilde{x}}(1 + \tilde{x}) - e^{\tilde{x}}}{2(e^\ell - 1)} + A_R^{[1]} e^{-\tilde{x}} + B_R^{[1]}, & 0 \leq \tilde{x} < \delta \ell, \\ \frac{p_D}{2} \frac{\ell(1 - \delta)}{e^\ell - 1} \left(\frac{e^{\tilde{x}}}{\lambda_-^{[2]}} - \frac{e^{\ell - \tilde{x}}}{\lambda_+^{[2]}} \right) + A_R^{[2]} e^{\frac{\tilde{x} \kappa}{\ell(1 - \delta)}} + B_R^{[2]}, & \delta \ell \leq \tilde{x} < \ell, \end{cases} \quad (5.61a)$$

- Case (ii): $h/(L - a) = \sqrt{Dr} \neq h/a$, $(\lambda_-^{[2]} = 0 \neq \lambda_-^{[1]})$

$$\tilde{P}_R(\tilde{x}) = \begin{cases} \frac{p_D}{2} \frac{\ell \delta}{e^\ell - 1} \left(\frac{e^{\ell - \tilde{x}}}{\lambda_-^{[1]}} - \frac{e^{\tilde{x}}}{\lambda_+^{[1]}} \right) + A_R^{[1]} e^{-\frac{\tilde{x} \kappa}{\ell \delta}} + B_R^{[1]}, & 0 \leq \tilde{x} < \delta \ell, \\ \frac{p_D}{2} \frac{-2e^{\tilde{x}}(1 - \tilde{x}) + e^{\ell - \tilde{x}}}{2(e^\ell - 1)} + A_R^{[2]} e^{\tilde{x}} + B_R^{[2]}, & \delta \ell \leq \tilde{x} < \ell, \end{cases} \quad (5.61b)$$

- Case (iii): $h/a = h/(L - a) = \sqrt{Dr}$, $(\lambda_-^{[1]} = \lambda_-^{[2]} = 0)$

$$\tilde{P}_R(\tilde{x}) = \begin{cases} \frac{p_D}{2} \frac{2e^{\ell - \tilde{x}}(1 + \tilde{x}) - e^{\tilde{x}}}{2(e^\ell - 1)} + A_R^{[1]} e^{-\tilde{x}} + B_R^{[1]}, & 0 \leq \tilde{x} < \delta \ell, \\ \frac{p_D}{2} \frac{-2e^{\tilde{x}}(1 - \tilde{x}) + e^{\ell - \tilde{x}}}{2(e^\ell - 1)} + A_R^{[2]} e^{\tilde{x}} + B_R^{[2]}, & \delta \ell \leq \tilde{x} < \ell, \end{cases} \quad (5.61c)$$

where the constants $A_R^{[1]}, A_R^{[2]}, B_R^{[1]}, B_R^{[2]}$ differ for each case, and can be calculated using the final value theorem, e.g. $A_R^{[1]} = \lim_{s \rightarrow 0} s \hat{A}_R^{[1]}(s)$.

5.C Solution for a “stop-and-start” model with deterministic returns in a static ratchet

In this appendix, I discuss how to obtain the steady-state solution for a “stop-and-start” resetting model. In this model, while diffusing in a ratchet potential, a particle stochastically switches off its diffusion, commencing the “resetting phase”. The resetting phase ends only upon the particle’s first passage to the origin, where it then switches its diffusion back on again, restarting the cycle. Since the particle does not diffuse during the resetting phase, the returns to the origin are deterministic. The dynamics are captured by the

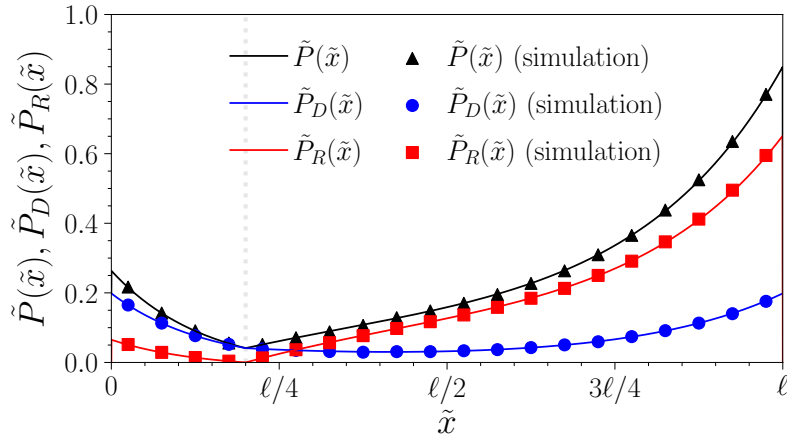


Figure 5.12: Steady-state probability densities $\tilde{P}_{D,R}(\tilde{x})$ for the “stop-and-start” model as a function of particle position $\tilde{x}$ for parameters $\ell = 4$, $\kappa = 1$, and $\delta = 0.2$. The vertical dotted line indicates the position of the ratchet apex $\tilde{x} = \delta\ell$. Simulation data are plotted as symbols and are in excellent agreement with the theoretical results obtained by the procedure described in Appendix 5.C.

following Langevin equations,

$$\dot{x}_D(t) = -V'(x_D) + \sqrt{2D_0}\xi(t), \quad (5.62a)$$

$$\dot{x}_R(t) = -V'(x_R), \quad (5.62b)$$

where the ratchet potential $V(x)$ is the same as the one defined in Equation (5.3). This model is similar to that considered in Ref. [143], for which the authors obtain numerical results. However, in that work, the ratchet potential is continuously differentiable, whereas I will continue to consider a piecewise-linear ratchet potential, Equation (5.3).

One way to solve this model is to first consider that the diffusion and resetting phases each have an associated finite diffusion constant, say D_D and D_R , respectively. After solving this more general model, the limit $D_R \rightarrow 0$ recovers the stop-and-start model. It turns out that solving the model in this way avoids an issue with solving the $D_R = 0$ case directly, namely that the usual resetting-phase boundary condition $P_R(0) = P_R(L) = 0$ no longer holds for $D_R = 0$ as the resetting-phase density has a finite value at the origin in this case [140, 144]. Solving the more general model for finite D_R allows one to keep the usual resetting-phase boundary condition. However, care needs to be taken as the limits $x \rightarrow 0$ and $D_R \rightarrow 0$ do not commute in this case [119]. Hence, taking the limit $D_R \rightarrow 0$ in the more general model recovers the $D_R = 0$ result everywhere except at $x = 0$, where the solution abruptly drops to 0 due to the boundary condition.

The steady-state Fokker-Planck equations for the model with finite D_R can be cast in

the following dimensionless form,

$$0 = \frac{\partial^2 \tilde{P}_D^{[1]}(\tilde{x})}{\partial \tilde{x}^2} + \tilde{V}'^{[1]} \frac{\partial \tilde{P}_D^{[1]}(\tilde{x})}{\partial \tilde{x}} - \tilde{P}_D^{[1]}(\tilde{x}) - \tilde{J}_R^{[1]}(0^+) \delta(\tilde{x}), \quad (5.63a)$$

$$0 = \frac{\partial^2 \tilde{P}_D^{[2]}(\tilde{x})}{\partial \tilde{x}^2} + \tilde{V}'^{[2]} \frac{\partial \tilde{P}_D^{[2]}(\tilde{x})}{\partial \tilde{x}} - \tilde{P}_D^{[2]}(\tilde{x}) + \tilde{J}_R^{[2]}(\ell^-) \delta(\tilde{x}), \quad (5.63b)$$

$$0 = \alpha \frac{\partial^2 \tilde{P}_R^{[1]}(\tilde{x})}{\partial \tilde{x}^2} + \tilde{V}'^{[1]} \frac{\partial \tilde{P}_R^{[1]}(\tilde{x})}{\partial \tilde{x}} + \tilde{P}_D^{[1]}(\tilde{x}) + \tilde{J}_R^{[1]}(0^+) \delta(\tilde{x}), \quad (5.63c)$$

$$0 = \alpha \frac{\partial^2 \tilde{P}_R^{[2]}(\tilde{x})}{\partial \tilde{x}^2} + \tilde{V}'^{[2]} \frac{\partial \tilde{P}_R^{[2]}(\tilde{x})}{\partial \tilde{x}} + \tilde{P}_D^{[2]}(\tilde{x}) - \tilde{J}_R^{[2]}(\ell^-) \delta(\tilde{x}), \quad (5.63d)$$

where I have introduced $\alpha = D_R/D_0$ as a new dimensionless parameter and all other symbols retain the same definitions from the main text. One can verify that the Boltzmann solution, i.e. $\tilde{P}(\tilde{x}) = \tilde{P}_R(\tilde{x}) + \tilde{P}_D(\tilde{x}) \propto \exp(-\tilde{V}(\tilde{x}))$ is recovered for $\alpha = 1$. The stop-and-start model is recovered in the limit $\alpha \rightarrow 0$.

I will now describe how to obtain the solution to Equation (5.63). Since the procedure is mostly analogous to that of Appendix 5.B, I will omit most of the details. As in Appendix 5.B, I first solve for the diffusion-phase density, and then fix the constants of integration using the periodic boundary conditions $\tilde{P}_D^{[1]}(0) = \tilde{P}_D^{[2]}(\ell)$, density continuity condition $\tilde{P}_D^{[1]}(\delta\ell) = \tilde{P}_D^{[2]}(\delta\ell)$, current continuity condition $\tilde{J}_D^{[1]}(\delta\ell) = \tilde{J}_D^{[2]}(\delta\ell)$, and jump condition at $\tilde{x} = 0$, which can be found by integrating Equations (5.63a)–(5.63b) over the region $\tilde{x} \in [-\epsilon, \epsilon]$, recalling $-\epsilon \sim \ell - \epsilon$, and then taking $\epsilon \rightarrow 0^+$, resulting in

$$\left. \frac{\partial \tilde{P}_D^{[1]}(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow 0^+} - \left. \frac{\partial \tilde{P}_D^{[2]}(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow \ell^-} + \frac{\kappa}{\ell\delta(1-\delta)} \tilde{P}_D^{[1]}(0) = - \left(\tilde{J}_R^{[2]}(\ell^-) - \tilde{J}_R^{[1]}(0^+) \right), \quad (5.64)$$

where $\tilde{J}_R^{[2]}(\ell^-) - \tilde{J}_R^{[1]}(0^+)$ can be fixed using the normalisation condition $p_D + p_R = 1$. The solution for $\tilde{P}_D(\tilde{x})$ can then be inserted into Equations (5.63c)–(5.63d) to solve for $\tilde{P}_R(\tilde{x})$, the procedure of which is analogous to the above. The resulting expressions for the densities of both phases are too complicated to write down here. However, they are plotted in Figure 5.12, where the analytic expressions obtained by the procedure above are shown to be in good agreement with simulations.

5.D Relation between normalisation conditions, Equations (5.20) and (5.21)

In this appendix, I show that Equation (5.21) can be derived from Equation (5.20) without the need for an ad-hoc justification based solely on physical arguments [118].

I begin by multiplying both sides of Equation (5.20), $p_D + p_R = 1$, by τ before rearranging the resulting expression to obtain

$$p_D = \frac{\tau}{\tau + \frac{\tau}{p_D} p_R}. \quad (5.65)$$

Next, I derive an expression for p_R in terms of the mean first-passage time $T_R(x)$. First,

I multiply the dimensionless Fokker-Planck equation (5.9b)–(5.9c) by the dimensionless mean first-passage time $\tilde{T}_R(x)$, and then integrate over the entire region. This results in

$$0 = \int_0^\ell d\tilde{x} \tilde{T}_R(x) \left[\frac{\partial^2 \tilde{P}_R(\tilde{x})}{\partial \tilde{x}^2} + \frac{\partial}{\partial \tilde{x}} \left(\tilde{V}'(\tilde{x}) \tilde{P}_R(\tilde{x}) \right) + \tilde{P}_D(\tilde{x}) - \left(\tilde{J}_R(\ell^-) - \tilde{J}_R(0^+) \right) \delta(\tilde{x}) \right] \quad (5.66a)$$

$$= \int_0^\ell d\tilde{x} \left[\frac{\partial^2 \tilde{T}_R(\tilde{x})}{\partial \tilde{x}^2} - \tilde{V}'(\tilde{x}) \frac{\partial \tilde{T}_R(\tilde{x})}{\partial \tilde{x}} \right] \tilde{P}_R(\tilde{x}) + \int_0^\ell d\tilde{x} \tilde{P}_D(\tilde{x}) \tilde{T}_R(\tilde{x}) \quad (5.66b)$$

where, in the second equality, I integrated by parts with the resulting boundary terms vanishing due to the absorbing boundary conditions satisfied by $\tilde{P}_R(\tilde{x})$ and $\tilde{T}_R(\tilde{x})$. The term proportional to $\delta(\tilde{x})$ also vanishes because $\tilde{T}_R(0) = 0$. The term in the square brackets on the right-hand side of Equation (5.66b) simplifies to -1 using the definition of the mean first-passage time (see Equation (5.68) below). Hence, the first integral on the right-hand side of Equation (5.66b) simplifies to $-\int_0^\ell d\tilde{x} \tilde{P}_R(\tilde{x}) = -p_R$, whence

$$p_R = \int_0^\ell d\tilde{x} \tilde{P}_D(\tilde{x}) \tilde{T}_R(\tilde{x}). \quad (5.67)$$

Substituting this expression into Equation (5.65) (which is just a rearrangement of Equation (5.20)) recovers Equation (5.21) in the main text, thus concluding the derivation.

5.E Mean first-passage time in the resetting phase

In this appendix, I derive the (unconditional) mean first-passage time (MFPT) $T_R(x_0)$ of the particle in the resetting phase, i.e. the average time taken for a particle initialised at position $x_0 \in [0, L]$ in the resetting phase to exit the resetting phase by reaching either $x = 0$ or $x = L$. To be consistent with the main text, I define the units of length and time as $\sigma = \sqrt{D_0/r}$ and $\tau = 1/r$, respectively, despite the MFPT being independent of r . While the solution I derive below depends on the dimensionless parameters κ , δ and ℓ , the latter of which depends on r , the dependence on r vanishes after converting back to dimensionful parameters, as should be expected.

In dimensionless form, the MFPT obeys the following partial differential equation [56],

$$-1 = \frac{\partial^2 \tilde{T}_R(\tilde{x})}{\partial \tilde{x}^2} - \tilde{V}'(\tilde{x}) \frac{\partial \tilde{T}_R(\tilde{x})}{\partial \tilde{x}}, \quad (5.68)$$

where the advective term has the opposite sign compared to that of the probability densities (see, for example, Equations (5.9b)–(5.9c)), due to the MFPT obeying the backwards Kolmogorov equation. By definition, the MFPT satisfies the following absorbing boundary conditions

$$\tilde{T}_R^{[1]}(0) = \tilde{T}_R^{[2]}(\ell) = 0, \quad (5.69)$$

which impose that a particle initialised at either $\tilde{x} = 0$ or $\tilde{x} = \ell$ is absorbed instantly and thus takes zero time to exit the resetting phase. The MFPT is also subject to the

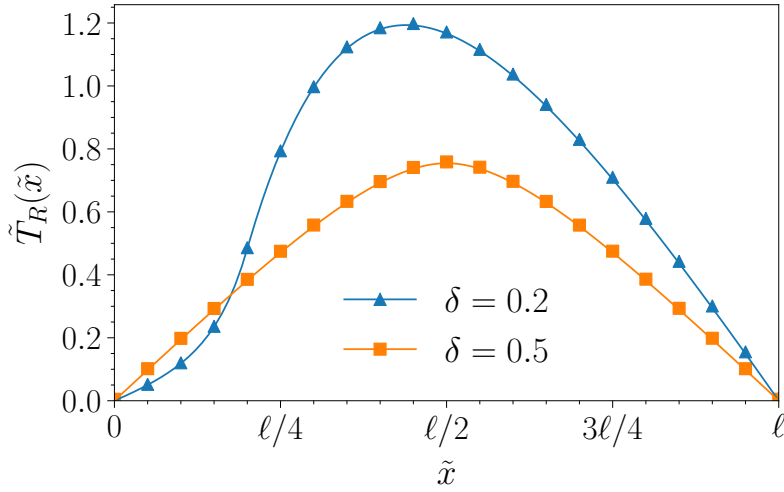


Figure 5.13: Mean first-passage time $\tilde{T}_R(\tilde{x})$ to exit the resetting phase, Equation (5.71), as a function of $\tilde{x}$ for $\ell = 4$, $\kappa = 4$, and $\delta = 0.2$ (blue) or $\delta = 0.5$ (orange). Simulation results are given by markers and are obtained by averaging over 10^6 realisations for each initial position $\tilde{x}/\ell = 0, 0.05, \dots, 1$.

following continuity conditions at the apex $\tilde{x} = \delta\ell$ [21],

$$\tilde{T}_R^{[1]}(\delta\ell) = \tilde{T}_R^{[2]}(\delta\ell), \quad (5.70a)$$

$$\left. \frac{\partial \tilde{T}_R^{[1]}(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow \delta\ell^-} = \left. \frac{\partial \tilde{T}_R^{[2]}(\tilde{x})}{\partial \tilde{x}} \right|_{\tilde{x} \rightarrow \delta\ell^+}. \quad (5.70b)$$

Equation (5.68) can then be solved in a similar manner to that of the probability densities in Appendix 5.B, resulting in

$$\tilde{T}_R(\tilde{x}) = \begin{cases} \frac{\delta\ell}{\kappa^2(e^\kappa - 1)} \left((1 - \delta)\ell e^{-\kappa} (e^{\frac{\kappa}{\delta\ell}\tilde{x}} - 1) + \kappa\tilde{x}(e^\kappa - 1) \right. \\ \left. - \ell(e^{\frac{\kappa}{\delta\ell}\tilde{x}} - 1)(1 - \kappa + \delta(2\kappa - 1)) \right), & 0 \leq \tilde{x} < \delta\ell, \\ \frac{(1-\delta)\ell}{\kappa^2(e^\kappa - 1)} \left(\delta\ell \left[e^{-\kappa \frac{\tilde{x}-\delta\ell}{(1-\delta)\ell}} - e^{-\kappa} \right] + e^\kappa \kappa(\ell - \tilde{x}) \right. \\ \left. - \ell e^{\kappa - \frac{\kappa}{(1-\delta)\ell}(\tilde{x}-\delta\ell)} (\delta + \kappa - 2\delta\kappa) + (\tilde{x}\kappa + \delta\ell(1 - 2\kappa)) \right), & \delta\ell \leq \tilde{x} < \ell. \end{cases} \quad (5.71)$$

The analytical expression for the MFPT, Equation (5.71), is plotted in Figure 5.13 and is in good agreement with simulation results.

6

Autonomous ratcheting of run-and-tumble particles

This chapter is based on the following publication:

C. Roberts and Z. Zhen. Run-and tumble motion in a linear ratchet potential: Analytic solution, power extraction, and first-passage properties, *Physical Review E* **108**, 014139 (2023) [21].

The necessary permissions to reproduce this publication as part of my thesis are included in Appendices B.1.1 and B.2.11.

Author contributions to original manuscript: ZZ and I jointly conceived the project. ZZ wrote the Mathematica scripts to calculate the various observables. I interpreted the analytical results, derived the entropy production rate, performed all simulations, produced all graphs and diagrams, and wrote the bulk of the manuscript.

Chapter summary

In this chapter, we return to work extraction from active matter. In particular, I explore the properties of a run-and-tumble particle moving in a ratchet potential by deriving exact results for the system’s steady-state probability density, current, entropy production rate, extractable power, and thermodynamic efficiency. In contrast with Chapter 5, the potential here does not need to be modulated in time to sustain a steady-state current. Instead, the ratchet potential’s broken spatial symmetry autonomously rectifies the particle’s self-propelled motion. The resulting current is found to peak at finite values of the diffusion strength, ratchet height, and particle self-propulsion speed, while similar non-monotonic behaviour is also found for the entropy production, extractable power, and efficiency. One significant result is that the efficiency of the work extraction becomes arbitrarily perfect in certain parameter regimes, though this is mainly due to several simplifications afforded by modelling so-called “dry” active particles. In the final part, I derive the mean first-passage time and splitting probabilities for different boundary conditions of this model.

6.1 Introduction

When immersed in asymmetric environments, active particles exhibit a net current [20, 22, 50, 176–182]. As discussed in detail in Chapters 1 and 2, a net current indicates broken time-reversal symmetry, which is formally quantified by the entropy production rate [38]. Prior to the work in this chapter being published, entropy production had been calculated for run-and-tumble (RnT) particles only in the case of symmetric confining potentials

[26, 42]. As far as I am aware, the work on which this chapter is based provided the first calculation of entropy production for RnT particles in an *asymmetric* confining potential [21].

The non-equilibrium behaviour of active matter results in first-passage properties that are significantly different to that of equilibrium systems. For instance, the mean escape time of a Brownian particle from a potential well depends only on the ratio of the relative height of the potential barrier to the particle’s thermal energy [183]. In contrast, the mean escape time of active particles can depend on the detailed shape of the potential [184]. Studying the first-passage properties of active matter is particularly relevant to biology, which is often concerned with the time it takes motile agents to reach certain locations, such as in chemotaxis [185]. For the specific case of RnT particles, first-passage properties have been studied both with [27] and without [19, 67, 185, 186] the presence of diffusive noise. The noiseless case allows analytic results for run-and-tumble particles to be obtained in the case of partially absorbing boundaries [19, 185], encounter-based absorption [187, 188], and in the presence of symmetric confining potentials [68]. Even for the more general case of non-negligible diffusive noise, it is possible to obtain analytic results for the first-passage time density on a semi-infinite line, as well as the splitting probabilities and mean first-passage times on a finite interval [27]. It is therefore of interest to see how the combination of asymmetric potentials and diffusion, both of which will be considered in this chapter, generalise these known results.

In this chapter, I obtain exact analytic results for RnT particles in the presence of an external piecewise-linear “ratchet” potential on a periodic interval. In addition, I consider the application of an external counterforce, assuming the role of an external load, to the resulting rectified motion. The counterforce allows for the study of work extraction and is therefore relevant to the operation of active engines. This model of RnT motion is implemented through the addition of active telegraphic noise to the motion of an overdamped Brownian particle in a ratchet. This can describe several physically equivalent non-equilibrium systems, discussed further in Section 6.2.

In what follows, the derivation and discussion of new results begin in Section 6.3 with a calculation of the state-dependent probability densities at stationarity, which are obtained by solving the governing coupled Fokker-Planck equations of the system and then confirmed through Monte Carlo simulations of the Langevin equation. From these densities, in Section 6.4, I obtain the corresponding currents and observe non-monotonic dependencies on the system parameters, similarly to other non-equilibrium systems [189–192]. Then, following the formalism outlined in Ref. [76], I derive the steady-state entropy production rate in Section 6.5, which paves the way for the study of the power output and thermodynamic efficiency in Section 6.6. Finally, in Section 6.7, I study the transport properties of this system, namely, the mean first-passage times for the separate cases of absorbing and reflecting boundary conditions and the splitting probabilities for the particle to exit from either end of the ratchet.

Given the large number of quantities of interest, the aim of this chapter is not to

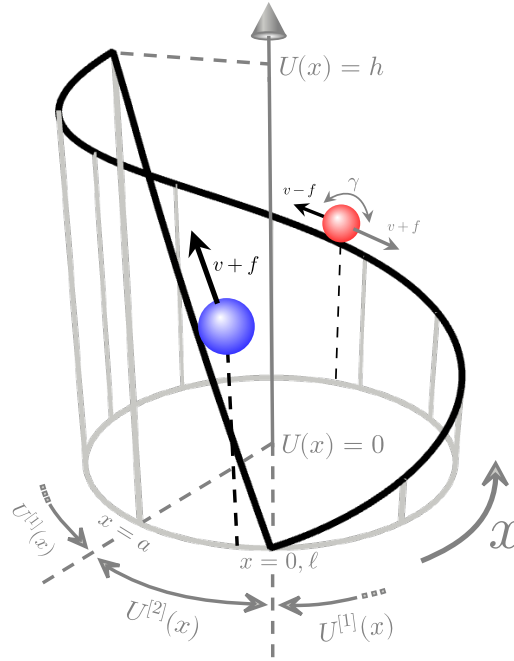


Figure 6.1: Schematic representation of RnT particles subject to a periodic piecewise-linear ratchet potential $U(x) = U(x + \ell)$, Equation (6.1), with maximum amplitude $U(a) = h$. Due to the contribution imparted by the external force f , the overall drift of an RnT particle alternates, with Poissonian rate γ , between $v - f$, corresponding to the right-moving state $\sigma(t) = 1$ (red sphere, background), and $-(v + f)$, corresponding to the left-moving state $\sigma(t) = -1$ (blue sphere, foreground).

provide a full characterisation of the high-dimensional phase space in each case, but to give an overview of the most interesting and relevant features.

As in Chapter 4, the terms “particle” and “particles” are used interchangeably here due to the following results applying equally to a single particle or an ensemble of *non-interacting* particles.

6.2 Model

I consider an RnT particle, whose self-propulsion speed $w(t) \in \{v, -v\}$, where $v > 0$, alternates or “tumbles” between two values with Poissonian rate γ , while moving at position $x \in [0, \ell)$ in a piecewise-linear ratchet potential of length ℓ . A more detailed overview of the RnT model can be found in Chapter 2. The ratchet has maximum amplitude h at the apex $x = a$, and periodic boundary conditions at $x = 0$ and $x = \ell$, see Figure 6.1. The particle is therefore subject to the potential,

$$U(x) = \begin{cases} U^{[1]}(x) = \frac{h}{a}x, & 0 \leq x < a \\ U^{[2]}(x) = \frac{h}{\ell-a}(\ell - x), & a \leq x < \ell \end{cases}. \quad (6.1)$$

Henceforth, any reference to the position $x = 0$ can be assumed to equally refer to $x = \ell$, due to the periodicity, and I will thus refer only to the former. Without loss of generality,

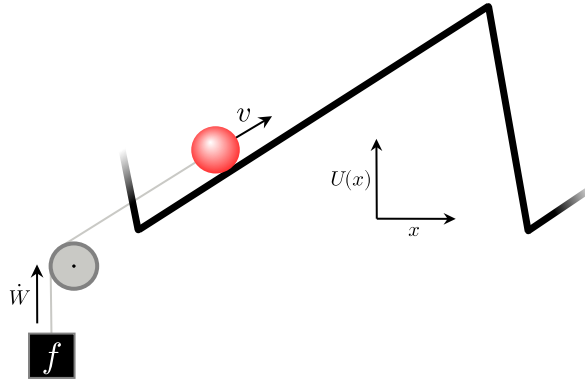


Figure 6.2: By applying an external counterforce of magnitude f , work W can be extracted from the rectified motion of an RnT particle. Here, the counterforce is represented schematically as an external load being raised on a pulley. However, more practical implementations could include rotatable ratchet gears [50] or passive movable obstacles [23, 51].

in Sections 6.3–6.6, I consider only $h \geq 0$ since replacing $h \rightarrow -h$ simply generates the mirror-image of the ratchet, i.e. $a \rightarrow \ell - a$, up to an (irrelevant) constant offset $-h$ after translating space by $x \rightarrow x - a$. For $a \neq \ell/2$, the ratchet is asymmetric and can therefore rectify the motion of the RnT particle. The rectified motion results in a current which can be exploited to perform useful work by applying a counterforce of magnitude f , such as an external load, see Figure 6.2. In the following, I take this counterforce to act to the left, i.e. in the negative- x direction, corresponding to a potential fx , so that work is done *by* the particle when both f and the current are positive, and there is thus still a net drift of particles to the right. I will consider the overdamped regime where forces, such as from the ratchet or the external counterforce, are equivalent to velocities up to a factor of the friction coefficient, which is set to unity (see Chapter 2).

The model considered in this chapter has several physically equivalent interpretations depending primarily on whether the breaking of detailed balance is attributed to external forcing or particle motility. For instance, f has been introduced as a counterforce, but it could also be viewed as an asymmetry parameter of a biased RnT motion with self-propulsion $\bar{w}(t) \in \{v - f, -(v + f)\}$, Figure 6.1. Alternatively, f could be considered a property of the ratchet by defining the potential $V(x) = U(x) + fx$, so that $-f$ is the tilt parameter of the tilted ratchet potential $V(x)$ [193–195]. Similarly, the tumble rate γ could be viewed as the switching rate of a time-fluctuating ratchet $V(x, t) = \{U(x) - (v - f)x, U(x) + (v + f)x\}$ acting on a (non-propelling) Brownian particle. The latter is the case for Brownian motors, whose underlying principle is the rectification of thermal fluctuations through time-varying external forces [161, 162, 196, 197]. Other interpretations can be formulated or devised from suitable combinations of the above.

I will occasionally draw on different interpretations when it offers additional insight, but the focus of this chapter is on the single perspective of an RnT particle with symmetric self-propulsion $w(t) \in \{v, -v\}$ moving in the potential $U(x)$, Equation (6.1), whilst subject to an additional external counterforce f . Regardless, the results presented in this chapter

apply to all of the aforementioned interpretations as, in any case, the motion of the particle is governed by the same Langevin equation in the overdamped limit, i.e.

$$\dot{x}(t) = -U'(x) + v\sigma(t) - f + \sqrt{2D}\xi(t), \quad (6.2)$$

where t is time, $U'(x)$ is the x -derivative of $U(x)$, the telegraphic noise $\sigma(t) \in \{1, -1\}$ switches sign with rate γ , the diffusion constant is D , and $\xi(t)$ is Gaussian white noise with correlator $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$. As is the case for thermal fluctuations, the diffusion considered here is translational and therefore superimposed on the active component of the particle's motion. Henceforth, I will refer to particles as being “right movers” or in the “right-moving state” when $\sigma(t) = 1$ and as “left movers” or in the “left-moving state” when $\sigma(t) = -1$.

The corresponding Fokker-Planck equation to Equation (6.2) reads

$$\frac{\partial P_R^{[i]}(x, t)}{\partial t} = D \frac{\partial^2 P_R^{[i]}(x, t)}{\partial x^2} - (v - f - U'^{[i]}) \frac{\partial P_R^{[i]}(x, t)}{\partial x} - \gamma (P_R^{[i]}(x, t) - P_L^{[i]}(x, t)), \quad (6.3a)$$

$$\frac{\partial P_L^{[i]}(x, t)}{\partial t} = D \frac{\partial^2 P_L^{[i]}(x, t)}{\partial x^2} - (-v - f - U'^{[i]}) \frac{\partial P_L^{[i]}(x, t)}{\partial x} - \gamma (P_L^{[i]}(x, t) - P_R^{[i]}(x, t)), \quad (6.3b)$$

where $P_R^{[i]}(x, t)$ and $P_L^{[i]}(x, t)$ are the probability densities at position x and time t of right movers and left movers respectively. The superscript $i \in \{1, 2\}$ indicates the section of the ratchet on which the probability densities $P_{R,L}^{[i]}(x, t)$ are valid. For the uphill section (from the perspective of a right mover) $x \in [0, a)$, the densities are given by $P_{R,L}^{[1]}(x, t)$, and for the downhill section $x \in [a, \ell)$, the densities are given by $P_{R,L}^{[2]}(x, t)$. Hence, each $U'^{[i]}$ of Equation (6.1) is in fact constant, specifically $U'^{[1]} = h/a$ and $U'^{[2]} = -h/(\ell - a)$, which has allowed the constants $(\pm v - f - U'^{[i]})$ to be brought in front of $\partial_x P_{R,L}^{[i]}(x, t)$ in Equation (6.3).

Unless specified otherwise, the default parameter values used in the figures throughout this chapter are $\ell = 1$, $a = 0.9$, $h = 4$, $D = 1$, $v = 1$, $\gamma = 1$ and $f = 0$. I have chosen these parameters as they correspond to the case where the particle is confined to the potential minimum at $x = 0$ when $D = 0$, since $v - f < h/a$ and $v + f < h/(\ell - a)$ represent the conditions for right movers and left movers to be confined respectively. In this “confined” case, or “locked” state [182, 198], a net current can be generated only by diffusive fluctuations that allow the particle to cross the top of the potential barrier at $x = a$. I will treat this confined case extensively because of its non-trivial behaviour that becomes apparent for $D > 0$ (c.f. the trivial $D = 0$ solution for the confined case in Appendix 6.B and Ref. [20]), as well as its greater relevance, such as to the activated escape of particles via noise-induced transitions [184].

Finally, I have opted to keep the discussion of all results in terms of physically meaningful dimensional parameters, $\ell, a, h, D, v, \gamma, f$, rather than reducing the description

of the system to five dimensionless parameters. In short, there is less benefit to non-dimensionalisation in this case compared to, say, Chapter 5 where the number of parameters almost halves from five to three through non-dimensionalisation.

6.3 Probability densities

The probability densities at stationarity $P_{R,L}^{[i]}(x) \equiv \lim_{t \rightarrow \infty} P_{R,L}^{[i]}(x, t)$ are derived from solving the coupled Fokker-Planck equations (6.3) with the left-hand sides set to zero, i.e. $\partial_t P_R^{[i]}(x) = \partial_t P_L^{[i]}(x) = 0$. For the specific case of $f = 0$, the steady-state solution to Equation (6.3) has been derived in the context of molecular motors [162], and was used principally to investigate how the steady-state current varies with the switching rate (equivalent to γ here) of the potential. However, this solution has never been studied in the context of RnT motion. The current of an RnT particle moving in a piecewise-linear potential has been studied for the less general case of $D = 0$ [20]. However, to the best of my knowledge, a detailed study of the more general $D > 0$ solution for RnT particles does not exist in the literature. Furthermore, the subsequent derivations of the entropy production, power output, thermodynamic efficiency and first-passage properties, as well as the generalisation to $f \neq 0$, are all novel results.

To obtain the steady-state probability densities, I make the following ansatz $P_{R,L}^{[i]}(x) = \mathcal{Z}_{R,L}^{[i]} \exp(\lambda^{[i]} x)$ [162]. Substituting this ansatz into Equation (6.3) for $\partial_t P_{R,L}(x, t) = 0$ results in four linearly independent solutions for each of the particle species, right movers and left movers, and for each section of the ratchet, $i = 1$ and $i = 2$, totalling 16 degrees of freedom. Each set of eigenvalues $\lambda^{[i]}$, $i \in \{1, 2\}$, is found by solving a quartic characteristic equation, see Appendix 6.A. One of the eigenvalues in each set vanishes and so the probability densities have the general solution

$$P_{R,L}^{[i]}(x) = \mathcal{A}_{R,L}^{[i]} e^{\lambda_{\mathcal{A}}^{[i]} x} + \mathcal{B}_{R,L}^{[i]} e^{\lambda_{\mathcal{B}}^{[i]} x} + \mathcal{C}_{R,L}^{[i]} e^{\lambda_{\mathcal{C}}^{[i]} x} + \mathcal{D}_{R,L}^{[i]}, \quad (6.4)$$

with the 16 coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$ to be determined.

These coefficients are fixed by demanding each linearly independent term in Equation (6.4) individually satisfies Equation (6.3) in the steady state, i.e. the resulting prefactors after substitution of each $\exp(\lambda^{[i]} x)$ term must be zero [162]. This fixes half of the 16 degrees of freedom in Equation (6.4). The remaining half is fixed through continuity of the probability densities and currents for each species across $x = 0$ and $x = a$, as well as the normalisation condition $\int_0^\ell dx P(x) = 1$, where $P(x) = P_R(x) + P_L(x)$ is the total probability density. Hence, in principle, the steady-state densities for RnT particles in a piecewise-linear ratchet potential can be obtained in closed form. However, solving 16 coupled equations unsurprisingly results in unwieldy expressions for the coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$, so the bulk of the calculations was performed using Mathematica. The resulting solutions are too long to conveniently display as equations and so most of the results are displayed as graphs alongside descriptions of their qualitative behaviour in the main text. Nevertheless, I emphasise that all results presented in this chapter originate

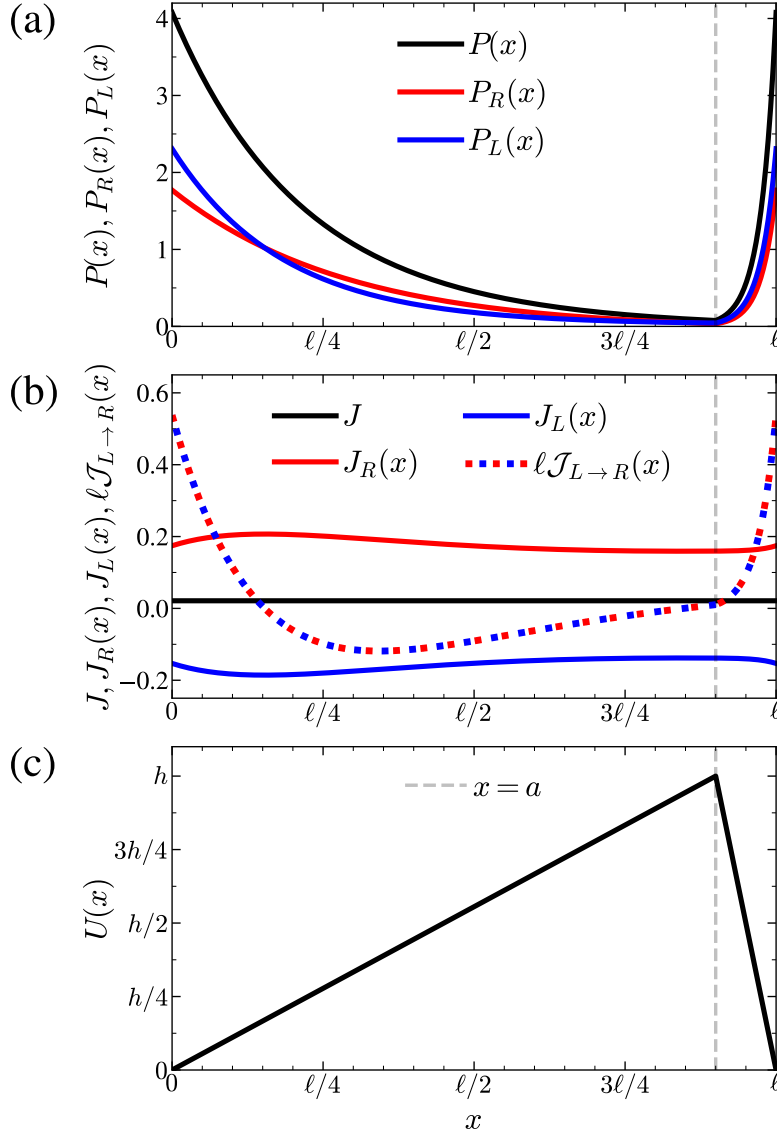


Figure 6.3: (a) Steady-state probability densities $P(x), P_R(x), P_L(x)$, Equation (6.4), (b) and corresponding currents $J, J_R(x), J_L(x), \mathcal{J}_{L \rightarrow R}(x)$, Equations (6.6)–(6.8), for a ratchet potential $U(x)$ shown in subfigure (c). The vertical dashed lines indicate the position of the ratchet apex, $x = a$.

from exact expressions. In fact, any observable that can be written exclusively in terms of the system parameters and the coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$, such as the steady-state current, Equation (6.8), and the steady-state entropy production rate, Equation (6.21), can be written in closed form. The full details of how the expressions for the densities were obtained are left to Appendix 6.A. I also derive the steady-state probability densities for the non-trivial $D = 0$ case in Appendix 6.B. This simplification ultimately leads to closed-form expressions for the corresponding particle current that are compact enough to be written down, see Equations (6.46)–(6.49).

The solutions for the steady-state probability densities, Equation (6.4), are plotted in

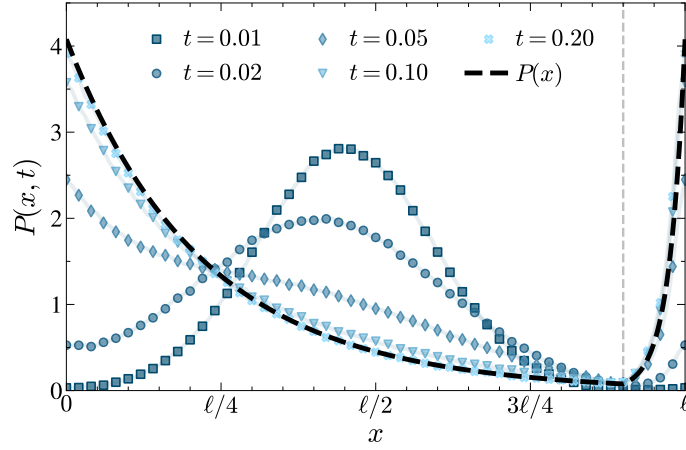


Figure 6.4: Time evolution of the overall probability density $P(x, t) = P_R(x, t) + P_L(x, t)$ obtained from averaging 10^6 stochastic trajectories of an RnT particle moving in a ratchet potential $U(x)$, Equation (6.1). In each realisation, a particle is initialised with an equal probability of being a right mover or a left mover at $x = \ell/2$ and $t = 0$, i.e. $P_R(x, 0) = P_L(x, 0) = \delta(x - \ell/2)/2$, before it is evolved in time by numerically integrating Equation (6.2) in timesteps of $dt = 10^{-5}$. At large times $t \rightarrow \infty$, the simulated densities converge to the theoretical steady-state density $P(x) = P_R(x) + P_L(x)$, Equation (6.4). The vertical dashed line indicates the position of the ratchet apex, $x = a$.

Figure 6.3(a). The solutions for the densities were confirmed by Monte Carlo simulations of the Langevin equation (6.2) by demonstrating the average density of 10^6 realisations of the stochastic dynamics converges to the theoretical steady-state density $P(x)$ as $t \rightarrow \infty$, Figure 6.4.

In Figure 6.3(a), particles are mostly aggregated around the minimum of the ratchet and their density decays further up either slope of the potential. Left movers are more likely to be found close to $x = 0$ than right movers as their preferred direction of motion is against the steeper slope of the potential resulting in greater confinement. The strength of the confinement can be adjusted by varying h . For $h \rightarrow 0$, the densities tend to uniform distributions $P_R(x) = P_L(x) = 1/(2\ell)$, since particles are unconfined. Uniform densities are similarly obtained for $v \rightarrow \infty$, $f \rightarrow \infty$ or $D \rightarrow \infty$ as these cases result in the particle essentially decoupling from the potential. For $h \rightarrow \infty$, particles are confined to the point $x = 0$ and so $P_{R,L}(x) \rightarrow \delta(x)/2$. In the equilibrium limit, $v \rightarrow 0$ or $\gamma \rightarrow \infty$, the density tends to a Boltzmann distribution $P^{[i]}(x) \propto \exp(-(U^{[i]} + f)x/D)$. In the limit $\gamma \rightarrow 0$, right movers and left movers decouple and the solution reduces to that of two drift-diffusive species in the ratchet potential $U(x)$. Finally, taking $D \rightarrow 0$ with $f = 0$ yields agreement with the $D = 0$ case studied in Ref. [20].

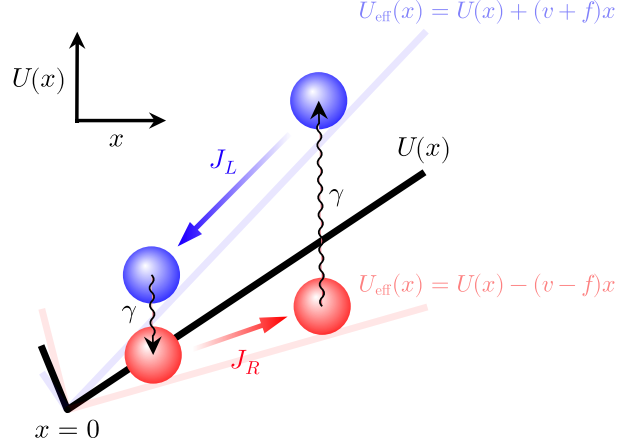


Figure 6.5: The currents for each species, $J_R(x)$ and $J_L(x)$, are greater in magnitude close to the potential minimum at $x = 0$ due to a recycling of particles that tumble before crossing the potential barrier. When in the right-moving state (red spheres, bottom), particles experience a weaker effective potential $U_{\text{eff}}(x) = U(x) - (v - f)x$ than when in the left-moving state (blue spheres, top), resulting in, on average, a greater number of right movers diffusing up the slope before tumbling and returning back down as left movers.

6.4 Currents

The currents for right movers and left movers are, respectively,

$$J_R^{[i]}(x, t) = \left(v - f - U'^{[i]} \right) P_R^{[i]}(x, t) - D \frac{\partial P_R^{[i]}(x, t)}{\partial x}, \quad (6.5a)$$

$$J_L^{[i]}(x, t) = \left(-v - f - U'^{[i]} \right) P_L^{[i]}(x, t) - D \frac{\partial P_L^{[i]}(x, t)}{\partial x}, \quad (6.5b)$$

where, again, I distinguish the separate contributions for the different regions of the ratchet (denoted by the superscript $[i]$) and recall each $U'^{[i]}$ is constant, see Section 6.2. The Fokker-Planck equation (6.3) can be rewritten as a continuity equation in terms of the currents defined in Equation (6.5),

$$\frac{\partial P_R^{[i]}(x, t)}{\partial t} + \frac{\partial J_R^{[i]}(x, t)}{\partial x} - \mathcal{J}_{L \rightarrow R}^{[i]}(x, t) = 0, \quad (6.6a)$$

$$\frac{\partial P_L^{[i]}(x, t)}{\partial t} + \frac{\partial J_L^{[i]}(x, t)}{\partial x} + \mathcal{J}_{L \rightarrow R}^{[i]}(x, t) = 0, \quad (6.6b)$$

where I have also defined the flux density of transitions from the left-moving state to the right-moving state as

$$\mathcal{J}_{L \rightarrow R}^{[i]}(x, t) = \gamma \left(P_L^{[i]}(x, t) - P_R^{[i]}(x, t) \right) = -\mathcal{J}_{R \rightarrow L}^{[i]}(x, t). \quad (6.7)$$

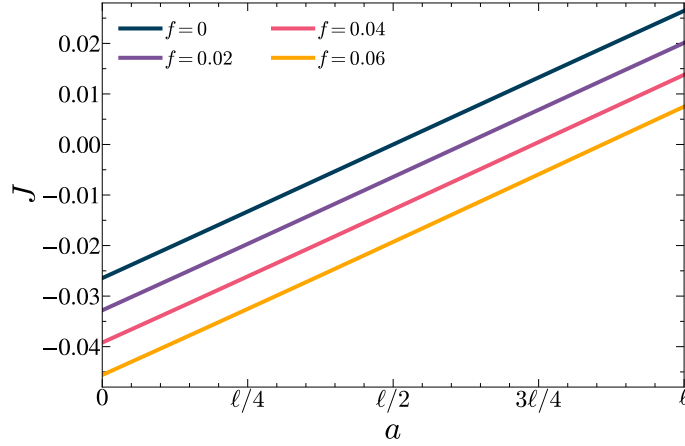


Figure 6.6: Steady-state current J , Equation (6.8), as a function of the position of the ratchet apex a for various external forces f . Maximum current occurs for $a \rightarrow \ell^-$ using the default parameters defined in Section 6.2.

The net current is given by $J(x, t) = J_R(x, t) + J_L(x, t)$. By summing Equations (6.6a) and (6.6b), it can be seen that the stationary condition $\partial_t P^{[i]}(x) = 0$ implies the net current at stationarity is constant across space since this leads to $\partial_x J^{[i]} = 0$. Hence, J can be calculated from the probability densities on just a single section $i \in \{1, 2\}$ of the ratchet since the other section must have the same current. If we choose $i = 1$, corresponding to $x \in [0, a)$, then the resulting expression for $J = J_R^{[1]}(x) + J_L^{[1]}(x)$ can be simplified significantly by setting $x = 0$, yielding a closed-form expression in terms of the known coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$ from Equation (6.4),

$$J = \sum_{\mathcal{Z}=\mathcal{A}}^c \left[v \mathcal{Z}_-^{[1]} - \left(f + \frac{h}{a} + D \lambda_{\mathcal{Z}}^{[1]} \right) \mathcal{Z}_+^{[1]} \right] - \left(f + \frac{h}{a} \right) \mathcal{D}^{[i]}, \quad (6.8)$$

where I have defined $\mathcal{Z}_{\pm}^{[i]} := \mathcal{Z}_R^{[i]} \pm \mathcal{Z}_L^{[i]}$ and have used that $\mathcal{D}_R^{[i]} = \mathcal{D}_L^{[i]} := \mathcal{D}^{[i]}$, see Appendix 6.A.

The currents, Equations (6.5) and (6.8), and flux density of transitions, Equation (6.7), are plotted in Figure 6.3(b). The currents for each species, $J_R(x)$ and $J_L(x)$, are greater in magnitude close to the potential minimum at $x = 0$. This results from particles that tumble before crossing the top of the potential barrier at $x = a$ and so are recycled to the bottom of the potential, e.g. right movers travel part way up the slope $U'^{[1]}$, spanning $0 \leq x < a$, before they tumble and return down the slope as left movers (and vice versa for particles on the opposite slope $U'^{[2]}$). This phenomenon is still present when particles are confined, e.g. one can still have $J_R(x) > 0$ on $U'^{[1]}$ despite $v - f < U'^{[1]}$. As illustrated in Figure 6.5, this is because particles experience different “effective” potentials $U_{\text{eff}}(x)$ depending on their internal state. Specifically, a right-mover can be viewed as a Brownian particle moving in an effective potential $U_{\text{eff}}(x) = U(x) - (v - f)x$. Assuming $v - f > 0$, right movers experience a smaller $U_{\text{eff}}^{[1]}$ than left movers. This asymmetry in $U_{\text{eff}}^{[1]}$ means, on average, a greater number of right movers than left movers will diffuse up the slope

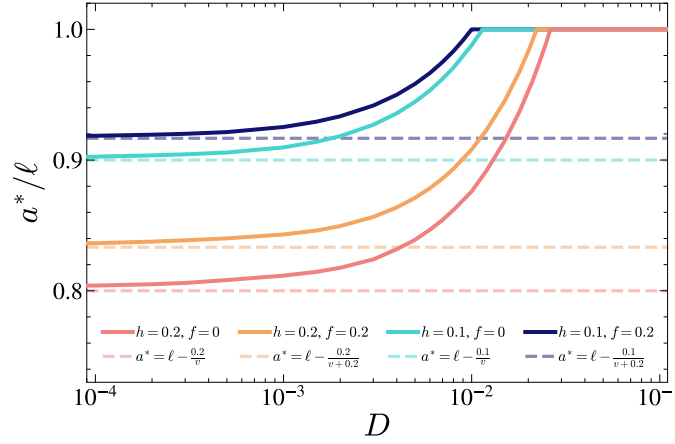


Figure 6.7: Position of the ratchet apex a^* resulting in maximum current J , Equation (6.8), as a function of diffusion strength D . Maximum current occurs for $a = \ell - h/(v + f)$ for $D \rightarrow 0$ and $a \rightarrow \ell^-$ for large D .

$U'^{[1]}$. When these additional right movers tumble, they will return down the slope as left movers, resulting in a current for each particle species just as in the unconfined case. As D is decreased, these confined currents become more localised around $x = 0$ as the chance of a particle crossing the potential barrier becomes increasingly unlikely.

Based on the mechanism described above and in Figure 6.5, each particle is expected to contribute $\sim \gamma$ to the currents $J_{R,L}(x)$ in the confined case. As will become apparent for the entropy production in Section 6.5, a particularly relevant case is the form of the confined currents as $D \rightarrow 0$. In this equilibrium-like case, the current obeys the Arrhenius law $J \sim \exp(-H/D) \approx 0$, see inset of Figure 6.9, where H is the “effective” height of the potential adjusted for particle activity [184]. Hence, one can assume particles almost never overcome the potential barrier as $D \rightarrow 0$, and can thus approximate the barrier height h to be effectively infinite. Taking the slope $U'^{[1]}$ as an example, the largest contribution to the left-moving current $J_L(x)$ at a position x will come from right movers that tumble higher up the slope, and so $|J_L^{[1]}(x)| \approx \gamma \int_x^\infty dx' P_R^{[1]}(x')$. Since the confined case is effectively equilibrium, then the right-moving probability density is given by a Boltzmann distribution $P_R^{[1]}(x) \sim \exp(-x/l_D)/l_D$, assuming relaxation to the steady state occurs much faster than transmutation between species and where $l_D = D/(U'^{[1]} - v + f) > 0$ is the characteristic length scale of diffusive spreading. Hence, when particles are confined, $0 < v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$, the current in the limit of vanishing diffusion is

$$\lim_{D \rightarrow 0} |J_L^{[1]}(x)| \sim \gamma e^{-\frac{x}{l_D}}. \quad (6.9)$$

Since $J \rightarrow 0$ for $D \rightarrow 0$ in the confined case, then $|J_R(x)| \approx |J_L(x)|$ and so $|J_R^{[1]}(x)|$ is also approximately equal to the right-hand side of Equation (6.9) in the confined case. Similar arguments can be used to calculate the contributions $J_{R,L}^{[2]}(x)$ to the confined currents on the other slope $U'^{[2]}$ for $D \rightarrow 0$.

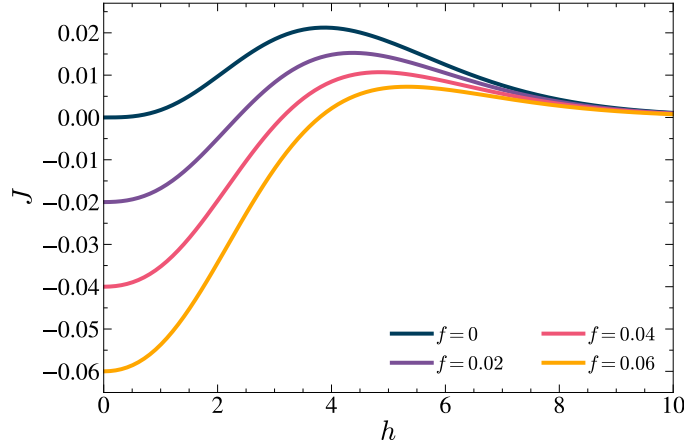


Figure 6.8: Steady-state current J , Equation (6.8), as a function of the ratchet height h for various external forces f . For $h = 0$, the current is given by $J = -f/\ell$. The current vanishes for all f as $h \rightarrow \infty$, due to the confinement at $x = 0$ being infinitely strong. The current peaks around $h \approx 4$, reflecting a compromise in choosing a potential $U(x)$, Equation (6.1), that rectifies the symmetric RnT motion while not confining particles too strongly.

Figure 6.6 shows that motion is rectified to the right ($J > 0$) for $a > \ell/2$ and is rectified to the left ($J < 0$) for $a < \ell/2$ when $f = 0$. Contrary to that of the $D = 0$ case studied in Ref. [20], where maximum positive current occurs for $a = \ell - h/(v + f)$, one finds for the parameters used in Figure 6.6 that maximum current occurs for $a \rightarrow \ell^-$, i.e. when there is an infinitely steep slope $U'^{[2]}$ opposing the motion of left movers. While taking $D \rightarrow 0$ in this model recovers the result of Ref. [20], Figure 6.7 shows that the position of the ratchet apex resulting in maximum current, denoted a^* , occurs at some non-trivial $\ell - h/(v + f) < a^* < \ell$ for small but finite diffusion, $D > 0$. As an explanation, consider first a^* for the $D = 0$ case, which arises by choosing the exact a at which left movers are *only just* confined by the potential, i.e. $v + f = h/(\ell - a)$, in order to not increase the uphill distance the unconfined right movers must traverse. However, for finite diffusion, $D > 0$, left movers are able to overcome the barrier to the left, even for $v + f < h/(\ell - a)$. Hence, to achieve maximum current J for $D > 0$, one must increase a to hinder the left movers' ability to overcome the barrier, while still bearing in mind the compromise that applies to right movers in the $D = 0$ case. As D is increased further, a^* also increases up until the “best” one can do to minimise the left-moving current $J_L(x)$ is simply to set $a \rightarrow \ell^-$.

The effect of varying the ratchet height h on the current is plotted in Figure 6.8. In the absence of a potential $U(x)$, i.e. $h = 0$, the current is given by $J = -f/\ell$. As $h \rightarrow \infty$, the current vanishes as particles become confined by infinitely steep slopes on both sides of $x = 0$. Between these extremes, J peaks at a finite value of h . This reflects that the potential $U(x)$ that optimises the current must be suitably strong to rectify each particle's symmetric RnT motion while not confining the particles too strongly.

The current J similarly peaks at finite values of v and D , the latter of which is plotted

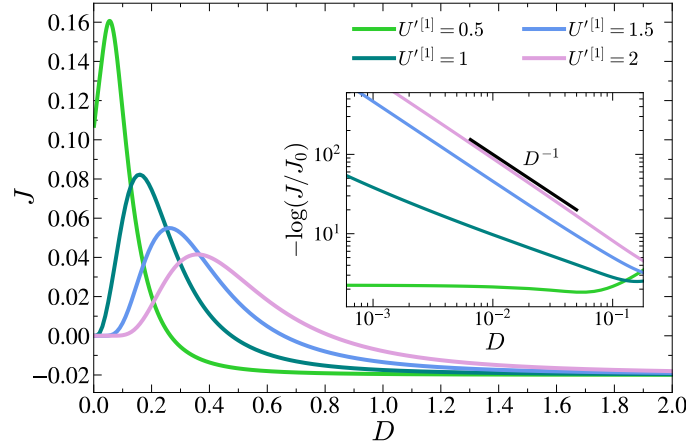


Figure 6.9: Steady-state current J , Equation (6.8), as a function of diffusion D for various magnitudes of the slope $U'^{[1]} = h/a$ for fixed $a = 0.9$ and $f = 0.02$. I have also defined $J_0 = 1 \text{ s}^{-1}$ for dimensional consistency in the logarithm. For $D \rightarrow \infty$, the current asymptotically approaches $J = -f/\ell$. For $D \rightarrow 0$, the current vanishes if the particle is confined, i.e. $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$. If the particle is unconfined, $v - f > U'^{[1]}$, then positive current is possible for $D \rightarrow 0$, as illustrated by the line for $U'^{[1]} = 0.5$. The inset log-log plot demonstrates that agreement with the Arrhenius equation $J \sim \exp(-H/D)$ for small D improves with increasing confinement.

in Figure 6.9. As $v \rightarrow \infty$ or $D \rightarrow \infty$, the particle decouples from the potential such that $J \rightarrow -f/\ell$. This is also the case for when the external force dominates, i.e. $|f| \rightarrow \infty$. The behaviour of J for $D \rightarrow 0$ depends on whether the particle is confined. If the particle's self-propulsive force is not large enough to penetrate the potential barrier, i.e. $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$, then the particle is confined to the potential well at $x = 0$ and thus $J = 0$, see Figure 6.9. If the particle is unconfined, $v - f > U'^{[1]}$ or $v + f > |U'^{[2]}|$, then there is a non-zero net current J as $D \rightarrow 0$.

For $\gamma = 0$, the net current J is the average for that of uncoupled drift-diffusive right movers and left movers. For $\gamma \rightarrow \infty$, the current tends to $J \rightarrow -f/\ell$ since the dynamics effectively reduce to that of a purely diffusive particle moving in a potential $U(x) + fx$.

For completeness, I provide a detailed derivation of the $D = 0$ current j in Appendix 6.B, resulting in closed-form expressions that are compact enough to be written down, Equations (6.46)–(6.49). This derivation generalises the results of Ref. [20] to include an additional linear external force $f \neq 0$ or, equivalently, to allow for asymmetric self-propulsion speeds between right movers and left movers.

6.5 Entropy production

The entropy production rate $\dot{S}_i$ quantifies the degree to which time-reversal symmetry is broken and therefore distinguishes between non-equilibrium, $\dot{S}_i > 0$, and equilibrium, $\dot{S}_i = 0$, systems. In the model considered in this chapter, there are several sources of symmetry breaking, such as asymmetric effective drift speeds between species due to the external force f , and that particles tend to run faster down the sides of the ratchet potential

$U(x)$, Equation (6.1), when the force due to the potential is aligned with the particle's own self-propulsion speed v , similarly to RnT particles in a harmonic potential [42]. Starting from the Gibbs-Shannon entropy [77], I take the same approach as in Chapter 2 to obtain an exact expression for the entropy production rate at stationarity, Equation (6.21) below.

The Gibbs-Shannon entropy for the present system is defined as

$$S(t) = - \sum_{k=R,L} \int_0^\ell dx P_k(x,t) \log \left(\frac{P_k(x,t)}{P_0} \right), \quad (6.10)$$

where P_0 , with $[P_0] = 1/\ell$, is for dimensional consistency in the logarithm but will drop out of the final expression for $\dot{S}_i$. The time derivative of Equation (6.10) is

$$\dot{S}(t) = - \sum_{k=R,L} \int_0^\ell dx \frac{\partial P_k(x,t)}{\partial t} \left(\log \left(\frac{P_k(x,t)}{P_0} \right) + 1 \right). \quad (6.11)$$

After relating $\partial_t P_k(x,t)$ in Equation (6.11) to the currents $J_k(x,t)$ and $\mathcal{J}_{L \rightarrow R}(x,t)$ through the continuity equations (6.6), followed by integrating by parts, and then dropping the boundary terms due to the periodic boundary conditions, one eventually obtains

$$\dot{S}(t) = - \int_0^\ell dx \left(\sum_{k=R,L} \frac{J_k(x,t)}{P_k(x,t)} \frac{\partial P_k(x,t)}{\partial x} + \mathcal{J}_{L \rightarrow R}(x,t) \log \left(\frac{P_R(x,t)}{P_L(x,t)} \right) \right). \quad (6.12)$$

Using the definition of the currents for each species, Equation (6.5), $\partial_x P_k(x,t)$ in Equation (6.12) can be rewritten in terms of these currents to yield

$$\begin{aligned} \dot{S}(t) = \int_0^\ell dx \left[\sum_{k=R,L} \frac{J_k^2(x,t)}{D P_k(x,t)} + \frac{f + U'(x)}{D} J(x,t) \right. \\ \left. - \frac{v}{D} (J_R(x,t) - J_L(x,t)) + \mathcal{J}_{L \rightarrow R}(x,t) \log \left(\frac{P_L(x,t)}{P_R(x,t)} \right) \right], \end{aligned} \quad (6.13)$$

where I have used that $J_R(x,t) + J_L(x,t) = J(x,t)$.

At this point, the time derivative of the entropy can be separated into the contributions $\dot{S}(t) = \dot{S}_i(t) - \dot{S}_e(t)$. The positive-definite terms in Equation (6.13) are identified as those corresponding to the internal entropy production rate of the system $\dot{S}_i(t)$ [26, 38, 75], i.e.

$$\dot{S}_i(t) = \dot{S}_R(t) + \dot{S}_L(t) + \dot{S}_{R \leftrightarrow L}(t) \quad (6.14)$$

where

$$\dot{S}_{R/L}(t) = \int_0^\ell dx \dot{s}_{R/L}(x,t) = \int_0^\ell dx \frac{J_{R/L}^2(x,t)}{D P_{R/L}(x,t)} \quad (6.15)$$

is the entropy production of right/left movers and $\dot{s}_{R/L}(x,t) = J_{R/L}^2(x,t)/(D P_{R/L}(x,t))$ is the local entropy production *density* of right/left movers at position x and time t [26, 42].

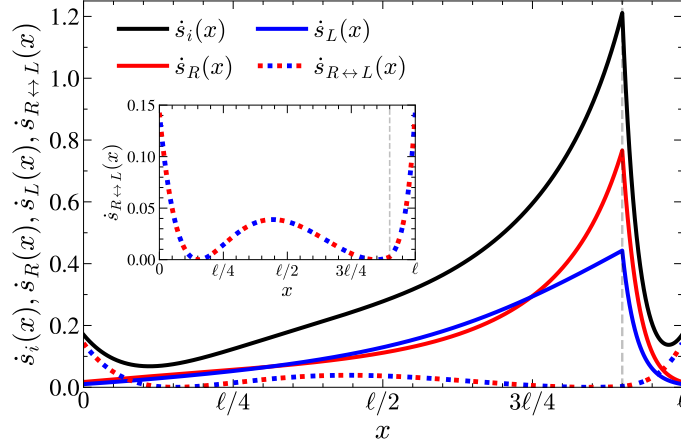


Figure 6.10: Steady-state entropy production densities for right movers $\dot{s}_R(x)$, Equation (6.15), left movers $\dot{s}_L(x)$, Equation (6.15), transitions between states $\dot{s}_{R \leftrightarrow L}(x)$, Equation (6.16) (inset), and their sum $\dot{s}_i(x) = \dot{s}_R(x) + \dot{s}_L(x) + \dot{s}_{R \leftrightarrow L}(x)$. The vertical dashed lines indicate the position of the ratchet apex, $x = a$.

Similarly,

$$\dot{S}_{R \leftrightarrow L}(t) = \int_0^\ell dx \dot{s}_{R \leftrightarrow L}(x, t) = \int_0^\ell dx \mathcal{J}_{L \rightarrow R}(x, t) \log \left(\frac{P_L(x, t)}{P_R(x, t)} \right) \quad (6.16)$$

is the entropy production due to transitions between right movers and left movers, with $\dot{s}_{R \leftrightarrow L}(x, t) = \mathcal{J}_{L \rightarrow R}(x, t) \log (P_L(x, t)/P_R(x, t))$ its local density. Note that $\dot{S}_{R \leftrightarrow L}(t) \geq 0$ for all t since $\mathcal{J}_{L \rightarrow R}(x, t)$, Equation (6.7), and $\log (P_L(x, t)/P_R(x, t))$ are both positive when $P_L(x, t) > P_R(x, t)$ and both negative when $P_L(x, t) < P_R(x, t)$.

The steady-state entropy production densities, as given by $\dot{s}_{R/L}(x) \equiv \lim_{t \rightarrow \infty} \dot{s}_{R/L}(x, t)$ and $\dot{s}_{R \leftrightarrow L}(x) \equiv \lim_{t \rightarrow \infty} \dot{s}_{R \leftrightarrow L}(x, t)$ in Equations (6.15) and (6.16) respectively, are plotted in Figure 6.10 for the same parameters as in Figure 6.3. The overall contribution from right movers to the steady-state entropy production $\dot{s}_R(x)$ is larger than that from left movers $\dot{s}_L(x)$ in the case where motion is rectified to the right, i.e. $J > 0$ as a result of $a > \ell/2$. This is expected since left movers are confined more strongly than right movers for $a > \ell/2$ (and $f = 0$). The entropy production densities for both states, $\dot{s}_R(x)$ and $\dot{s}_L(x)$, are most concentrated around $x = a$, where the magnitude of the current per particle $J/P(x)$, i.e. the mean local velocity, is greatest. The total entropy production density $\dot{s}_i(x)$ has a local maximum at $x = 0$ as a result of the entropy production from transitions between states $\dot{s}_{R \leftrightarrow L}(x)$, Equation (6.16). The confinement due to the ratchet results in a higher concentration of particles around $x = 0$, see Figure 6.3(a), and thus a greater number of tumbles occur in this region, which produces a local peak in the entropy production density. The density for transitions between states $\dot{s}_{R \leftrightarrow L}(x)$, essentially the Kullback-Leibler divergence of $P_R(x)$ and $P_L(x)$ [40], has another local maximum in the bulk. In the case of the default parameters used in Figure 6.10, this local maximum occurs between $x = \ell/4$ and $x = \ell/2$, coinciding with a large local difference between the probability densities for each species, $P_R(x)$ and $P_L(x)$, as seen in Figure 6.3.

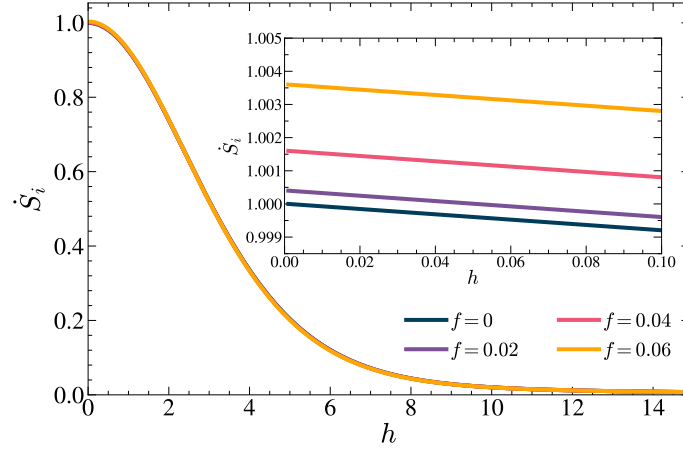


Figure 6.11: Steady-state entropy production rate $\dot{S}_i$, Equation (6.21), as a function of the ratchet height h for various external forces f . In the absence of a ratchet, $h = 0$, the entropy production is given by $\dot{S}_i = (v^2 + f^2)/D$ (inset), whilst $\dot{S}_i \rightarrow 0$ as $h \rightarrow \infty$ for all f .

After identifying the terms contributing to the internal entropy production rate $\dot{S}_i(t)$, Equation (6.14), the remaining terms in the time derivative of the total entropy $\dot{S}(t)$, Equation (6.13), are identified as the entropy flux lost from the system to the environment, i.e.

$$\dot{S}_e(t) = \frac{1}{D} \int_0^\ell dx [v(J_R(x, t) - J_L(x, t)) - (f + U'(x)) J(x, t)]. \quad (6.17)$$

At stationarity, $\dot{S} = 0$ implies $\dot{S}_i = \dot{S}_e$, where $\dot{S} \equiv \lim_{t \rightarrow \infty} \dot{S}(t)$ etc. Thus, it is convenient to evaluate the steady-state entropy production $\dot{S}_i$ through the simpler expression for the steady-state entropy flux $\dot{S}_e$, Equation (6.17), whence

$$\dot{S}_i = \frac{1}{D} \int_0^\ell dx [v(J_R(x) - J_L(x)) - (f + U'(x))J]. \quad (6.18)$$

Then, using that J is constant across space, Equation (6.8), and that $U(x)$ is periodic,

$$\dot{S}_i = \frac{v}{D} \int_0^\ell dx (J_R(x) - J_L(x)) - \frac{f\ell J}{D}. \quad (6.19)$$

After reinserting the expressions for the individual currents $J_{R,L}(x)$ from Equation (6.5), and applying the normalisation $\int_0^\ell dx P(x) = 1$ and periodic boundary conditions $P_{R,L}(0) = P_{R,L}(\ell)$, Equation (6.19) becomes

$$\dot{S}_i = \frac{v^2}{D} - \frac{f\ell J}{D} - \frac{v}{D} \int_0^\ell dx U'(x) (P_R(x) - P_L(x)), \quad (6.20)$$

which, in the absence of an external counterforce f and ratchet potential $U(x)$, recovers the entropy production rate of a free particle v^2/D , see Chapter 2. Finally, splitting the integral in Equation (6.20) into separate contributions for each region of the ratchet and

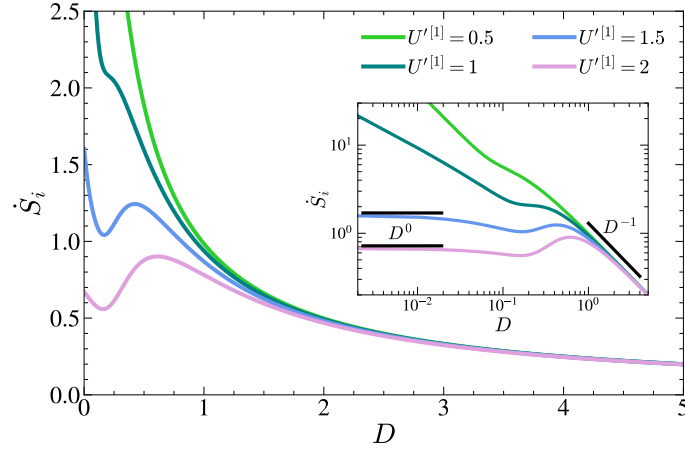


Figure 6.12: Steady-state entropy production rate $\dot{S}_i$, Equation (6.21), as a function of diffusion D for various magnitudes of $U'^{[1]} = h/a$ for fixed $a = 0.9$ and $f = 0$. The entropy production vanishes as $D \rightarrow \infty$. For $D \rightarrow 0$, $\dot{S}_{\text{int}}$ diverges or remains finite depending on whether the particle is confined, i.e. whether $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$.

inserting the expressions for the probability densities $P_{R,L}(x)$, Equation (6.4), results in an expression in terms of the known coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$,

$$\dot{S}_i = \frac{v^2}{D} - \frac{f\ell J}{D} - \frac{v}{D} \sum_{\mathcal{Z}=\mathcal{A}}^c \left(\frac{h}{a} \mathcal{Z}_-^{[1]} \frac{e^{\lambda_{\mathcal{Z}}^{[1]} a} - 1}{\lambda_{\mathcal{Z}}^{[1]}} - \frac{h}{\ell - a} \mathcal{Z}_-^{[2]} \frac{e^{\lambda_{\mathcal{Z}}^{[2]} \ell} - e^{\lambda_{\mathcal{Z}}^{[2]} a}}{\lambda_{\mathcal{Z}}^{[2]}} \right), \quad (6.21)$$

where I have used $\mathcal{D}_R^{[i]} = \mathcal{D}_L^{[i]}$, see Appendix 6.A, and have adopted the same shorthand notation, i.e. $\mathcal{Z}_-^{[i]} = \mathcal{Z}_R^{[i]} - \mathcal{Z}_L^{[i]}$, used in Equation (6.8).

The entropy production $\dot{S}_i$, Equation (6.21), is plotted in Figure 6.11 against the height h of the ratchet. For $h = 0$, the entropy production reduces to $\dot{S}_i = (v^2 + f^2)/D$, see inset of Figure 6.11, which is that of a free RnT particle v^2/D plus a positive contribution f^2/D originating from the asymmetry in the overall drift speeds breaking time-reversal symmetry. The entropy production monotonically decreases with h , and vanishes as $h \rightarrow \infty$, since particles become completely confined to the potential minimum at $x = 0$ and therefore the system contains only stationary particles that are trivially at equilibrium.

As is typically the case for active particles [26, 42], $\dot{S}_i$ monotonically increases with v and diverges as $v \rightarrow \infty$, see Chapter 2. For $D \rightarrow \infty$, the entropy production vanishes since any differences between the deterministic components of the forward and time-reversed trajectories of the RnT particle are washed out by diffusive noise. For $v \rightarrow 0$, $\dot{S}_i$ tends to a positive value due to there still being a current from the remaining drift $-f$.

As for the current J in Section 6.4, the $D \rightarrow 0$ limit of $\dot{S}_i$ depends on whether particles are confined, i.e. whether $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$. In typical systems of RnT particles [26, 42], the entropy production diverges as $D \rightarrow 0$, since the dynamics become more deterministic and it thus becomes easier to distinguish between forward and time-reversed trajectories. However, this effect competes with the increasing confinement of the particles as $D \rightarrow 0$ for $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$. This results in the entropy

production $\dot{S}_i$ remaining finite in the confined case, but diverging in the unconfined case, as $D \rightarrow 0$, see Figure 6.12. It is somewhat remarkable that the confining case results in $\dot{S}_i > 0$ for $D \rightarrow 0$ as one may naïvely expect $\dot{S}_i$ to vanish if the particles are confined. However, the non-vanishing entropy production as $D \rightarrow 0$ is a result of the confined currents, $J_R(x)$ and $J_L(x)$, discussed in Section 6.4. There, it was argued the magnitude of these currents scales approximately as $|J_{R,L}^{[1]}(x)| \sim \gamma \exp(-x/l_D)$, Equation (6.9), for $D \rightarrow 0$ on the slope $U'^{[1]}$, where $l_D = D/(U'^{[1]} - v + f)$. By inserting Equation (6.9) into Equation (6.19), the entropy production in the confined case is

$$\begin{aligned} \lim_{D \rightarrow 0} \dot{S}_i &\sim \lim_{D \rightarrow 0} \gamma \frac{v}{D} \int_0^a dx e^{-\frac{x}{l_D}} + \int_a^\ell dx \dots \\ &\sim \gamma \frac{v}{U'^{[1]} - v + f} + \dots, \end{aligned} \quad (6.22)$$

where $\dots$ indicates additional non-diverging contributions from the confined currents on the $i = 2$ section of the ratchet, spanning $a \leq x < \ell$. Equation (6.22) demonstrates that $\dot{S}_i$ remains finite as $D \rightarrow 0$ in the confined case, see also Figure 6.12.

Figure 6.12 shows that $\dot{S}_i$ has two local extrema in its dependence on D in the confined case. As an explanation, first note in Figure 6.9 that $J \sim \exp(-H/D) \approx 0$ for small D in the confined case but picks up abruptly as D is increased. Thus, it is expected that $\dot{S}_i$ should initially decrease with D in the confined case since the particle dynamics become less deterministic, while there is no significant gain in the net current J until diffusion-mediated barrier crossings significantly increase in frequency. As D is increased further, the onset of the rapid increase in J results in a similar increase in $\partial \dot{S}_i / \partial D$, as can be seen by comparing Figures 6.9 and 6.12 (bearing in mind the slight difference in external forces f used in each figure). The entropy production $\dot{S}_i$ thus attains a local minimum once there becomes an appreciable rise in diffusion-mediated barrier crossings that allow particles to escape confinement. However, as D is increased further, the particles eventually decouple from the potential $U(x)$, and so $\dot{S}_i$ decreases again as D becomes large. As a result, the entropy production also attains a local maximum in the confined case before eventually decaying like that of a free particle, i.e. $\dot{S}_i \sim 1/D$, see inset of Figure 6.12.

For $a < \ell/2$, it was found that the entropy production $\dot{S}_i$ is a monotonically increasing function of the external force f since increasing the external force enhances the existing bias of the system to rectify motion to the left which, in turn, increases the degree to which time-reversal symmetry is broken. In the confined case, $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$, for $a > \ell/2$, increasing the external force f initially decreases the overall bias $J > 0$ of the system, and so the entropy production $\dot{S}_i$ attains a global minimum at finite f before increasing with f again. As $|f| \rightarrow \infty$, the entropy production tends to $\dot{S}_i \rightarrow f^2/D$ as the external force dominates over the ratchet force $U'(x)$ and the self-propulsion v .

For $\gamma \rightarrow 0$, the entropy production $\dot{S}_i$ reduces to the average for that of uncoupled drift-diffusive right movers and left movers moving in a potential $U(x) + fx$. The entropy production also monotonically increases with γ and asymptotically approaches a value $\dot{S}_i \leq (v^2 + f^2)/D$ as $\gamma \rightarrow \infty$.

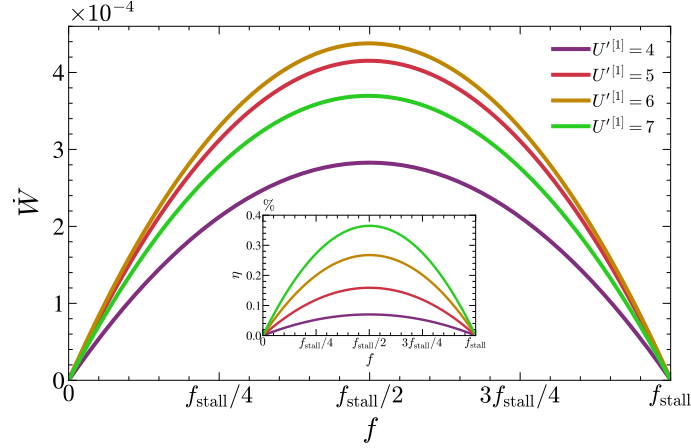


Figure 6.13: Steady-state power output $\dot{W}$, Equation (6.23), as a function of the external force f (renormalised in terms of f_{stall} , see main text) for various magnitudes of $U^{[1]} = h/a$ for fixed $a = 0.9$. Maximum power output occurs for $U^{[1]} \approx 6$ using the default parameters defined in Section 6.2. The power output $\dot{W}$ and thermodynamic efficiency η (inset) are non-zero for external forces $0 < f < f_{\text{stall}}$. The stall forces in this case are $f_{\text{stall}} \approx 0.054, 0.083, 0.112, 0.138$ for each $U^{[1]} = 4, 5, 6, 7$ respectively.

6.6 Power output and efficiency

By applying an external force $f > 0$ (in the negative- x direction, see Section 6.2), work W can be extracted from an RnT particle provided $J > 0$. The average rate of work, i.e. power, that can be extracted from the particle in the steady state is

$$\dot{W} = J\ell f, \quad (6.23)$$

where $\dot{W} > 0$ indicates work is being done *by* the particle. The dependence of $\dot{W}$ on the system parameters is thus the same as for that of the current J , Equation (6.8), for constant f and ℓ . Hence, much of the asymptotic behaviour of the extractable power, Equation (6.23), can be readily obtained from that of the current J in Section 6.4 by simply multiplying by ℓf . I will therefore omit this repetitive discussion. The only qualitatively different behaviour for $\dot{W}$ is obtained by varying the external force f , which is plotted in Figure 6.13 alongside the thermodynamic efficiency $\eta = \dot{W}/P_{\text{in}} = \dot{W}/(\dot{W} + D\dot{S}_i)$ [51] for gradients $U^{[1]} = h/a$ close to that achieving maximum extractable power for the default parameters defined in Section 6.2. For these particular parameters, the current can be approximated by $J \approx J_0(1 - f/f_{\text{stall}})$ for $f_{\text{stall}} \neq 0$, where f_{stall} is the stall force at which the current vanishes, $J = 0$, i.e. the point at which the force from the external load exactly cancels the current generated by the rectified motion. Hence, for these parameters where the approximation $J \approx J_0(1 - f/f_{\text{stall}})$ holds, the maximum extractable power $\dot{W}$, Equation (6.23), and in turn the maximum efficiency η , occur for $f \approx f_{\text{stall}}/2$, as seen in Figure 6.13. In the absence of an external force $f = 0$, no work W is produced and the efficiency of the power extraction is thus also $\eta = 0$. For $f < 0$, work is done *on* the particle and so $\dot{W} < 0$ and $\eta < 0$. For $f = f_{\text{stall}}$, $\dot{W} = 0$ and $\eta = 0$ because of the absence

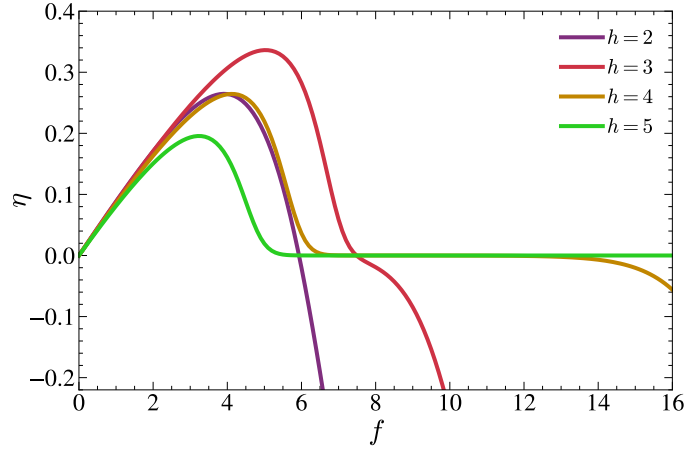


Figure 6.14: Steady-state efficiency η as a function of the external force f for various heights h of the ratchet and for particle parameters $v = 10$, $\gamma = 1$, and $D = 0.1$. For $h \gtrsim 4$, there is a range of external forces for which $\eta \approx 0$.

of a current $J = 0$. For forces greater than the stall force $f > f_{\text{stall}}$, work is done *on* the particle because the current generated by the force f outweighs that generated by the rectification, causing the particle to be “dragged” backwards by the force. As $|f| \rightarrow \infty$, the power $\dot{W} \rightarrow -f^2$ and thus the efficiency $\eta \rightarrow -\infty$ since $D\dot{S}_i \rightarrow f^2$, see Section 6.5.

Figure 6.13 shows the efficiency of the work extraction is relatively poor $\eta < 0.01$ for the default parameter values defined in Section 6.2 since, in this confined case, a current J can be generated only by rare diffusion-mediated barrier crossings. However, the efficiency η is vastly improved in the case where the particle is not confined by the potential $U(x)$, Equation (6.1). Using system parameters $L = 1$ and $a = 0.9$, this is illustrated in Figure 6.14 for particle parameters $v = 10$, $\gamma = 1$, and $D = 0.1$, corresponding to a Péclet number $\text{Pe} = v^2/(D\gamma) = 1000$ on the order of that of an *E. coli* bacterium.¹ These parameters are seen to result in a much higher efficiency, for instance $\eta \approx 0.35$ for $h = 3$ and $f \approx 5$. However, these parameters are by no means those that result in the maximum possible efficiency η for this system. In fact, efficiencies approaching unity can be obtained by taking $D \rightarrow 0$ and $\gamma \rightarrow 0$ while choosing the ratchet parameters in such a way that left movers are confined, $v + f < |U^{[2]}|$, but right movers are not, $v - f > U^{[1]}$, and an external force f slightly smaller than the stall force f_{stall} to minimise dissipation $D\dot{S}_i$ while maintaining positive power output $\dot{W}$. In this case, the ratchet acts as a mechanical diode since right movers produce useful work W against the external force f , while left movers are confined to $x = 0$ and therefore do not contribute negatively to the efficiency η . This highlights, however, the limitations of so-called “dry” active matter considered here, for which hydrodynamic interactions are neglected and thus particles do not dissipate energy while stuck at walls [2]. The efficiency η of this system is expected to be lower for the

¹The typical run speed and tumble rate of an *E. coli* are $v \approx 15 \mu\text{m s}^{-1}$ and $\gamma \approx 1 \text{ s}^{-1}$ respectively [109]. The *thermal* diffusion constant D of an *E. coli* can be calculated from the Stokes-Einstein equation $D = k_B T / (6\pi\eta_{\text{vis}} r)$. By approximating an *E. coli* as a sphere of radius $r = 1 \mu\text{m}$ immersed in water (of dynamic viscosity $\eta_{\text{vis}} \approx 10^{-3} \text{ Pa s}$), this gives $D \approx 0.2 \mu\text{m}^2 \text{ s}^{-1}$ at room temperature $T = 300 \text{ K}$. Thus, the Péclet number of an *E. coli* is on the order of $\text{Pe} = v^2/(D\gamma) \approx 1000$.

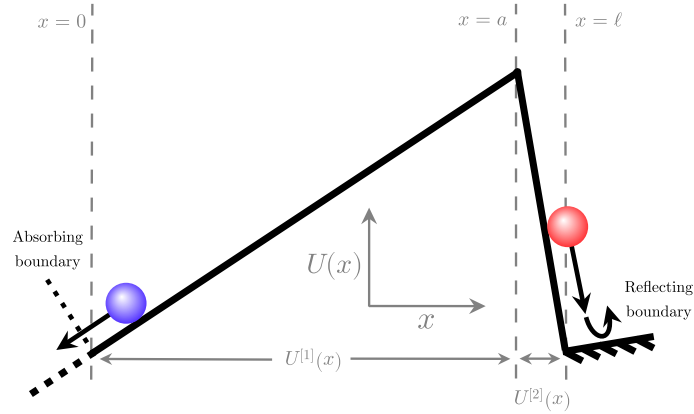


Figure 6.15: Schematic representation of configuration (ii) in Section 6.7, used to study the mean first-passage time of RnT particles in a ratchet potential with a reflecting boundary at $x = \ell$ and an absorbing boundary at $x = 0$. Configuration (i) is the same as configuration (ii) but with the reflecting boundary at $x = \ell$ replaced by an absorbing boundary.

more realistic case of “wet” active matter where particles still dissipate energy even when pinned against the walls of a container.

In Figure 6.14, for $h = 4$ and $h = 5$, we observe a range of external forces f for which the efficiency is $\eta \approx 0$. This is possible for external forces that satisfy $f_{\text{stall}} < f < h/(\ell - a) - v$, as these are larger than the stall force, resulting in motion to the right being suppressed, but still small enough that the combination of the external force f and self-propulsion v is not enough to overcome the potential barrier to the left, and so motion to the left is also suppressed. In the case of small but non-vanishing diffusion D in Figure 6.14, there is still an appreciable chance of the particle overcoming the barrier as a result of diffusive fluctuations and so the range of forces f for which $\eta \approx 0$ does not extend the *entire* way to $f = h/(\ell - a) - v$.

Regarding the maximum power $\dot{W}$, Equation (6.23), that can be extracted from this system, it is known in the case of $D = 0$ that maximum current j , and hence maximum power $\dot{W}$, is achieved by taking $h \rightarrow 0$ and $\ell \rightarrow 0$ for fixed $a = \ell - h/(v + f) > \ell/2$ [20], corresponding to an optimal ratchet on a ring of vanishing circumference that a particle circumnavigates infinitely quickly. However, this diverging $D = 0$ current j fails to take into account the finite size of the particles, which puts physical limitations on how small the ratchet height h and length ℓ can become. Instead, for given particle parameters v and γ , and physically appropriate values of h and ℓ , one could find the optimal power $\dot{W}$ in the $D = 0$ case by using that maximum current occurs for an apex position $a = \ell - h/(v + f)$, which then leaves the external force f as the only remaining parameter to be optimised.

6.7 First-passage properties

In this section, I calculate the mean first-passage times $\tau_{R,L}(x_0)$ and splitting probabilities $\Pi_{R,L}(x_0)$ for an RnT particle in a ratchet potential $U(x)$, Equation (6.1), on a finite interval $x \in [0, \ell]$. Firstly, the mean first-passage times can be calculated for the cases of (i) two

absorbing boundary conditions at $x = 0$ and $x = \ell$, and (ii) a single reflecting boundary at $x = \ell$ and an absorbing boundary at $x = 0$, Figure 6.15. The mean first-passage time $\tau_{R/L}(x_0)$ is the average time it takes the RnT particle to be absorbed at a boundary, and thus leave the system, given the particle was initialised in the right/left-moving state at position $x = x_0 \in [0, \ell]$. The mean first-passage times can be shown to satisfy the backward equations [56]

$$-1 = D \frac{d^2 \tau_R^{[i]}(x)}{dx^2} + (v - f - U'^{[i]}) \frac{d\tau_R^{[i]}(x)}{dx} - \gamma (\tau_R^{[i]}(x) - \tau_L^{[i]}(x)), \quad (6.24a)$$

$$-1 = D \frac{d^2 \tau_L^{[i]}(x)}{dx^2} + (-v - f - U'^{[i]}) \frac{d\tau_L^{[i]}(x)}{dx} - \gamma (\tau_L^{[i]}(x) - \tau_R^{[i]}(x)), \quad (6.24b)$$

with boundary conditions (i) $\tau_{R,L}^{[1]}(0) = \tau_{R,L}^{[2]}(\ell) = 0$, and (ii) $\tau_{R,L}^{[1]}(0) = 0$ and $\partial_x \tau_{R,L}^{[2]}(x)|_{x=\ell} = 0$, for each system configuration. The solutions for the mean first-passage time have the form

$$\tau_{R,L}^{[i]}(x) = \tilde{\mathcal{A}}_{R,L}^{[i]} e^{\tilde{\lambda}_A^{[i]} x} + \tilde{\mathcal{B}}_{R,L}^{[i]} e^{\tilde{\lambda}_B^{[i]} x} + \tilde{\mathcal{C}}_{R,L}^{[i]} e^{\tilde{\lambda}_C^{[i]} x} + \tilde{\mathcal{D}}_{R,L}^{[i]} + \frac{x}{f + U'^{[i]}}, \quad (6.25)$$

where, compared to the general solution for the probability densities $P_{R,L}^{[i]}(x)$ in Equation (6.4), an additional term that is linear in x arises from the particular solution to the non-homogeneous Equation (6.24), see Appendix 6.C.a. Again, as for the probability densities $P_{R,L}^{[i]}(x)$ in Section 6.3, the 16 coefficients $\tilde{\mathcal{A}}_R^{[1]}, \tilde{\mathcal{A}}_L^{[1]}, \tilde{\mathcal{A}}_R^{[2]}, \dots, \tilde{\mathcal{D}}_L^{[2]}$ are fixed by requiring each linearly independent term in Equation (6.25) to satisfy Equation (6.24), before applying boundary conditions and continuity conditions, see Appendix 6.C.a.

For configuration (i), the presence of two absorbing boundaries allows one to also calculate the splitting probabilities $\Pi_{R,L}(x)$ for the system. The splitting probabilities $\Pi_{R,L}(x_0)$ are the probabilities of a particle being absorbed at the left-hand boundary $x = 0$ (before being absorbed at the right-hand boundary $x = \ell$) given it was initialised as a right mover $\Pi_R(x)$ or as a left mover $\Pi_L(x)$ at position $x = x_0 \in [0, \ell]$. The splitting probabilities at the opposite boundary $x = \ell$ are readily obtained from $1 - \Pi_{R,L}(x)$ and their discussion is therefore omitted. Similarly to the mean first-passage times $\tau_{R,L}(x)$, Equation (6.25), the splitting probabilities obey the backward equations [56]

$$0 = D \frac{d^2 \Pi_R^{[i]}(x)}{dx^2} + (v - f - U'^{[i]}) \frac{d\Pi_R^{[i]}(x)}{dx} - \gamma (\Pi_R^{[i]}(x) - \Pi_L^{[i]}(x)), \quad (6.26a)$$

$$0 = D \frac{d^2 \Pi_L^{[i]}(x)}{dx^2} + (-v - f - U'^{[i]}) \frac{d\Pi_L^{[i]}(x)}{dx} - \gamma (\Pi_L^{[i]}(x) - \Pi_R^{[i]}(x)), \quad (6.26b)$$

which are homogeneous, meaning the solutions $\Pi_{R,L}^{[i]}(x)$ to Equation (6.26) can be obtained in a similar manner to that of the homogeneous Equation (6.3), i.e

$$\Pi_{R,L}^{[i]}(x) = \check{\mathcal{A}}_{R,L}^{[i]} e^{\check{\lambda}_A^{[i]} x} + \check{\mathcal{B}}_{R,L}^{[i]} e^{\check{\lambda}_B^{[i]} x} + \check{\mathcal{C}}_{R,L}^{[i]} e^{\check{\lambda}_C^{[i]} x} + \check{\mathcal{D}}_{R,L}^{[i]}, \quad (6.27)$$

where expressions for the 16 coefficients $\check{\mathcal{A}}_R^{[1]}, \check{\mathcal{A}}_L^{[1]}, \check{\mathcal{A}}_R^{[2]}, \dots, \check{\mathcal{D}}_L^{[2]}$ are once again found by

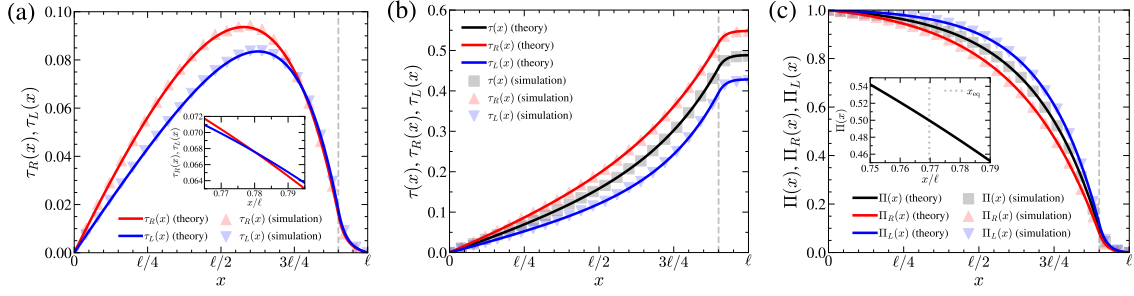


Figure 6.16: Comparison between simulations (markers) and theoretical results (lines) for mean first-passage times $\tau_{R/L}(x)$, Equation (6.25), in the case of (a) absorbing boundaries at $x = 0$ and $x = \ell$, and (b) an absorbing boundary at $x = 0$ and a reflecting boundary at $x = \ell$, and for (c) splitting probabilities $\Pi_{R/L}(x)$, Equation (6.26), for initialisation of an RnT particle as a right/left mover. As in Figure 6.4, simulations were performed by numerically integrating the Langevin equation (6.2) in timesteps of $\Delta t = 10^{-5}$. The simulation data were obtained from the average time it takes the particle to escape the interval, in the case of (a) and (b), and the proportion of times it escapes through $x = 0$, in the case of (c), for 10^5 realisations at each $x/\ell = 0, 0.01, \dots, 1$. The vertical dashed lines indicate the position of the ratchet apex, $x = a$. The theoretical results, Equations (6.25) and (6.27), are in good agreement with simulations.

first requiring each linearly independent term in Equation (6.27) to satisfy Equation (6.26), before applying the boundary conditions $\Pi_{R,L}^{[1]}(0) = 1$ and $\Pi_{R,L}^{[2]}(\ell) = 0$, as well as analogous continuity conditions to that of the mean first-passage times $\tau_{R,L}^{[i]}(x)$, see Appendix 6.C.b.

In Figure 6.16(a), I plot the mean first-passage times $\tau_{R,L}(x)$, Equation (6.25), using the default parameter values, Section 6.2, for absorbing boundaries at $x = 0$ and $x = \ell$. Both $\tau_R(x)$ and $\tau_L(x)$ are skewed to the right compared to a symmetric distribution, which is the case for a Brownian particle in free space, i.e. the maximum mean first-passage times both occur for $x > \ell/2$, due to the asymmetry $a > \ell/2$ of the system. This asymmetry becomes more pronounced as the distance $|a - \ell/2|$ from the symmetric potential is increased, see Figure 6.17(c). The ratchet breaks the symmetry in the mean first-passage times $\tau_{R,L}(x)$ of an RnT particle in the absence of a potential, which satisfies $\tau_R(x) = \tau_L(\ell - x)$ [27], see Figure 6.17(b). For $a > \ell/2$, a particle initialised at $x \in [0, a)$ experiences an average force to the left, assuming $v - f < U^{[1]}$, and thus has a higher chance to escape through the left-hand boundary at $x = 0$ than in the free case. This is seen in the splitting probabilities $\Pi(x)$ plotted in Figure 6.16(c), where an equal chance of escaping through either boundary, i.e. $\Pi(x) = 0.5$, occurs at $x = x_{\text{eq}} \approx 3\ell/4$. For the default parameters, Section 6.2, this position x_{eq} also approximately coincides with the point where the mean first-passage times for right movers and left movers are the same, i.e. $\tau_R(x_{\text{eq}}) \approx \tau_L(x_{\text{eq}})$, Figure 6.16(a). As D is increased, the effect of the ratchet on the mean first-passage times $\tau_{R,L}(x)$ is diminished, resulting in an average time to exit the interval that is symmetric about $x = \ell/2$, Figure 6.17(a). Similarly, large diffusion results in the familiar form $\Pi(x) = 1 - x/\ell$ for the splitting probability, see inset of Figure 6.17(a).

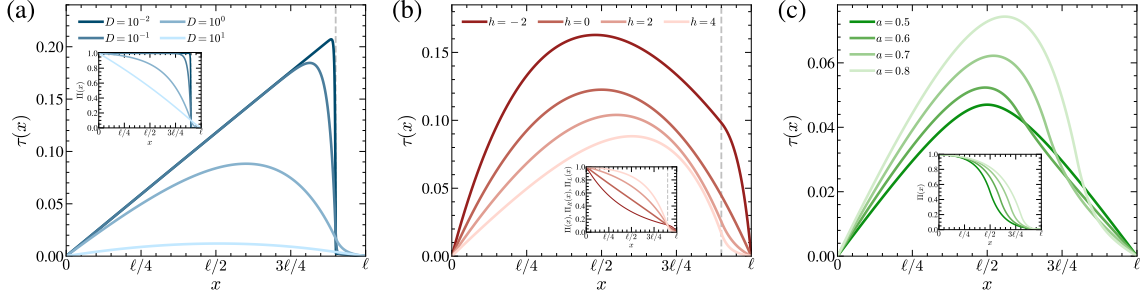


Figure 6.17: Mean first-passage times $\tau(x)$, Equation (6.25), and corresponding splitting probabilities $\Pi(x)$ (insets), Equation (6.27), for varying (a) the diffusion constant D , (b) the height of the ratchet h , and (c) the position of the ratchet peak a , in the case of absorbing boundaries at $x = 0$ and $x = \ell$. In (a) and (b), vertical dashed lines indicate the position of the ratchet apex, $x = a$. In (c), the apexes are indicated by star data points for each curve.

The bounded interval also allows exploration of the first-passage properties for the case $h < 0$, which is no longer degenerate, as in Sections 6.2–6.6, since the boundaries break translational symmetry. The resulting inverted potential for $h < 0$ has the characteristics of a confining potential well, rather than a potential barrier, similarly to the potential $U(x) \sim |x|$ considered in Refs. [68, 199]. However, in the present case, this framework allows exploration of a more general asymmetric variation of this piecewise-linear potential well. As seen in Figure 6.17(b), $h < 0$ results in an increase in the mean first-passage time $\tau(x)$ for all x , as well as concave distributions in the region $a \leq x \leq \ell$ for both $\tau(x)$ and the splitting probability $\Pi(x)$, compared to that of the convex distributions that occur for $h > 0$ due to the resulting favourable gradient towards the right-hand boundary.

For configuration (ii), where the absorbing boundary at $x = \ell$ is replaced with a reflecting boundary, the mean first-passage time of a right mover is trivially greater than that of a left mover for any initial position due to the initial self-propulsion of a right mover always being directed away from the only available exit to the interval, Figure 6.16(b). This is also reflected in the splitting probabilities $\Pi_{R,L}(x)$ in Figure 6.16(c), where the probability for the particle to exit at the left-hand boundary at $x = 0$ is always greater for an initial left mover than an initial right mover.

Finally, for completeness, in Appendix 6.C.c I demonstrate how to derive the “conditional splitting probabilities” $\pi_{X|Y}(x_0)$ for a particle initialised in state $Y \in \{R, L\}$ at $x = x_0$ to leave through the left-hand boundary at $x = 0$ in the self-propulsion state $X \in \{R, L\}$. This generalises what was first derived in Ref. [54] to incorporate piecewise-linear potentials $U(x)$, Equation (6.1). In the free case [54], conditional splitting probabilities allow for the study of particles that exit an interval via diffusive fluctuations even when the particle’s self-propulsion is directed away from the boundary, e.g. a right mover exiting through the left-hand boundary at $x = 0$. The derivation of the conditional splitting probabilities in this chapter can be used to study the combined role that diffusion and potentials play in this phenomenon.

6.8 Conclusion

In this chapter, I studied in detail the motion of run-and-tumble particles subject to a piecewise-linear “ratchet” potential $U(x)$, Equation (6.1), and an external counterforce f for the purpose of extracting useful work. I derived the stationary probability densities $P_{R,L}(x)$, Equation (6.4), in Section 6.3 and Appendix 6.A for both right-moving and left-moving particle species, see Figure 6.3(a), and confirmed the numerically simulated time-dependent densities converge to these expressions as $t \rightarrow \infty$, Figure 6.4.

From the densities $P_{R,L}(x)$, I calculated the corresponding steady-state currents $J_R(x)$, $J_L(x)$, and $J = J_R(x) + J_L(x)$, Equation (6.8), in Section 6.4 and analysed how they depend on the system’s parameters. The current J was found to peak at a finite value of the ratchet potential height h and to vanish in the limit $h \rightarrow \infty$, Figure 6.8. The current J displays similar non-monotonic dependencies on the magnitude of the particle’s self-propulsion speed v and the translational diffusion D . Depending on the strength of the diffusion D , the position of the apex a resulting in maximum current J occurs between $a = \ell - h/(v + f)$ for $D = 0$ and $a \rightarrow \ell^-$ for large D , Figure 6.7. As $D \rightarrow 0$, the current J either remains finite or vanishes depending on whether the particle is confined, Figure 6.9, i.e. whether $v - f < h/a$ and $v + f < h/(\ell - a)$, representing confinement conditions for right movers and left movers respectively. Simple closed-form expressions were obtained for the $D = 0$ current in both the unconfined, Equation (6.46), and confined, Equation (6.48), cases in Appendix 6.B. The currents for each particle species, $J_R(x)$ and $J_L(x)$, are greater in magnitude close to the potential minimum at $x = 0$ due to contributions from particles that tumble before crossing the potential barrier, see Figure 6.3(b). This phenomenon is present even when particles are confined because of weaker “effective” potentials that particles experience as a result of their self-propulsion, Figure 6.5. While many ratchet models exhibit current reversals [200], where particles preferentially flow against the steeper slope of the potential, no such phenomenon is found in the model studied in this chapter. This is in agreement with the findings of Ref. [192], where there is no current reversal for overdamped active particles moving in a piecewise-linear potential, but a current reversal is observed for underdamped active particles. Hence, introducing inertia into the present system could result in a current reversal and thus allow power extraction from a “negative load”, $f < 0$, i.e. an external force applied in the opposite direction to that considered in this chapter, which could be explored in future work.

In Section 6.5, I derived the steady-state entropy production rate $\dot{S}_i$, Equation (6.21), and entropy production densities $\dot{s}_R(x)$, $\dot{s}_L(x)$, and $\dot{s}_{R \leftrightarrow L}(x)$, Equations (6.15) and (6.16), for each particle species. The total entropy production density $\dot{s}_i(x) = \dot{s}_R(x) + \dot{s}_L(x) + \dot{s}_{R \leftrightarrow L}(x)$ is greatest at the apex $x = a$ of the ratchet where the mean local velocity of particles is greatest, Figure 6.10. The steady-state entropy production $\dot{S}_i$ was found to decrease monotonically with the height h of the potential, Figure 6.11. Remarkably, the entropy production $\dot{S}_i$ can have a non-monotonic dependence on diffusion D and, in the limit $D \rightarrow 0$, remains finite when particles are confined due to the Arrhenius-like form of the currents for each particle species, Figure 6.12. Similar behaviour would be

expected for the entropy production of run-and-tumble particles in confining potentials of the form $U_p(x) \sim |x|^p$ for $p \leq 1$, studied in Ref. [68] for the case $D = 0$. Therefore, studying how the entropy production of run-and-tumble particles subject to potentials of the form $U_p(x) \sim |x|^p$ varies with D would be an interesting avenue for further research. It would also be interesting to consider smooth ratchet potentials, where particles can become confined to a finite region rather than a single point, to verify whether entropy production diverges in the confined case as $D \rightarrow 0$. Furthermore, throughout this chapter I have calculated average values for the observables of interest. A study of higher-order moments, such as fluctuations of the entropy production, would be interesting to consider for future work.

The system studied in this chapter can be interpreted as an autonomous engine extracting work W from a run-and-tumble particle. For such an “active engine”, I studied the extractable power $\dot{W}$, Equation (6.23), and the thermodynamic efficiency η in Section 6.6. Relatively poor efficiencies $\eta < 0.01$ are observed in the case where the particle is strongly confined by the potential, since a current J can be generated only through diffusive fluctuations, Figure 6.13. However, efficiencies η arbitrarily close to 1 are possible for $\gamma \rightarrow 0$ and $D \rightarrow 0$ in the case where right movers are unconfined, $v - f > U'^{[1]}$, but left movers are confined, $v + f < |U'^{[2]}|$, as this prevents left movers from dissipating wasted energy (at least when particles are modelled as “dry” active matter). It would be interesting to calculate the maximum efficiency η of this system in the case of “wet” active matter where momentum is conserved through hydrodynamic interactions.

Finally, in Section 6.7 and Appendix 6.C, I derived the mean first-passage times $\tau_{R,L}(x)$, Equation (6.25), and splitting probabilities $\Pi_{R,L}(x)$, Equation (6.27), for this system under different boundary conditions and explored how they depend on the system’s parameters, Figures 6.16 and 6.17.

CHAPTER 6 APPENDICES

6.A Derivation of steady-state probability densities

To solve the coupled Fokker-Planck equations, Equation (6.3), for the steady-state probability densities $P_{R,L}^{[i]}(x)$, I first rewrite Equation (6.3) as a four-dimensional first-order ODE system for both $i = 1$ and $i = 2$. Introducing $\eta_{R,L}^{[i]}(x) := P_{R,L}^{[i]}(x)$, the steady-state Fokker-Planck equations, i.e. Equation (6.3) with $\partial_t P_{R,L}^{[i]} = 0$, can be rewritten as

$$\mathbf{y}'(x) = \mathbf{A}\mathbf{y}(x), \quad (6.28)$$

where $\mathbf{y}'$ is the derivative of $\mathbf{y}$ with respect to x , and I have defined

$$\mathbf{y}(x) = \begin{pmatrix} P_R^{[i]}(x) \\ \eta_R^{[i]}(x) \\ P_L^{[i]}(x) \\ \eta_L^{[i]}(x) \end{pmatrix} \quad \text{and} \quad \mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{\gamma}{D} & \frac{v-f-U'^{[i]}}{D} & -\frac{\gamma}{D} & 0 \\ 0 & 0 & 0 & 1 \\ -\frac{\gamma}{D} & 0 & \frac{\gamma}{D} & \frac{-v-f-U'^{[i]}}{D} \end{pmatrix}. \quad (6.29)$$

As Equation (6.28) is linear and homogeneous for both $i = 1$ and $i = 2$, I make the ansatz $P_{R,L}^{[i]}(x) = \mathcal{Z}_{R,L}^{[i]} \exp(\lambda^{[i]}x)$, where the $\lambda^{[i]}$ are the eigenvalues of $\mathbf{A}$. After substituting this ansatz into Equation (6.28), the eigenvalues $\lambda^{[i]}$ are found to satisfy a quartic characteristic equation (arising from two coupled quadratic equations),

$$0 = D^2(\lambda^{[i]})^4 + (\lambda^{[i]})^3 \left(2Df + 2DU'^{[i]} \right) + (\lambda^{[i]})^2 \left(-2\gamma D + f^2 + 2fU'^{[i]} + \left(U'^{[i]} \right)^2 - v^2 \right) - \lambda^{[i]} \left(2\gamma f + 2\gamma U'^{[i]} \right). \quad (6.30)$$

The solutions $\lambda^{[i]}$ to Equation (6.30) are too long to display in full. However, one of the solutions to Equation (6.30) is $\lambda^{[i]} = 0$ for both $i \in \{1, 2\}$, and so the general solution to the matrix differential equation (6.28) is

$$P_{R,L}^{[i]}(x) = \mathcal{A}_{R,L}^{[i]} e^{\lambda_{\mathcal{A}}^{[i]}x} + \mathcal{B}_{R,L}^{[i]} e^{\lambda_{\mathcal{B}}^{[i]}x} + \mathcal{C}_{R,L}^{[i]} e^{\lambda_{\mathcal{C}}^{[i]}x} + \mathcal{D}_{R,L}^{[i]}, \quad (6.31)$$

where $\lambda_{\mathcal{A}}^{[i]}, \lambda_{\mathcal{B}}^{[i]}, \lambda_{\mathcal{C}}^{[i]}$ are the other three non-zero solutions (for a given $[i]$) to the quartic equation (6.30).

It remains to calculate the 16 coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$ in Equation (6.31). First, the ratios of the coefficients $\mathcal{A}_R^{[i]}/\mathcal{A}_L^{[i]}$, representing half of the degrees of freedom, are fixed from substituting Equation (6.31) into Equation (6.28) and requiring the resulting prefactor of each linearly independent $\exp(\lambda^{[i]}x)$ term to vanish. This results in

$$\frac{\mathcal{Z}_R^{[i]}}{\mathcal{Z}_L^{[i]}} = \frac{\gamma}{\gamma + (v - f - U'^{[i]}) \lambda_{\mathcal{Z}}^{[i]} - D(\lambda_{\mathcal{Z}}^{[i]})^2}, \quad \text{and} \quad \mathcal{D}_R^{[i]} = \mathcal{D}_L^{[i]}, \quad (6.32)$$

where $\mathcal{Z} \in \{\mathcal{A}, \mathcal{B}, \mathcal{C}\}$. The remaining eight degrees of freedom are fixed through normalisation as well as continuity of the probability densities $P_{R,L}^{[i]}(x)$ and currents $J_{R,L}^{[i]}(x)$, Equation (6.5), for each species across $x = 0$ and $x = a$. Specifically, the continuity conditions are

$$P_{R,L}^{[1]}(0) = P_{R,L}^{[2]}(\ell), \quad (6.33a)$$

$$J_{R,L}^{[1]}(0) = J_{R,L}^{[2]}(\ell), \quad (6.33b)$$

$$P_{R,L}^{[1]}(a) = P_{R,L}^{[2]}(a), \quad (6.33c)$$

$$J_{R,L}^{[1]}(a) = J_{R,L}^{[2]}(a). \quad (6.33d)$$

Finally, we also have the normalisation condition

$$\int_0^a dx \left(P_R^{[1]}(x) + P_L^{[1]}(x) \right) + \int_a^\ell dx \left(P_R^{[2]}(x) + P_L^{[2]}(x) \right) = 1. \quad (6.34)$$

Only 15 of the resulting 16 equations from Equations (6.32) and (6.33) are linearly independent. After removing any one of these equations, the steady-state densities $P_{R,L}^{[i]}(x)$ for RnT particles moving in a piecewise-linear ratchet potential $U(x)$, Equation (6.1), can be obtained in closed form by solving the remaining Equations (6.32), (6.33) and (6.34) for the coefficients $\mathcal{A}_R^{[1]}, \mathcal{A}_L^{[1]}, \mathcal{A}_R^{[2]}, \dots, \mathcal{D}_L^{[2]}$.

6.B Derivation of $D = 0$ steady-state probability densities and currents

Here, I derive the steady-state probability densities $p_{R,L}^{[i]}(x)$ and currents $j_{R,L}^{[i]}(x)$ for $D = 0$. Setting $D = 0$ in Equation (6.3), the coupled Fokker-Planck equations in the absence of diffusion become

$$\frac{\partial p_R^{[i]}(x, t)}{\partial t} = - \left(v - f - U'^{[i]} \right) \frac{\partial p_R^{[i]}(x, t)}{\partial x} - \gamma \left(p_R^{[i]}(x, t) - p_L^{[i]}(x, t) \right), \quad (6.35a)$$

$$\frac{\partial p_L^{[i]}(x, t)}{\partial t} = - \left(-v - f - U'^{[i]} \right) \frac{\partial p_L^{[i]}(x, t)}{\partial x} - \gamma \left(p_L^{[i]}(x, t) - p_R^{[i]}(x, t) \right). \quad (6.35b)$$

The currents for right movers and left movers then become, respectively,

$$j_R^{[i]}(x, t) = \left(v - f - U'^{[i]} \right) p_R^{[i]}(x, t), \quad (6.36a)$$

$$j_L^{[i]}(x, t) = \left(-v - f - U'^{[i]} \right) p_L^{[i]}(x, t). \quad (6.36b)$$

To solve the coupled Fokker-Planck equations (6.35) in the steady state, $\partial_t p_{R,L}^{[i]} = 0$, I again rewrite them in matrix form, i.e.

$$\hat{\mathbf{y}}'(x) = \hat{\mathbf{A}}\hat{\mathbf{y}}(x), \quad (6.37)$$

where

$$\hat{\mathbf{y}}(x) = \begin{pmatrix} p_R^{[i]}(x) \\ p_L^{[i]}(x) \end{pmatrix} \quad \text{and} \quad \hat{\mathbf{A}} = \begin{pmatrix} -\frac{\gamma}{v-f-U'^{[i]}(x)} & \frac{\gamma}{v-f-U'^{[i]}(x)} \\ \frac{\gamma}{-v-f-U'^{[i]}(x)} & -\frac{\gamma}{-v-f-U'^{[i]}(x)} \end{pmatrix}. \quad (6.38)$$

As Equation (6.37) is homogenous, I again make the ansatz $p_{R,L}^{[i]}(x) = \hat{\mathcal{Z}}_{R,L}^{[i]} \exp(\hat{\lambda}^{[i]}x)$, where $\hat{\lambda}^{[i]}$ are the eigenvalues of $\hat{\mathbf{A}}$. The two eigenvalues are found to be

$$\hat{\lambda}_{\mathcal{A}}^{[i]} = \frac{2\gamma (f + U'^{[i]})}{(-v + f + U'^{[i]})(v + f + U'^{[i]})} \quad \text{and} \quad \hat{\lambda}_{\mathcal{B}}^{[i]} = 0. \quad (6.39)$$

The general solutions to the matrix ODE (6.37) are then

$$p_{R,L}^{[1]}(x) = \hat{\mathcal{A}}_{R,L}^{[1]} e^{\hat{\lambda}_{\mathcal{A}}^{[1]}x} + \hat{\mathcal{B}}_{R,L}^{[1]} + \hat{\mathcal{C}}_{R,L} \delta(x), \quad (6.40a)$$

$$p_{R,L}^{[2]}(x) = \hat{\mathcal{A}}_{R,L}^{[2]} e^{\hat{\lambda}_{\mathcal{A}}^{[2]}x} + \hat{\mathcal{B}}_{R,L}^{[2]}, \quad (6.40b)$$

where the term proportional to $\delta(x)$ in Equation (6.40a) has been added to account for the possibility of particles becoming trapped at $x = 0$ in the absence of diffusion. There are 10 coefficients $\hat{\mathcal{A}}_R^{[1]}, \hat{\mathcal{A}}_L^{[1]}, \hat{\mathcal{A}}_R^{[2]}, \dots, \hat{\mathcal{B}}_L^{[2]}, \hat{\mathcal{C}}_R, \hat{\mathcal{C}}_L$ in Equation (6.40), but only 9 of these need to be fixed at any given time since $\hat{\mathcal{C}}_R$ and $\hat{\mathcal{C}}_L$ are both non-zero *only* in the case where the particle is completely confined, i.e. $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$. In this case, the solutions are trivially given by $p_{R,L}(x) = \delta(x)/2$. Therefore, to fix the 9 coefficients that are non-zero, I first substitute Equation (6.40) into the Fokker-Planck equation (6.35), and require the resulting prefactor of each linearly independent $\exp(\hat{\lambda}^{[i]}x)$ to vanish, resulting in

$$\frac{\hat{\mathcal{A}}_R^{[i]}}{\hat{\mathcal{A}}_L^{[i]}} = \frac{\gamma}{\gamma + (v - f - U'^{[i]}(x))\hat{\lambda}_{\mathcal{A}}^{[i]}} \quad \text{and} \quad \hat{\mathcal{B}}_R^{[i]} = \hat{\mathcal{B}}_L^{[i]}, \quad (6.41)$$

and leaving 5 degrees of freedom to fix.

Continuity in the densities $p_{R,L}^{[i]}(x)$ is no longer a viable condition to fix the degrees of freedom since the absence of diffusion ceases to smooth out the solutions to Equation (6.37), resulting in the densities becoming discontinuous at $x = 0$ and $x = a$. The form of the solutions depends on the relations between the self-propulsion v and the slopes of the potential, $U'^{[1]} = h/a$ and $U'^{[2]} = -h/(\ell - a)$, in particular whether or not the particle is confined. For instance, the particle could climb over both slopes of the potential, i.e. $v - f > U'^{[1]}$ and $v + f > |U'^{[2]}|$, only one slope, $v - f > U'^{[1]}$ or $v + f > |U'^{[2]}|$, or be completely confined, $v - f < U'^{[1]}$ and $v + f < |U'^{[2]}|$. At $x = 0$, if the particle is confined by the barrier to the left, $v + f < |U'^{[2]}|$, then there is a $\delta(x)$ contribution to the left-moving density $p_L^{[1]}(x)$ with prefactor $\hat{\mathcal{C}}_L$. A tumbling event from a left mover to a right mover thus results in an instantaneous contribution $\gamma \hat{\mathcal{C}}_L$ to the right-moving current $j_R^{[1]}(x)$ at $x = 0$. Similarly, if the particle were instead confined to the right, $v - f < U'^{[1]}$, then there would be a $\delta(x)$ contribution to the right-moving density $p_R^{[1]}(x)$ with prefactor $\hat{\mathcal{C}}_R$, and therefore a contribution $-\gamma \hat{\mathcal{C}}_R$ to the left-moving current $j_L^{[1]}(x)$ at $x = 0$. Hence, in the case where the particle is confined only to the left, $v + f < |U'^{[2]}|$ and $v - f > U'^{[1]}$,

the continuity conditions are

$$j_R^{[1]}(0) = j_R^{[2]}(\ell) + \gamma \hat{\mathcal{C}}_L, \quad (6.42a)$$

$$j_R^{[1]}(a) = j_R^{[2]}(a), \quad (6.42b)$$

$$p_L^{[1]}(a) = 0, \quad (6.42c)$$

$$p_L^{[2]}(a) = 0, \quad (6.42d)$$

where, since the particle cannot cross the left barrier, there is no contribution to the left-moving probability density $p_L(x)$ at $x = a$. Similarly, in the case where the particle is instead confined only to the right, $v + f > |U'^{[2]}|$ and $v - f < U'^{[1]}$, the continuity conditions are

$$j_L^{[1]}(0) = j_L^{[2]}(\ell) - \gamma \hat{\mathcal{C}}_R, \quad (6.43a)$$

$$j_L^{[1]}(a) = j_L^{[2]}(a), \quad (6.43b)$$

$$p_R^{[1]}(a) = 0, \quad (6.43c)$$

$$p_R^{[2]}(a) = 0. \quad (6.43d)$$

Finally, if the particle can overcome both barriers, $v - f > U'^{[1]}$ and $v + f > |U'^{[2]}|$, then the continuity conditions are

$$j_{R,L}^{[1]}(0) = j_{R,L}^{[2]}(\ell), \quad (6.44a)$$

$$j_{R,L}^{[1]}(a) = j_{R,L}^{[2]}(a). \quad (6.44b)$$

The remaining degree of freedom is then fixed through the normalisation condition,

$$\int_0^a dx \left(p_R^{[1]}(x) + p_L^{[1]}(x) \right) + \int_a^\ell dx \left(p_R^{[2]}(x) + p_L^{[2]}(x) \right) = 1. \quad (6.45)$$

The net current $j = j_R(x) + j_L(x)$ has a closed-form expression that is compact enough to be written down. In the case where the particle is unconfined and therefore able to cross both barriers, $v + f > |U'^{[2]}|$ and $v - f > U'^{[1]}$, the current is given by

$$j_{\leftrightarrow} = \frac{2\gamma(af + h)^2(af - f\ell + h)^2 (e^{\kappa + \delta\ell} - e^{\delta a})}{\theta(e^{\delta a} - e^{\kappa + \delta\ell}) + h^2\ell^2v^2(e^{\kappa} - 1)(e^{\delta a} - e^{\delta\ell})}, \quad (6.46)$$

where

$$\delta = \frac{2\gamma(a - \ell)(af - f\ell + h)}{(af - f\ell + h)^2 - v^2(a - \ell)^2}, \quad (6.47a)$$

$$\kappa = \frac{2\gamma a^2(af + h)}{(af + h)^2 - a^2v^2}, \quad (6.47b)$$

$$\theta = 2\gamma\ell(af + h)(af - f\ell + h)(a(af + 2h) - \ell(af + h)). \quad (6.47c)$$

However, when the particle is confined only to the left, $v + f < |U'^{[2]}|$ and $v - f > U'^{[1]}$, the current is given by

$$j_{\nrightarrow} = \frac{2\gamma(af + h)^2(af - f\ell + h)^2}{\tilde{\theta}_1 e^{-\kappa} + \tilde{\theta}_2 e^{\delta(\ell-a)} + \tilde{\theta}_3 - \theta}, \quad (6.48)$$

where

$$\tilde{\theta}_1 = (af - f\ell + h)^2(a(f + v) + h)^2, \quad (6.49a)$$

$$\tilde{\theta}_2 = -(af + h)^2(h + (a - \ell)(f + v))^2, \quad (6.49b)$$

$$\tilde{\theta}_3 = h\ell^2 v^2(2af + h) - 2h\ell v(af + h)(af + h - f\ell) - 2h\ell av^2(af + h). \quad (6.49c)$$

Finally, the net current $j_{\nrightarrow}$ in the case where the particle is confined only to the right, $v + f > |U'^{[2]}|$ and $v - f < U'^{[1]}$, can be found by inverting the overall sign in Equation (6.48) and replacing $a \rightarrow \ell - a$ in Equations (6.47), (6.48), and (6.49) above.

6.C Derivation of first-passage properties

6.C.a Mean first-passage times

As the coupled ODEs for the mean first-passage time $\tau_{R,L}^{[i]}(x)$, Equation (6.24), are similar to the coupled Fokker-Planck equations (6.3) for the steady-state probability density $P_{R,L}^{[i]}(x)$, the procedure for solving Equation (6.24) follows similarly to solving Equation (6.3) in Appendix 6.A. However, Equation (6.24) is non-homogeneous and so one must also find a particular solution satisfying the equation. Again, Equation (6.24) can be rewritten as a four-dimensional system of first-order ODEs for both $i = 1$ and $i = 2$. As in the previous appendices, introducing $\tilde{\eta}_{R,L}^{[i]}(x) = \tau_{R,L}^{\prime[i]}(x)$ allows Equation (6.24) to be written as

$$\tilde{\mathbf{y}}'(x) = \tilde{\mathbf{A}}\tilde{\mathbf{y}}(x) + \tilde{\mathbf{b}} \quad (6.50)$$

where

$$\tilde{\mathbf{y}}(x) = \begin{pmatrix} \tau_R^{[i]}(x) \\ \tilde{\eta}_R^{[i]}(x) \\ \tau_L^{[i]}(x) \\ \tilde{\eta}_L^{[i]}(x) \end{pmatrix}, \quad \tilde{\mathbf{A}} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{\gamma}{D} & \frac{-v+f+U'^{[i]}}{D} & -\frac{\gamma}{D} & 0 \\ 0 & 0 & 0 & 1 \\ -\frac{\gamma}{D} & 0 & \frac{\gamma}{D} & \frac{v+f+U'^{[i]}}{D} \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{b}} = \begin{pmatrix} -1 \\ 0 \\ -1 \\ 0 \end{pmatrix}. \quad (6.51)$$

First, the solution to the homogeneous equation is found by substituting the ansatz $\tau_{R,L}^{[i]}(x) = \tilde{\mathcal{Z}}_{R,L}^{[i]} \exp(\tilde{\lambda}^{[i]}x)$ into Equation (6.50) to obtain a quartic equation for the eigenvalues $\tilde{\lambda}^{[i]}$,

$$0 = D^2(\tilde{\lambda}^{[i]})^4 - (\tilde{\lambda}^{[i]})^3 \left(2Df + 2DU'^{[i]} \right) + (\tilde{\lambda}^{[i]})^2 \left(-2\gamma D + f^2 + 2fU'^{[i]} + \left(U'^{[i]} \right)^2 - v^2 \right) + \tilde{\lambda}^{[i]} \left(2\gamma f + 2\gamma U'^{[i]} \right), \quad (6.52)$$

which differs to Equation (6.30) only in the sign of the eigenvalues, i.e. $\lambda^{[i]} \rightarrow -\tilde{\lambda}^{[i]}$. As in Appendix 6.A, one eigenvalue for each of $i = 1$ and $i = 2$ vanishes and so the solution to the homogeneous part of Equation (6.50) has the same form as for $P_{R,L}^{[i]}(x)$ in Equation (6.31), i.e.

$$\tau_{R,L}^{[i]} \Big|_{\text{H}}(x) = \tilde{\mathcal{A}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{A}}^{[i]} x} + \tilde{\mathcal{B}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{B}}^{[i]} x} + \tilde{\mathcal{C}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{C}}^{[i]} x} + \tilde{\mathcal{D}}_{R,L}^{[i]}. \quad (6.53)$$

Next, it is easily verified that the particular solution satisfies

$$\tau_{R,L}^{[i]} \Big|_{\text{P}}(x) = \tilde{\mathcal{E}}_{R,L}^{[i]} x + \tilde{\mathcal{F}}_{R,L}^{[i]}, \quad (6.54)$$

and after substituting Equation (6.54) into Equation (6.50), one obtains

$$(v - f - U'^{[i]}) \tilde{\mathcal{E}}_R^{[i]} - \gamma(\tilde{\mathcal{E}}_R^{[i]} x + \tilde{\mathcal{F}}_R^{[i]} - \tilde{\mathcal{E}}_L^{[i]} x - \tilde{\mathcal{F}}_L^{[i]}) = 0, \quad (6.55a)$$

$$(-v - f - U'^{[i]}) \tilde{\mathcal{E}}_L^{[i]} - \gamma(\tilde{\mathcal{E}}_L^{[i]} x + \tilde{\mathcal{F}}_L^{[i]} - \tilde{\mathcal{E}}_R^{[i]} x - \tilde{\mathcal{F}}_R^{[i]}) = 0. \quad (6.55b)$$

As Equations (6.55a) and (6.55b) are valid for all $x \in [0, \ell]$, then equating terms linear in x yields

$$\tilde{\mathcal{E}}_R^{[i]} = \tilde{\mathcal{E}}_L^{[i]}, \quad (6.56)$$

and equating the remaining terms gives

$$(v - f - U'^{[i]}) \tilde{\mathcal{E}}_R^{[i]} - \gamma(\tilde{\mathcal{F}}_R^{[i]} - \tilde{\mathcal{F}}_L^{[i]}) = 0, \quad (6.57a)$$

$$(-v - f - U'^{[i]}) \tilde{\mathcal{E}}_L^{[i]} - \gamma(\tilde{\mathcal{F}}_L^{[i]} - \tilde{\mathcal{F}}_R^{[i]}) = 0. \quad (6.57b)$$

Adding Equations (6.57a) and (6.57b), then combining with Equation (6.56), yields

$$\tilde{\mathcal{E}}_R^{[i]} = \tilde{\mathcal{E}}_L^{[i]} = \frac{1}{f + U'^{[i]}}. \quad (6.58)$$

Absorbing the constant $\tilde{\mathcal{F}}_{R,L}^{[i]}$ into $\tilde{\mathcal{D}}_{R,L}^{[i]}$, the full solution to Equation (6.50) is therefore

$$\tau_{R,L}^{[i]}(x) = \tau_{R,L}^{[i]} \Big|_{\text{H}}(x) + \tau_{R,L}^{[i]} \Big|_{\text{P}}(x) = \tilde{\mathcal{A}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{A}}^{[i]} x} + \tilde{\mathcal{B}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{B}}^{[i]} x} + \tilde{\mathcal{C}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{C}}^{[i]} x} + \tilde{\mathcal{D}}_{R,L}^{[i]} + \frac{x}{f + U'^{[i]}}. \quad (6.59)$$

As for the probability densities $P_{R,L}^{[i]}(x)$ in Appendix 6.A, the ratios $\tilde{\mathcal{Z}}_R^{[i]}/\tilde{\mathcal{Z}}_L^{[i]}$, where $\tilde{\mathcal{Z}} \in \{\tilde{\mathcal{A}}, \tilde{\mathcal{B}}, \tilde{\mathcal{C}}, \tilde{\mathcal{D}}\}$, are fixed by requiring each linearly independent term in Equation (6.59) to satisfy Equation (6.50), resulting in

$$\frac{\tilde{\mathcal{Z}}_R^{[i]}}{\tilde{\mathcal{Z}}_L^{[i]}} = \frac{\gamma}{\gamma - (v - f - U'^{[i]}) \tilde{\lambda}_{\tilde{\mathcal{Z}}}^{[i]} - D(\tilde{\lambda}_{\tilde{\mathcal{Z}}}^{[i]})^2}, \quad \text{and} \quad \tilde{\mathcal{D}}_R^{[i]} = \tilde{\mathcal{D}}_L^{[i]}. \quad (6.60)$$

The remaining degrees of freedom are then fixed from the boundary conditions and con-

tinuity conditions,

$$\tau_{R,L}^{[1]}(0) = 0, \quad (6.61a)$$

$$\tau_{R,L}^{[1]}(a) = \tau_{R,L}^{[2]}(a), \quad (6.61b)$$

$$\left. \frac{d\tau_{R,L}^{[1]}(x)}{dx} \right|_{x=a} = \left. \frac{d\tau_{R,L}^{[2]}(x)}{dx} \right|_{x=a}, \quad (6.61c)$$

and

$$(i) \quad \tau_{R,L}^{[2]}(\ell) = 0, \quad \text{or} \quad (ii) \quad \left. \frac{d\tau_{R,L}^{[2]}(x)}{dx} \right|_{x=\ell} = 0, \quad (6.61d)$$

depending on whether the system has (i) an absorbing boundary or (ii) a reflecting boundary at $x = \ell$ (see, for instance, Ref. [201]).

6.C.b Splitting probabilities

To derive the splitting probabilities $\Pi_{R,L}^{[i]}(x)$, I define $\check{\eta}_{R,L}^{[i]}(x) = \Pi_{R,L}^{[i]}(x)$ and $\check{\mathbf{y}}(x) = (\pi_R^{[i]}(x), \check{\eta}_R^{[i]}(x), \pi_L^{[i]}(x), \check{\eta}_L^{[i]}(x))$ such that the governing equations (6.26) for the splitting probabilities $\Pi_{R,L}^{[i]}(x)$ can be written as a four-dimensional system of first-order ODEs, $\check{\mathbf{y}}'(x) = \tilde{\mathbf{A}}\check{\mathbf{y}}(x)$, where $\tilde{\mathbf{A}}$ is the same operator acting on the mean first-passage times $\tau_{R,L}^{[i]}(x)$ and is defined in Equation (6.51). Thus, the splitting probabilities $\Pi_{R,L}^{[i]}(x)$ obey the same (backward) equations as for that of the mean first-passage times $\tau_{R,L}^{[i]}(x)$, Equations (6.50)–(6.51), aside from being homogeneous, i.e. $\tilde{\mathbf{b}} = \mathbf{0}$. Hence, the splitting probabilities have the same form of general solution as for the homogeneous part to the mean first-passage times, Equation (6.53), but with different coefficients, i.e.

$$\Pi_{R,L}^{[i]}(x) = \check{\mathcal{A}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{A}}^{[i]} x} + \check{\mathcal{B}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{B}}^{[i]} x} + \check{\mathcal{C}}_{R,L}^{[i]} e^{\tilde{\lambda}_{\mathcal{C}}^{[i]} x} + \check{\mathcal{D}}_{R,L}^{[i]}, \quad (6.62)$$

where the eigenvalues $\tilde{\lambda}^{[i]}$ are the same as those obtained through solving Equation (6.52) and the ratios $\check{\mathcal{Z}}_{R,L}^{[i]}/\check{\mathcal{Z}}_L^{[i]}$, where $\check{\mathcal{Z}} \in \{\check{\mathcal{A}}, \check{\mathcal{B}}, \check{\mathcal{C}}, \check{\mathcal{D}}\}$, also satisfy equations analogous to that of the mean first-passage times $\tau_{R,L}^{[i]}(x)$, i.e. Equation (6.60). The remaining degrees of freedom in the general solution for the splitting probabilities $\Pi_{R,L}^{[i]}(x)$, Equation (6.62), are fixed from the boundary conditions and continuity conditions,

$$\Pi_{R,L}^{[1]}(0) = 1, \quad (6.63a)$$

$$\Pi_{R,L}^{[2]}(\ell) = 0, \quad (6.63b)$$

$$\Pi_{R,L}^{[1]}(a) = \Pi_{R,L}^{[2]}(a), \quad (6.63c)$$

$$\left. \frac{d\Pi_{R,L}^{[1]}(x)}{dx} \right|_{x=a} = \left. \frac{d\Pi_{R,L}^{[2]}(x)}{dx} \right|_{x=a}, \quad (6.63d)$$

recalling that $\Pi_{R,L}(x)$ is defined to be the splitting probabilities for a right/left mover to exit at the *left*-hand boundary of the system at $x = 0$.

6.C.c Conditional splitting probabilities

The splitting probabilities $\Pi_{R,L}^{[i]}(x)$ calculated above can be generalised to be conditioned on the particle's self-propulsion state as it exits the interval. Following the calculation in Ref. [54], I define $\pi_{X|Y}(x_0)$ as the “conditional splitting probability” for a particle initialised in state $Y \in \{R, L\}$ at $x = x_0$ to leave through the left-hand boundary at $x = 0$ in the self-propulsion state $X \in \{R, L\}$. Hence, there are four conditional splitting probabilities that exist for each boundary, obtained from every possible permutation of $X, Y \in \{R, L\}$. Introducing $\check{\eta}_{X|Y}^{[i]}(x) = \pi'_{X|Y}^{[i]}(x)$, the conditional splitting probabilities satisfy $\check{\mathbf{y}}'_{R,L}(x) = \tilde{\mathbf{A}}\check{\mathbf{y}}_{R,L}(x)$ where $\tilde{\mathbf{A}}$ is the same operator, defined in Equation (6.51), acting on the “unconditional” splitting probabilities $\Pi_{R,L}^{[i]}(x)$ and mean first-passage times $\tau_{R,L}^{[i]}(x)$, and $\check{\mathbf{y}}_{R,L}(x) = (\pi_{R,L|R}^{[i]}(x), \check{\eta}_{R,L|R}^{[i]}(x), \pi_{R,L|L}^{[i]}(x), \check{\eta}_{R,L|L}^{[i]}(x))$. Hence, the conditional splitting probabilities satisfy two different sets of coupled ODEs, one for each conditional exit state. As these ODEs are the same as for that of the unconditional splitting probabilities, Equation (6.26), they thus have the same general solution given in Equation (6.62), i.e.

$$\pi_{X|Y}^{[i]}(x) = \check{\mathcal{A}}_{X|Y}^{[i]} e^{\tilde{\lambda}_{\mathcal{A}}^{[i]} x} + \check{\mathcal{B}}_{X|Y}^{[i]} e^{\tilde{\lambda}_{\mathcal{B}}^{[i]} x} + \check{\mathcal{C}}_{X|Y}^{[i]} e^{\tilde{\lambda}_{\mathcal{C}}^{[i]} x} + \check{\mathcal{D}}_{X|Y}^{[i]}, \quad (6.64)$$

where $X, Y \in \{R, L\}$ and the eigenvalues $\tilde{\lambda}^{[i]}$ are found by solving Equation (6.52). The coefficients $\check{\mathcal{A}}_{X|Y}^{[1]}, \check{\mathcal{A}}_{X|Y}^{[2]}, \dots, \check{\mathcal{D}}_{X|Y}^{[2]}$ are fixed in the same manner as for the mean first-passage times $\tau_{R,L}^{[i]}(x)$ and splitting probabilities $\Pi_{R,L}^{[i]}(x)$ above, by requiring each linearly independent term to satisfy the ODEs before applying boundary conditions and continuity conditions. The boundary conditions of the ODEs are

$$\pi_{R|R}^{[1]}(0) = \pi_{L|L}^{[1]}(0) = 1, \quad (6.65a)$$

$$\pi_{R|L}^{[1]}(0) = \pi_{L|R}^{[1]}(0) = 0, \quad (6.65b)$$

$$\pi_{R|R}^{[2]}(\ell) = \pi_{L|L}^{[2]}(\ell) = 0, \quad (6.65c)$$

$$\pi_{R|L}^{[2]}(\ell) = \pi_{L|R}^{[2]}(\ell) = 0, \quad (6.65d)$$

and the continuity conditions are analogous to that of the unconditional splitting probabilities in Equation (6.63), i.e.

$$\pi_{R,L|R}^{[1]}(a) = \pi_{R,L|R}^{[2]}(a), \quad (6.66a)$$

$$\pi_{R,L|L}^{[1]}(a) = \pi_{R,L|L}^{[2]}(a), \quad (6.66b)$$

$$\left. \frac{d\pi_{R,L|R}^{[1]}(x)}{dx} \right|_{x=a} = \left. \frac{d\pi_{R,L|R}^{[2]}(x)}{dx} \right|_{x=a}, \quad (6.66c)$$

$$\left. \frac{d\pi_{R,L|L}^{[1]}(x)}{dx} \right|_{x=a} = \left. \frac{d\pi_{R,L|L}^{[2]}(x)}{dx} \right|_{x=a}. \quad (6.66d)$$

7

Optimising work extraction from active particles

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L. Cocconi, J. Knight, and C. Roberts. Optimal power extraction from active particles with hidden states, *Physical Review Letters* **131**, 188301 (2023) [54].

The necessary permissions to reproduce this publication as part of my thesis are included in Appendices B.1.1, B.2.2, and B.2.5.

Author contributions to original manuscript: LC supervised the project, performed the bulk of the main derivation, and wrote the bulk of the manuscript. JK performed the simulations of the boundary-update protocol and derived exact expressions for the conditional moments of the active Ornstein-Uhlenbeck particle in Appendix 7.E. I studied the conditional splitting probabilities as a method of predicting a run-and-tumble particle’s hidden internal state, derived the exact expressions for the conditional splitting probabilities, and compared these against simulations. LC and I derived the positional moments for the canonical active particles in harmonic potentials in Appendix 7.C. All authors contributed to the formulation of the boundary-update protocol, interpretation of the results, and editing of the manuscript.

Chapter summary

Equipped with a thorough overview of work extraction from active particles, this chapter now aims to identify generic protocols that achieve *optimal* power extraction from a single active particle subject to continuous feedback control. This is under the assumption that the particle’s spatial trajectory, but *not* its instantaneous self-propulsion force, is accessible to direct observation. The central protocol is based on a Bayesian approach which draws on the Onsager-Machlup path integral formalism and is exemplified in the cases of free run-and-tumble and active Ornstein-Uhlenbeck dynamics in one dimension. This protocol establishes an upper bound on the power output and suggests that positive work extraction is possible even in models characterised by time-symmetric positional trajectories and thus vanishing informational entropy production rates. This bound is verified by an independent (and novel) “boundary-update” protocol and is arguably that with which the performance of *realistic* active matter engines should be compared.

7.1 Introduction

Macroscopic living creatures such as horses and oxen have been utilised by humans for millennia to do useful work. A question of current theoretical and practical interest is the extent to which energy can be efficiently harvested from *microscopic* active systems [51, 202–206], whose motion is subject to non-negligible noise. The efficiency of existing many-particle microscopic active matter engines is heavily limited by the difficulty of rectifying the incoherent motion of collections of individual swimmers with weak alignment interactions in the bulk [50, 207, 208]. Even under idealised conditions, where individual active particles can be manipulated independently, strict upper bounds on extractable power are not well understood, particularly when only a subset of the observables characterising active motion are accessible to direct observation [22, 209, 210]. In this chapter, I present a generic framework for the identification of continuous-feedback protocols achieving optimal power extraction from a single active particle under the assumption that its instantaneous net velocity, $\dot{x}(t)$, but *not* its fluctuating self-propulsion, $w(t)$, is observable. In other words, the dynamics are non-Markovian. This is typically the case for realistic active matter engines, such as in Refs. [50, 51]. The Bayesian approach, which draws on the Onsager-Machlup path integral formalism [211], applies to a generic stochastic self-propulsion process and is illustrated in the cases of free run-and-tumble (RnT) [42] and active Ornstein-Uhlenbeck (AOU) [73] dynamics in one dimension, see Chapter 2. Both models are characterised by time-symmetric positional trajectories (see Appendix 7.A) and thus vanishing informational entropy production rates (iEPRs) [212, 213], defined as the Kullback-Leibler divergence [40] per unit time of the ensemble of forward paths and their time-reversed counterparts [214, 215].

In the Markovian case, where all degrees of freedom are observable, the iEPR of these active particle models is proportional to the thermodynamic dissipation and thus provides a (loose) upper bound to the extractable power. This relation fails to apply in the presence of hidden states [210, 216, 217]. Indeed, this chapter demonstrates that positive average power extraction remains possible even for vanishing iEPR upon Bayesian inference of the hidden state (cf. [44], where it is argued that vanishing local iEPR implies zero extractable work). Finally, of note is that the measurement-driven protocols of the type discussed in the following incur a thermodynamic maintenance cost [218, 219], but are not constrained by Landauer’s principle in the same way as equilibrium information engines [206, 220].

7.2 Definition of the optimal protocol

Consider the overdamped Langevin equation for a generic active particle (see Chapter 2),

$$\dot{x}(t) = w(t) + F_{\text{ext}}(t) + \sqrt{2D_x}\xi(t), \quad (7.1)$$

where $\xi(t)$ is Gaussian white noise of unit covariance with associated diffusivity D_x , and $w(t)$ is a stochastic self-propulsion velocity, which for the time being I take to be measurable by an external observer tasked with controlling the external force $F_{\text{ext}}(t)$. In practice,

$F_{\text{ext}}(t)$ could be implemented using an optical trap [220] or, for a charged active colloid [221], using an external electric field of time-varying magnitude and direction. Positive average work is readily extracted by applying an external force $F_{\text{ext}}(t)$ smaller than and opposite to the particle's self-propulsion [21, 50, 51]. Over a time duration T , this generates a noise-averaged total work by the particle against the known external force, given by

$$\mathbb{E}_{\xi}[W_{\text{tot}}[F_{\text{ext}}]] = - \int_0^T dt F_{\text{ext}}(t) \mathbb{E}_{\xi}[\dot{x}(t)] = - \int_0^T dt F_{\text{ext}}(t)(w(t) + F_{\text{ext}}(t)), \quad (7.2)$$

which constitutes the key observable of a hypothetical experiment. Above and henceforth, $\mathbb{E}_{\phi}[\bullet]$ is used to denote an average with respect to the steady-state distribution of the random variable ϕ . I will subsequently refer to $F_{\text{ext}}(t)$ as “the protocol”. The integrand of Equation (7.2), corresponding to the instantaneous power output, can be maximised at each time t by applying the protocol $F_{\text{ext}}^*(t) = -w(t)/2$. The corresponding steady-state average power output is

$$\lim_{T \rightarrow \infty} \frac{\mathbb{E}_{\xi}[W_{\text{tot}}[F_{\text{ext}}]]}{T} = \frac{\bar{w}^2}{4} + \frac{\mathbb{E}_w[(w(t) - \bar{w})^2]}{4}, \quad (7.3)$$

where $\bar{w} := \mathbb{E}_w[w(t)]$, and ergodicity has been invoked to convert time averages to ensemble averages. I will henceforth refer to protocols $F_{\text{ext}}^*(t)$ achieving the maximum average power output allowed under a particular set of constraints as *optimal*.

Consider now the case where the underlying dynamics of the active particle (in the form of the full set of governing equations) are known but the instantaneous self-propulsion velocity $w(t)$ is not accessible to direct observation, i.e. it is a hidden variable. Naïvely, this suggests positive work extraction is unattainable since there is no immediate indication of which direction and magnitude should be chosen for $F_{\text{ext}}(t)$. However, since $w(t)$ can be partially inferred from the history of $x(t)$, positive work can be extracted during transient periods of persistent motion. To see this, let $\mathbb{P}(w(T) = v | \{x\}_0^T)$ denote the posterior probability density that the instantaneous self-propulsion velocity of the active particle at current time T equals v given a particular spatial trajectory $\{x\}_0^T$ has been observed. The expected work extracted during a time window of duration T can be expressed as the following functional of the generic protocol $F_{\text{ext}}(t)$,

$$\mathbb{E}_{\xi, w}[W_{\text{tot}}[F_{\text{ext}}]] = - \int_0^T dt \int_{-\infty}^{\infty} dv \mathbb{P}(v | \{x\}_0^t) F_{\text{ext}}(t)(v + F_{\text{ext}}(t)). \quad (7.4)$$

The optimal protocol $F_{\text{ext}}^*(t)$ is obtained from $\delta \mathbb{E}_{\xi, w}[W_{\text{tot}}[F_{\text{ext}}]] / \delta F_{\text{ext}}|_{F_{\text{ext}}^*} = 0$, whence

$$F_{\text{ext}}^*(T) = -\frac{1}{2} \int_{-\infty}^{\infty} dv \mathbb{P}(v | \{x\}_0^T) v = -\frac{\mathbb{E}_w[w(T) | \{x\}_0^T]}{2}, \quad (7.5)$$

where $\mathbb{E}_w[w(T) | \{x\}_0^T]$ denotes the posterior expectation of the self-propulsion velocity with respect to $\mathbb{P}(v | \{x\}_0^T)$. This is not to be confused with the expectation of $w(T)$ taken with

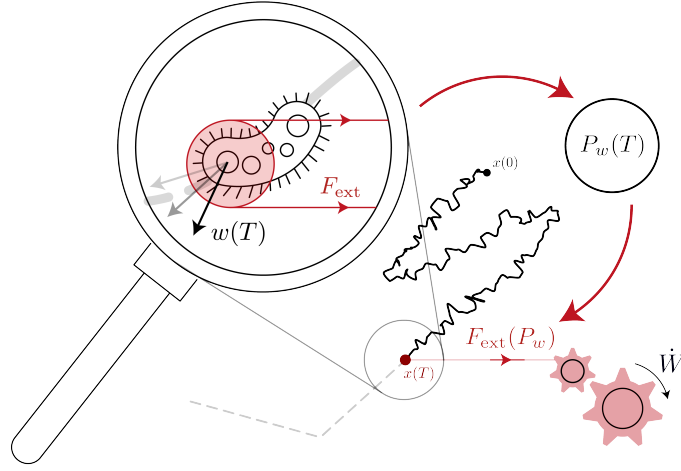


Figure 7.1: Optimal power extraction from an active particle (here visualised as a bacterium) with hidden self-propulsion velocity is achieved by subjecting the latter to continuous feedback control, whereby the magnitude and direction of the protocol $F_{\text{ext}}(t)$ are modulated according to the inferred self-propulsion velocity. [Figure credit: Luca Cocconi].

respect to the corresponding prior probability $\mathbb{P}(v) = \int \mathcal{D}x \mathbb{P}(v|\{x\}_0^T) \mathbb{P}(\{x\}_0^T)$, which is denoted $\bar{w}$ and assumed to be independent of T . Substituting the optimal protocol, Equation (7.5), into the expression for the instantaneous power output, the integrand in Equation (7.4) gives

$$\mathbb{E}_{\xi, w}[\dot{W}[F_{\text{ext}}^*(t)]] = \frac{\bar{w}^2}{4} + \frac{\mathbb{E}_w[(w(T) - \bar{w})|\{x\}_0^T]^2}{4}, \quad (7.6)$$

cf. Equation (7.3). In the following, I take $\bar{w} = 0$ to focus on the non-trivial term appearing on the right-hand side of Equation (7.6). Figure 7.1 schematises the idea of the feedback control described above.

7.3 Warm-up: The run-and-tumble particle

The problem of identifying the optimal protocol has been reduced to the evaluation of the posterior expectation $\mathbb{E}_w[w(T)|\{x\}_0^T]$, Equation (7.5). Now, I proceed to show how this can be done for the case of RnT motion in one dimension,

$$\dot{x}(t) = \nu w(t) + F_{\text{ext}}(t) + \sqrt{2D_x} \xi(t), \quad (7.7)$$

where ν is the magnitude of the self-propulsion, which has a binary internal self-propulsion $w(t)$ that constitutes the simplest example of a state-space amenable to non-trivial coarse graining.

In particular, let $w(t) \in \{-1, 1\}$ be a dimensionless telegraphic noise with symmetric transition rate α . Identification of the optimal protocol requires the posterior probability that the particle is a right self-propeller, $w(T) = +1$, given its positional trajectory up to the current time T , which I denote $P_+(T) = \mathbb{P}[w(T) = +1|\{x\}_0^T]$ for compactness.

The complementary probability is denoted $P_-(T) = \mathbb{P}[w(T) = -1|\{x\}_0^T]$. Defining the *confidence parameter* $Q[\{x\}_0^T] = \log(P_+(T)/P_-(T))$ and using $P_+(T) + P_-(T) = 1$, one can write

$$P_+(T) = \frac{e^Q}{1+e^Q} = \frac{1}{2} + \frac{e^Q - 1}{2(1+e^Q)}. \quad (7.8)$$

Equation (7.8) reduces to the prior probability $P_+ = 1/2$ when $Q = 0$. To calculate $P_+(T)$ via Q one thus needs to find an expression for the ratio of the conditional path probabilities. To do so, I first invoke Bayes' theorem,

$$\mathbb{P}[w(T) = \pm 1|\{x\}_0^T] = \frac{\mathbb{P}[\{x\}_0^T|w(T) = \pm 1]}{2\mathbb{P}[\{x\}_0^T]}, \quad (7.9)$$

where I have used $\mathbb{P}[w(T) = \pm 1] = 1/2$. Thus, the confidence parameter can be rewritten as

$$Q[\{x\}_0^T] = \log \frac{\mathbb{P}[\{x\}_0^T|w(T) = +1]}{\mathbb{P}[\{x\}_0^T|w(T) = -1]}, \quad (7.10)$$

reminiscent of a stochastic entropy [215]. I now introduce the notation for the average with respect to the distribution of $w(t)$ path probabilities conditioned on a particular final value $w(T)$,

$$\overline{\bullet}^{(v)} := \int \mathcal{D}w \bullet \mathbb{P}[\{w(t)\}_0^T|w(T) = v], \quad (7.11)$$

which allows one to express the path probabilities in Equation (7.10) as

$$\mathbb{P}[\{x\}_0^T|w(T) = +1] = \overline{\mathbb{P}[\{x\}_0^T|\{w\}_0^T]}^{(+1)}, \quad (7.12a)$$

$$\mathbb{P}[\{x\}_0^T|w(T) = -1] = \overline{\mathbb{P}[\{x\}_0^T|\{w\}_0^T]}^{(-1)}. \quad (7.12b)$$

Finally, I invoke the Onsager-Machlup path integral form [211] of the conditional path probability in the Stratonovich discretisation (such that the normal rules of calculus apply)

$$\mathbb{P}[\{x\}_0^T|\{w\}_0^T] \propto \exp\left(-\frac{1}{4D_x} \int_0^T dt (\dot{x}_c(t) - \nu w(t))^2\right), \quad (7.13)$$

where $\dot{x}_c = \dot{x} - F_{\text{ext}}$ denotes the velocity in the reference frame where the externally imposed drift from the protocol is subtracted away. Substituting Equation (7.13) into Equation (7.12), combining the resulting expressions with Equation (7.10), and cancelling common $w(t)$ -independent factors appearing in the numerator and denominator, results in

$$\begin{aligned} Q[\{x\}_0^T] = & \log \left(\overline{\exp\left(\frac{\nu}{2D_x} \int_0^T dt \dot{x}_c(t)w(t)\right)}^{(+1)} \right) \\ & - \log \left(\overline{\exp\left(\frac{\nu}{2D_x} \int_0^T dt \dot{x}_c(t)w(t)\right)}^{(-1)} \right), \end{aligned} \quad (7.14)$$

where I have also used $w^2(t) = 1$ for all $t \in [0, T]$. To make further progress, one can exploit the identity between the logarithm of a moment-generating function and its cumulant-generating function [105, 108], as well as the parity of the cumulants (see Appendix 7.B). This leads to

$$Q[\{x\}_0^T] = \sum_{n \text{ odd}}^{\infty} \frac{\text{Pe}^n}{2^{n-1}n!} \overline{Y^n[\{x\}_0^T]}^{(+1),c}, \quad (7.15)$$

with Péclet number $\text{Pe} = \nu^2/(D_x\alpha)$ and

$$Y^n[\{x\}_0^T] = \int_0^T dt_1 \dots dt_n \prod_{i=1}^n \left(\frac{\alpha \dot{x}_c(t_i)}{\nu} \right) w(t_i), \quad (7.16)$$

where the superscript c in expectations, e.g. $\overline{\bullet}^{(v),c}$, denotes the corresponding cumulant. Substituting Equation (7.15) into Equation (7.8), combined with Equation (7.5), returns the optimal protocol.

Computing the right-hand side of Equation (7.15) is unfeasible in general. However, $Q[\{x\}_0^T]$ can be computed analytically in the low-Pe asymptotic regime. To leading order in $\text{Pe} \ll 1$, only the first cumulant $\overline{Y[\{x\}_0^T]}^{(+1),c}$ is required, explicitly,

$$Q[\{x\}_0^T] = \text{Pe} \overline{Y[\{x\}_0^T]}^{(+1),c} + \mathcal{O}(\text{Pe}^3), \quad (7.17)$$

which in turn draws on $\overline{w(t)}^{(+1),c} = \overline{w(t)}^{(+1)} = \exp(-2\alpha(T-t))$, Appendix 7.B, whence

$$Q[\{x\}_0^T] = \text{Pe} \int_0^T dt \left(\frac{\alpha \dot{x}_c(t)}{\nu} \right) e^{-2\alpha(T-t)} + \mathcal{O}(\text{Pe}^3). \quad (7.18)$$

In order to conveniently apply the optimal protocol under continuous feedback control, one can differentiate Equation (7.18) with respect to T and use the Leibniz integration rule (assuming $\dot{x}_c(t) = 0$ for $t < 0$) to obtain a differential equation for the time evolution of Q , i.e.

$$\dot{Q}(T) = \frac{\nu}{D_x} \dot{x}_c(T) - 2\alpha Q(T). \quad (7.19)$$

Remarkably, upon substituting $\dot{x} - F_{\text{ext}}$ for $\dot{x}_c$ and rescaling time by the switching rate, $T' = \alpha T$, the Langevin equation for $Q(T')$ reads like that of the position of a RnT particle in a harmonic potential with self-propulsion speed and diffusivity both equal to Pe , i.e.

$$\frac{dQ(T')}{dT'} = \text{Pe} w(T') - 2Q(T') + \sqrt{2\text{Pe}} \xi(T'). \quad (7.20)$$

From this mapping, one finds (see Appendix 7.C)

$$\mathbb{E}_{\xi,w}[Q^2] = \frac{\text{Pe}}{2} \left(1 + \frac{\text{Pe}}{4} \right). \quad (7.21)$$

I now proceed to make the connection with the rate of work extraction. First of all,

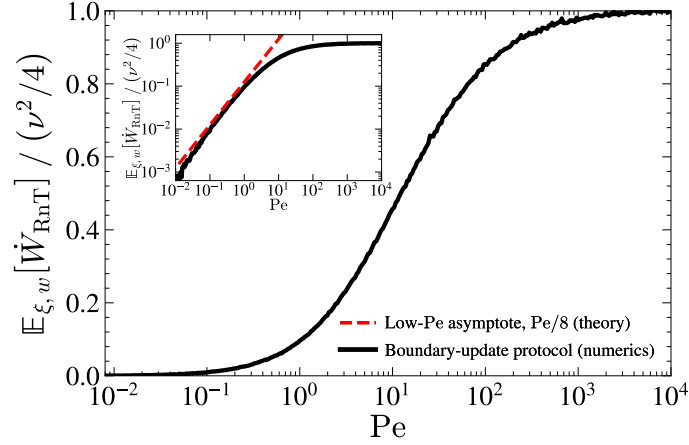


Figure 7.2: Average power extracted from a RnT particle with hidden self-propulsion velocity upon application of the boundary-update protocol, Section 7.4. The numerical implementation of the boundary-update protocol is discussed in detail in Appendix 7.F. The extractable power, which is positive for all Pe , asymptotically approaches that of the Markovian case where the internal state is known, Equation (7.3), as $\text{Pe} \rightarrow \infty$ and is in excellent agreement with the theoretical bound in the low- Pe limit, Equation (7.25).

from Equation (7.8),

$$P_{\pm}(T) = \frac{1}{2} \pm \frac{Q}{4} + \mathcal{O}(Q^2). \quad (7.22)$$

Then, by combining Equation (7.5) and Equation (7.22), the optimal protocol is given to leading order in $Q \sim \text{Pe}$ by

$$F_{\text{ext}}^*(T) = -\frac{\nu}{2}P_+(T) + \frac{\nu}{2}P_-(T) = -\frac{\nu}{4}Q + \mathcal{O}(Q^2). \quad (7.23)$$

When the optimal protocol is applied at all times, the resulting noise-averaged power output, Equation (7.6), is found to be

$$\mathbb{E}_{\xi}[\dot{W}_{\text{RnT}}[F_{\text{ext}}^*(t)]] = P_+F_{\text{ext}}(\nu + F_{\text{ext}}) + P_-F_{\text{ext}}(-\nu + F_{\text{ext}}) = \frac{\nu^2}{16}Q^2(T) + \mathcal{O}(\text{Pe}^2), \quad (7.24)$$

from inserting the small- Q expansions in Equations (7.22) and (7.23). Taking a further expectation of Equation (7.24) with respect to the telegraphic noise $w(t)$ and inserting Equation (7.21), the fully noise-averaged power output is

$$\frac{\mathbb{E}_{\xi,w}[\dot{W}_{\text{RnT}}(F_{\text{ext}}^*)]}{\nu^2/4} = \frac{\text{Pe}}{8} + \mathcal{O}(\text{Pe}^2), \quad (7.25)$$

which constitutes a tight upper bound to the average extractable power from a RnT particle with hidden self-propulsion velocity in the low-Péclet regime. Higher moments of the fluctuating power output under F_{ext}^* can be computed similarly, see Appendix 7.C.

7.4 A boundary-update protocol

I now introduce an independent approach to computing the posterior probability $P_+(T)$ in real time. This novel “boundary-update” protocol, described in full detail in Appendix 7.F, both saturates the bound (7.25) and is conjectured to achieve optimal work extraction for *all* Pe. The protocol draws on the *conditional* splitting probabilities of the RnT process, which, to the best of my knowledge, were computed for the first time in the work on which this chapter is based [54]. These are the probabilities that a particle initialised at $x_0 \in [-L/2, L/2]$ in a given statistical superposition of internal states exits said interval through either the left or right boundary in either a left or right self-propulsion state. Knowledge of these statistics is used in combination with Bayes’ theorem to update the posterior distribution of the internal state $w(t)$ each time the particle is observed to undergo a net displacement larger than $L/2$ in the reference frame where the deterministic drift from the protocol is subtracted away, $\dot{x}_c(t) = \dot{x}(t) - F_{\text{ext}}(t)$. In the limit $L \rightarrow 0$, the posterior updating frequency diverges suggesting that optimal inference is achieved. Figure 7.2 shows application of the boundary-update protocol indeed produces an average power output matching the bounds Equations (7.25) and (7.3) in the low- and high-Pe limits, respectively. Figure 7.3 illustrates the implementation of the boundary-update protocol for an example trajectory. Given the trajectory, the protocol predicts, and constantly updates, the probability of the particle’s time-dependent internal state $P_+(t)$. Using this prediction, the protocol applies a corresponding modulated external force $F_{\text{ext}}(t)$ to extract work over time.

7.5 A generic active particle

Having explored the particular case of RnT motion in some detail, the scope is now expanded to a one-dimensional active particle with self-propulsion velocity $w(t)$ evolving according to a *generic* (discrete- or continuous-state) stochastic process [222]. Following Equation (7.5), the identification of the optimal protocol requires computation of the posterior expectation of the self-propulsion velocity, which can be conveniently expressed as

$$\begin{aligned} \mathbb{E}_w[w(T)|\{x\}_0^T] &= \text{Tr}_v [v \mathbb{P}[w(T) = v | \{x\}_0^T]] \\ &= \frac{\text{Tr}_v \left[v \cdot \exp \left(-\frac{\text{Pe}}{4} \int_0^T dt \frac{\mu}{\sigma_w^2} (\dot{x}_c(t) - w(t))^2 \right)^{(v)} \mathbb{P}(v) \right]}{\text{Tr}_v \left[\exp \left(-\frac{\text{Pe}}{4} \int_0^T dt \frac{\mu}{\sigma_w^2} (\dot{x}_c(t) - w(t))^2 \right)^{(v)} \mathbb{P}(v) \right]} \end{aligned} \quad (7.26)$$

with $\text{Pe} = \sigma_w^2/(\mu D_x)$, $\sigma_w^2 = \mathbb{E}_w[w^2]$, and μ a characteristic inverse timescale associated with the self-propulsion dynamics. Here, Tr_v denotes either an integral or a sum depending on whether the state space is continuous or discrete, respectively. Bayes’ theorem was also

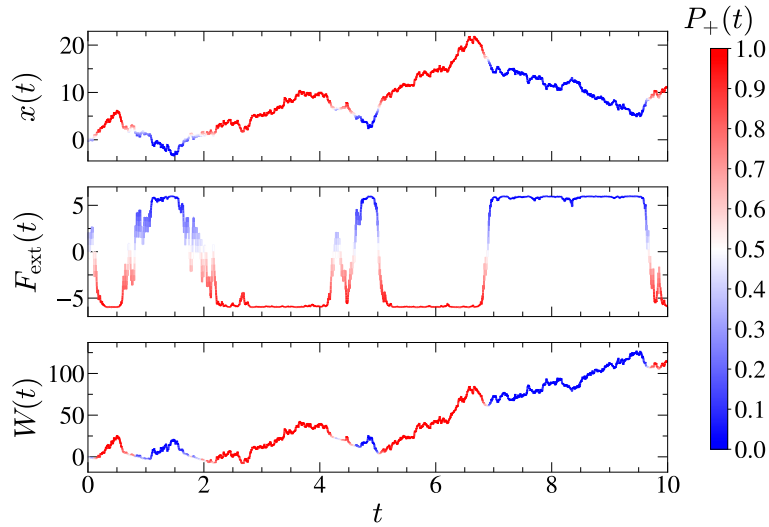


Figure 7.3: Implementation of the boundary-update protocol for an example stochastic trajectory of an RnT particle. (a) Particle position $x(t)$, (b) applied external force $F_{\text{ext}}(t)$, and (c) total amount of extracted work $W(t)$, are colour-coded according to the protocol's prediction of the particle's internal state $P_+(t)$. A redder (respectively, bluer) trajectory corresponds to the protocol predicting with greater certainty that the particle is in the right-moving (respectively, left-moving) state. Over long periods of time, the protocol extracts a positive amount of work from the particle.

invoked to write

$$\mathbb{P}[w(T) = v | \{x\}_0^T] = \frac{\mathbb{P}(v) \overline{\mathbb{P}[\{x\}_0^T | \{w(t)\}_0^T]^{(v)}}}{\mathbb{P}[\{x(t)\}_0^T]}, \quad (7.27)$$

where $\overline{\bullet}^{(v)}$ is defined as in Equation (7.11), and the normalisation condition $1 = \text{Tr}_v \mathbb{P}[w(T) = v | \{x\}_0^T]$ is used to divide by a factor of unity throughout, producing the same type of cancellations of v -independent terms observed in the RnT case. One can rewrite Equation (7.26) in a compact form as

$$\mathbb{E}_w[w(T) | \{x\}_0^T] = \frac{\text{Tr}_v \left[v \cdot e^{\mathcal{L}[\{x\}_0^T, v]} \mathbb{P}(v) \right]}{\text{Tr}_v \left[e^{\mathcal{L}[\{x\}_0^T, v]} \mathbb{P}(v) \right]} \quad (7.28)$$

by introducing the cumulant-generating function

$$\mathcal{L}[\{x\}_0^T, v] = \sum_{n=1}^{\infty} \frac{(-\text{Pe})^n}{2^{2n} n!} \left[\int_0^T dt \frac{\mu}{\sigma_w^2} (\dot{x}_c(t) - w(t))^2 \right]^{n^{(v),c}}. \quad (7.29)$$

If no further assumptions can be made regarding the process $w(t)$, one can now truncate the sum and substitute the resulting expression into Equation (7.28) to obtain, by invoking Equation (7.5) and recalling $\mathbb{E}_w[w] = 0$, the optimal protocol in the asymptotic case

$\text{Pe} \ll 1$,

$$F_{\text{ext}}^*(T) = \text{Tr}_v \left[v \frac{\text{Pe}}{8} \int_0^T dt \frac{\mu}{\sigma_w^2} \left(\overline{w^2(t)}^{(v),c} - 2\dot{x}_c(t) \overline{w(t)}^{(v),c} \right) \mathbb{P}(v) \right]. \quad (7.30)$$

The form of Equation (7.30) matches the RnT result, Equation (7.18), except for the appearance of a term depending on the second-order cumulant $\overline{w^2(t)}^{(v),c}$, which was absent in the RnT case due to the norm of the self-propulsion velocity being constant. The correlation functions of the hidden state $w(t)$ in Equation (7.30) can be reconstructed from observable trajectories (see Appendix 7.E). This allows relaxation *a posteriori* the requirement that the equations governing the dynamics of $w(t)$ be known.

In Appendix 7.D, the general result obtained above is applied to the specific case of a one-dimensional AOU process—the simplest canonical active particle model with a continuous self-propulsion state [73], see Chapter 2. The optimal average extractable power from an AOU particle with hidden self-propulsion velocity in the low-Péclet regime is found to be

$$\frac{\mathbb{E}_{\xi, w}[\dot{W}_{\text{AOU}}(F_{\text{ext}}^*)]}{\sigma_w^2/4} = \frac{\text{Pe}}{16} + \mathcal{O}(\text{Pe}^2). \quad (7.31)$$

The second moment of the power output distribution can be further computed with the aid of Appendix 7.C.

7.6 Langevin dynamics: high-Péclet asymptotics

When the dynamics of $w(t)$ are described by a Langevin equation, Equation (7.26) also allows one to explore the high-Péclet regime through a saddle-point expansion. For the particular case of the AOU process (as defined in Appendix 7.D), the exponential terms in Equation (7.26) can be written as (using the Onsager-Machlup form of $\mathbb{P}[\{w\}_0^T]$)

$$\overline{\exp \left(-\frac{\text{Pe}}{4} \int_0^T dt \frac{\mu}{\sigma_w^2} (\dot{x}_c(t) - w(t))^2 \right)}^{(v)} \propto \int \mathcal{D}w \, e^{-\mathcal{N}[w(t); \{x\}_0^T]} \delta(w(T) - v), \quad (7.32)$$

with the action-like functional

$$\mathcal{N}[w(t); \{x\}_0^T] = \mu \int_0^T dt \left[\text{Pe} \left(\frac{\dot{x}_c(t) - w(t)}{2\sigma_w} \right)^2 + \left(\frac{\dot{w}(t)/\mu + w(t)}{2\sigma_w} \right)^2 \right], \quad (7.33)$$

which combines a “potential” term $\propto (\dot{x}_c(t) - w(t))^2$, penalising departures from $w(t) = \dot{x}_c$, and a “kinetic” term $\propto (\dot{w}(t)/\mu + w(t))^2$ penalising changes in $w(t)$ that are exceedingly fast or slow compared to the characteristic inverse timescale μ of the self-propulsion dynamics. Even at high Pe , the second term cannot be ignored since the boundary condition $w(T) = v$ in general prevents $w(t) = \dot{x}_c(t)$ from being an accessible trajectory for the functional integral. I define $w^*(t; v)$ as the path that minimises Equation (7.33), i.e. $\delta \mathcal{N}[w]/\delta w|_{w^*} = 0$, whence

$$m\ddot{w}^*(t) = \mu^2(w^*(t) - \dot{x}_c(t)) + \mu^2 m w^*(t) \quad (7.34)$$

with $m = 1/\text{Pe}$ and boundary condition $w^*(T) = v$. Equation (7.34) is purposefully arranged to resemble the Newtonian dynamics of a particle of mass m in an unstable, time-dependent harmonic potential $V(w^*, t) = -[\mu^2(\dot{x}_c(t) - w^*)^2/2 + m\mu^2 w^{*2}/2]$. Remarkably, the high-Pe limit corresponds to the overdamped limit of Equation (7.34), whereby $m \rightarrow 0$ and the potential term dominates. For $m \ll 1$, Equation (7.34) is solved by combining an exponential ansatz with the particular solution $w^*(t; v) = \dot{x}_c(t) + \mathcal{O}(m)$, whence

$$w^*(t) = \dot{x}_c(t) + (v - \dot{x}_c(T))e^{\sqrt{\frac{1+m}{m}}\mu(t-T)} + \mathcal{O}(m). \quad (7.35)$$

Noting the second functional derivative of $\mathcal{N}$ is independent of $w(t)$, one can perform a change of variables $w(t) \rightarrow \delta w(t) + w^*(t; v)$ in the functional integral, Equation (7.32), to rewrite Equation (7.26) exactly as

$$\mathbb{E}_w[w(T)|\{x\}_0^T] = \frac{\int dv \, v \cdot e^{-\mathcal{N}[w^*(t;v);\{x\}_0^T]}\mathbb{P}(v)}{\int dv \, e^{-\mathcal{N}[w^*(t;v);\{x\}_0^T]}\mathbb{P}(v)}. \quad (7.36)$$

Substituting Equation (7.35) into Equation (7.33) yields, to leading order in large Pe,

$$\mathcal{N}[w^*(t)] = \frac{\sqrt{\text{Pe}}}{8} \left[\left(\frac{v - \dot{x}_c(T)}{\sigma_w} \right)^2 + \mathcal{O}(\text{Pe}^{-\frac{1}{2}}) \right], \quad (7.37)$$

which draws only on the potential-like term. Substituting Equation (7.37) into Equation (7.36) and then performing all the resulting Gaussian integrals in closed form, one arrives at the following expression for the posterior expectation of the self-propulsion velocity at high Pe,

$$\mathbb{E}_w[w(T)|\{x\}_0^T] = \left(1 - \frac{4}{\sqrt{\text{Pe}}} \right) \dot{x}_c(T) + \mathcal{O}(m). \quad (7.38)$$

Thus, the prior distribution $\mathbb{P}[w]$ weakly biases the posterior estimation $\mathbb{E}_w[w(T)|\{x\}_0^T]$ away from $\dot{x}_c(T)$ and towards the prior expectation $\mathbb{E}_w[w(T)] = 0$. Using Equation (7.6), the high-Pe asymptotic average power output from applying the optimal protocol is

$$\frac{\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}(F_{\text{ext}}^*)]}{\sigma_w^2/4} = \left(1 - \frac{8}{\sqrt{\text{Pe}}} \right) + \mathcal{O}(m). \quad (7.39)$$

7.7 Conclusion

In this final chapter of Part 2, I identified generic continuous feedback protocols achieving maximum average power extraction from active particles with a (zero-mean) hidden self-propulsion state. These optimal protocols can be written in closed form in the asymptotes $\text{Pe} \ll 1$, Equations (7.25) and (7.31), and $\text{Pe} \gg 1$, Equation (7.39), and provide upper bounds to the average extractable work by *any* such protocol. Arguably, these bounds are those against which the performance of autonomous active matter engines, which typically do not have access to the self-propulsion states of the individual constituent particles [51, 202], should be compared. Furthermore, the “boundary-update” protocol introduced

in this chapter enables work extraction in experimental settings where real-time particle tracking is unfeasible, since only the detection of first-passage events is required for its implementation.

The optimal protocol is generally non-Markovian. However, this difficulty can be circumvented at $Pe \ll 1$ by embedding the dynamics in a higher-dimensional phase space [223], e.g. via the auxiliary dynamics in Equation (7.20). Analogously to equilibrium information engines [206, 220], the thermodynamic cost of operating the feedback control can be identified with the increase in the total entropy production rate upon expanding the phase space to include such auxiliary variables [224]. In an idealised situation where the operating temperature of the measurement device is arbitrary, and can thus be chosen to be arbitrarily small, the associated dissipation is negligible [220].

The unique utility of information engines operating on active particles arises from their non-vanishing efficiency even when the measurement device and the particle are coupled to the same heat bath [206]. Future work should aim to characterise the efficiency of the optimal protocols in this case [169].

CHAPTER 7 APPENDICES

7.A Time-reversal symmetry of active motion with hidden self-propulsion

Consider a motile active particle with dynamics governed by the Langevin equation

$$\dot{x}(t) = w(t) + \sqrt{2D_x}\eta(t), \quad (7.40)$$

where $\eta(t)$ is a unit covariance white noise, D_x is the spatial diffusivity and $w(t)$ is a fluctuating self-propulsion velocity which is taken to be inaccessible to direct observation, i.e. to constitute a hidden state. In this appendix, I show that, when $w(t)$ is a *parity-time* (PT) symmetric stochastic process, the ensuing x -dynamics are time-reversal symmetric. This result applies to the particular cases of symmetric RnT and AOU dynamics discussed in the main text of this chapter, where $w(t)$ is given by a telegraph process and an Ornstein-Uhlenbeck process, respectively. Both of these are separately parity *and* time (and thus PT) symmetric. As a measure of time-reversal symmetry, I take the Kullback-Leibler divergence [40] of the ensemble of forward paths and their time-reversed counterparts, which also defines the average total informational entropy produced along a fluctuating trajectory [212, 213],

$$\Delta S[\{x\}_0^T] = \int \mathcal{D}x \, \mathbb{P}[\{x\}_0^T] \ln \left(\frac{\mathbb{P}[\{x\}_0^T]}{\mathbb{P}[\{x^R\}_0^T]} \right). \quad (7.41)$$

Here, $\mathbb{P}[\{x\}_0^T]$ denotes the probability density of a particular positional path and $\dot{x}^R(t) = -\dot{x}(T-t)$ denotes the time-reversed velocity, with the negative sign originating from odd parity of velocities under this transformation [78]. Using the law of total probability combined with the Onsager-Machlup [211] form of the positional path probability in the Stratonovich discretisation, one finds

$$\begin{aligned} \mathbb{P}[\{x\}_0^T] &= \int \mathcal{D}w \, \mathbb{P}[\{x\}_0^T | \{w\}_0^T] \mathbb{P}[\{w\}_0^T] \\ &\propto \int \mathcal{D}w \exp \left(-\frac{1}{4D_x} \int_0^T dt (\dot{x}(t) - w(t))^2 \right) \mathbb{P}[\{w\}_0^T], \end{aligned} \quad (7.42)$$

and similarly

$$\mathbb{P}[\{x^R\}_0^T] \propto \int \mathcal{D}w \exp \left(-\frac{1}{4D_x} \int_0^T dt (\dot{x}(t) + w^R(t))^2 \right) \mathbb{P}[\{w\}_0^T]. \quad (7.43)$$

Assuming PT symmetry of the w -statistics is equivalent to requiring that $\mathbb{P}[\{w\}_0^T] = \mathbb{P}[\{-w^R\}_0^T]$, Equation (7.43) becomes

$$\begin{aligned} \mathbb{P}[\{x^R\}_0^T] &\propto \int \mathcal{D}w \exp\left(-\frac{1}{4D_x} \int_0^T dt (\dot{x}(t) + w^R(t))^2\right) \mathbb{P}[\{-w^R\}_0^T] \\ &\propto \int \mathcal{D}\tilde{w} \exp\left(-\frac{1}{4D_x} \int_0^T dt (\dot{x}(t) - \tilde{w}(t))^2\right) \mathbb{P}[\{\tilde{w}\}_0^T], \end{aligned} \quad (7.44)$$

where I have used

$$\int \mathcal{D}w F[w^R(t)] = \int \mathcal{D}(-w^R) F[w^R(t)] = \int \mathcal{D}\tilde{w} F[-\tilde{w}(t)]. \quad (7.45)$$

Combining Equations (7.42) and (7.44) with Equation (7.41), one finds $\Delta S[\{x\}_0^T] = 0$, confirming the positional dynamics of the active particle are indeed time-reversal symmetric. It is worth restating that PT symmetry is a weaker constraint on the w -statistics compared to requiring that symmetry under parity reversal ($\mathbb{P}[\{w\}_0^T] = \mathbb{P}[\{-w\}_0^T]$) and time reversal ($\mathbb{P}[\{w\}_0^T] = \mathbb{P}[\{w^R\}_0^T]$) are separately satisfied. The simplest example of a stochastic process that is PT symmetric, but not individually P or T symmetric, is the zero-mean three-state Markov process taking values $w \in \{-1, 0, 1\}$ with transition rates $k_{0,1} = k_{1,-1} = k_{-1,0} = \alpha$ and $k_{1,0} = k_{-1,1} = k_{0,-1} = \beta$, where $k_{i,j}$ denotes the probability per unit time to transition from state j into state i and $\alpha \neq \beta$ are positive real numbers.

7.B Conditional correlations of the symmetric telegraph process

In this appendix, I derive the n -time correlation functions for a normalised telegraph process with symmetric transition rate α between states $w \in \{-1, +1\}$, conditioned on the process achieving a given state at some final time T (cf. the unconditional correlations derived in Appendix A of Ref. [225]). In particular, given an ordered set of n measurement times $0 < t_1 < t_2 < \dots < t_n \leq T$, the correlations are denoted

$$\begin{aligned} \overline{w(t_1)w(t_2)\dots w(t_n)}^{(+1)} &= \int \mathcal{D}w w(t_1)\dots w(t_n) \mathbb{P}(\{w\}_0^T | w(T) = +1) \\ &= \int \mathcal{D}w' w'(T - t_n)\dots w'(T - t_1) \mathbb{P}(\{w'\}_0^T | w'(0) = +1) \end{aligned} \quad (7.46a)$$

$$\begin{aligned} \overline{w(t_1)w(t_2)\dots w(t_n)}^{(-1)} &= \int \mathcal{D}w w(t_1)\dots w(t_n) \mathbb{P}(\{w\}_0^T | w(T) = -1) \\ &= \int \mathcal{D}w' w'(T - t_n)\dots w'(T - t_1) \mathbb{P}(\{w'\}_0^T | w'(0) = -1) \end{aligned} \quad (7.46b)$$

where, in the second equality of both Equations (7.46a) and (7.46b), I have used the invariance of the symmetric telegraph process statistics under time reversal to express the expectations in terms of conditioning on some initial state $w(0)$ of a trajectory of duration

T. I now introduce the transition probabilities

$$P_{+1,+1}(t) = \frac{1}{2} (1 + e^{-2\alpha t}) \quad (7.47a)$$

$$P_{-1,+1}(t) = \frac{1}{2} (1 - e^{-2\alpha t}) \quad (7.47b)$$

$$P_{+1,-1}(t) = \frac{1}{2} (1 - e^{-2\alpha t}) \quad (7.47c)$$

$$P_{-1,-1}(t) = \frac{1}{2} (1 + e^{-2\alpha t}) \quad (7.47d)$$

where $P_{i,j}(t)$ denotes the probability of a telegraph process initialised in state j to be found in state i after time t . Defining the matrix

$$M_w(t) = \begin{bmatrix} (+1)P_{+1,+1}(t) & (+1)P_{+1,-1}(t) \\ (-1)P_{-1,+1}(t) & (-1)P_{-1,-1}(t) \end{bmatrix}, \quad (7.48)$$

one can conveniently re-express the time-reversed conditional correlation functions above as

$$\overline{w(t_1)w(t_2)\dots w(t_n)}^{(+1)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}^T M_w(t_2 - t_1) M_w(t_3 - t_2) \dots M_w(T - t_n) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (7.49a)$$

$$\overline{w(t_1)w(t_2)\dots w(t_n)}^{(-1)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}^T M_w(t_2 - t_1) M_w(t_3 - t_2) \dots M_w(T - t_n) \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad (7.49b)$$

which differ only by the final column vector, responsible for the conditioning. For the particular case of a symmetric telegraph process,

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}^T M_w(t_2 - t_1) = e^{-2\alpha(t_2 - t_1)} \begin{bmatrix} 1 \\ -1 \end{bmatrix}^T, \quad (7.50)$$

and therefore

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}^T M_w(t_2 - t_1) M_w(t_3 - t_2) = e^{-2\alpha(t_2 - t_1)} \begin{bmatrix} 1 \\ 1 \end{bmatrix}^T, \quad (7.51)$$

whence

$$\overline{w(t_1)w(t_2)\dots w(t_n)}^{(+1)} = \begin{cases} \prod_{m=1}^{n/2} e^{-2\alpha(t_{2m} - t_{2m-1})}, & \text{for } n \text{ even} \\ e^{-2\alpha(T - t_n)} \prod_{m=1}^{n/2} e^{-2\alpha(t_{2m} - t_{2m-1})}, & \text{for } n \text{ odd} \end{cases}, \quad (7.52)$$

while

$$\overline{w(t_1)w(t_2)\dots w(t_n)}^{(-1)} = \begin{cases} \prod_{m=1}^{n/2} e^{-2\alpha(t_{2m} - t_{2m-1})}, & \text{for } n \text{ even} \\ -e^{-2\alpha(T - t_n)} \prod_{m=1}^{n/2} e^{-2\alpha(t_{2m} - t_{2m-1})}, & \text{for } n \text{ odd} \end{cases}, \quad (7.53)$$

where $//$ denotes integer division. The lowest-order correlation functions are thus given by

$$\overline{w(t_1)}^{(+1)} = e^{-2\alpha(T-t_1)}, \quad (7.54a)$$

$$\overline{w(t_1)w(t_2)}^{(+1)} = e^{-2\alpha(t_2-t_1)}, \quad (7.54b)$$

$$\overline{w(t_1)w(t_2)w(t_3)}^{(+1)} = e^{-2\alpha(t_2-t_1)}e^{-2\alpha(T-t_3)}. \quad (7.54c)$$

The odd cumulants up to the same order are, instead,

$$\overline{w(t_1)}^{(+1),c} = e^{-2\alpha(T-t_1)} \quad (7.55a)$$

$$\overline{w(t_1)w(t_2)w(t_3)}^{(+1),c} = -4e^{-2\alpha(T-t_1)}e^{-2\alpha(T-t_2)} \sinh[2\alpha(T-t_3)]. \quad (7.55b)$$

Note that, by symmetry of the w -statistics under parity reversal, $w(t) \rightarrow -w(t)$, we have

$$\overline{w(t_1)w(t_2)\dots w(t_n)}^{(+1),c} - \overline{w(t_1)w(t_2)\dots w(t_n)}^{(-1),c} = \begin{cases} 0, & \text{if } n \text{ even} \\ 2\overline{w(t_1)\dots w(t_n)}^{(+1),c} & \text{if } n \text{ odd} \end{cases}. \quad (7.56)$$

7.C Moments of position for active particles in harmonic potentials

In this appendix, I derive simple recurrence formulae for the moments of the position of RnT and AOU particles in harmonic potentials. The relevance of these results to this chapter originate from the mapping identified in the main text, via Equation (7.18), between the dynamics of the fluctuating extracted power from a RnT particle upon application of the optimal protocol $F_{\text{ext}}^*(t) = -\mathbb{E}_w[w(T)|\{x\}_0^T]/2$ and those of the position of such a harmonically-bound active particle. We will see that a similar mapping applies to the AOU particle, see Equation (7.76) below. While the exact form of the full probability densities are typically quite cumbersome (see, for example, Ref. [42]), these recurrence formulae allow one to easily extract key characteristics such as the mean power output and the associated coefficient of variation, defined as the standard deviation normalised to the mean.

7.C.a Run-and-tumble particle

I now derive the recurrence formulae for the steady-state positional moments of an RnT particle, which draw on the steady-state positional moments conditioned on the particle being in either of its accessible self-propelling modes. I arbitrarily choose to calculate the positional moments of the right-moving state ($w(t) = +\nu$), since those of the left-moving state ($w(t) = -\nu$) can be obtained by symmetry assuming, as I do here, that the switching rates are symmetric. I start from the coupled Fokker-Planck equations for the joint probability density $\mathcal{P}_{+/-}(x, t)$ to observe a particle in the right/left-moving state at

position x at time t ,

$$\partial_t \mathcal{P}_+ = D_x \partial_x^2 \mathcal{P}_+ + \kappa \partial_x (x \mathcal{P}_+) - \nu \partial_x \mathcal{P}_+ + \alpha (\mathcal{P}_- - \mathcal{P}_+), \quad (7.57a)$$

$$\partial_t \mathcal{P}_- = D_x \partial_x^2 \mathcal{P}_- + \kappa \partial_x (x \mathcal{P}_-) + \nu \partial_x \mathcal{P}_- - \alpha (\mathcal{P}_- - \mathcal{P}_+), \quad (7.57b)$$

where κ denotes the stiffness of the harmonic potential and I retain all other definitions of symbols from the main text. Since, at steady-state, $\mathcal{P}_+(x, t) = \mathcal{P}_-(-x, t)$ by symmetry, the final term in Equation (7.57a) is odd. It can be written equivalently as $\alpha (\mathcal{P}_- - \mathcal{P}_+) = \alpha (\mathcal{P} - 2\mathcal{P}_+)$ where the total density $\mathcal{P} = \mathcal{P}_+ + \mathcal{P}_-$ is an even function of x . At steady-state $\partial_t \mathcal{P}_+ = \partial_t \mathcal{P}_- = 0$, and after operating on Equation (7.57a) with $\int dx x^n$, performing all integrations by parts, and exploiting the even/odd symmetry of the final term, one eventually arrives at

$$0 = \begin{cases} D_x n(n-1) \mathbb{E}_x^+[x^{n-2}] - \kappa n \mathbb{E}_x^+[x^n] + \nu n \mathbb{E}_x^+[x^{n-1}] & \text{for even } n \geq 2 \\ D_x n(n-1) \mathbb{E}_x^+[x^{n-2}] - \kappa n \mathbb{E}_x^+[x^n] + \nu n \mathbb{E}_x^+[x^{n-1}] - 2\alpha \mathbb{E}_x^+[x^n] & \text{for odd } n \geq 1 \end{cases}, \quad (7.58)$$

where the steady-state conditional moments are given by $\mathbb{E}_x^+[x^n] := \lim_{t \rightarrow \infty} \int dx x^n \mathcal{P}_+(x, t)$ and all boundary terms vanish due to $\lim_{x \rightarrow \pm \infty} \mathcal{P}_+(x, t) = 0$. Equation (7.58) can be rearranged into the form of a recursive relation for the n^{th} conditional moment,

$$\mathbb{E}_x^+[x^n] = \begin{cases} \frac{1}{\kappa} (D_x(n-1) \mathbb{E}_x^+[x^{n-2}] + \nu \mathbb{E}_x^+[x^{n-1}]) & \text{for even } n \geq 2 \\ \frac{n}{n\kappa + 2\alpha} (D_x(n-1) \mathbb{E}_x^+[x^{n-2}] + \nu \mathbb{E}_x^+[x^{n-1}]) & \text{for odd } n \geq 1 \end{cases}. \quad (7.59)$$

Using Equation (7.59), the normalisation condition $\mathbb{E}_x^+[x^0] = \int dx \mathcal{P}_+(x) = 1/2$ readily gives rise to the $n = 1$ moment, $\mathbb{E}_x^+[x] = \nu/(2(\kappa + 2\alpha))$ which, in turn, can be used to obtain the $n = 2$ moment, $\mathbb{E}_x^+[x^2] = D_x/2\kappa + \nu^2/(2\kappa(\kappa + 2\alpha))$, in agreement with Ref. [42]. In fact, closed-form expressions for all higher-order conditional moments can be obtained in a similar manner, since any given conditional moment depends only on the two lower-order moments immediately preceding it.

The steady-state conditional moments for the left-moving state, denoted $\mathbb{E}_x^-[x^n] := \lim_{t \rightarrow \infty} \int dx x^n \mathcal{P}_-(x, t)$, and those of the total density $\mathcal{P}$ are readily obtained from the symmetry relation $\mathbb{E}_x^-[x^n] = (-1)^n \mathbb{E}_x^+[x^n]$ and the total probability relation $\mathbb{E}_x[x^n] = \mathbb{E}_x^+[x^n] + \mathbb{E}_x^-[x^n]$, respectively. It is thus straightforward to obtain the expression for the variance of the particle position,

$$\mathbb{E}_x[x^2] = \frac{D_x}{\kappa} + \frac{\nu^2}{\kappa(\kappa + 2\alpha)}. \quad (7.60)$$

As was shown in the main text, in the asymptotic regime $\text{Pe} \ll 1$, the dynamics of the fluctuating power extracted from an RnT process with hidden self-propulsion state $w(t)$ subject to the optimal protocol F_{ext}^* are identical to those of the square of the position of an RnT particle in a harmonic potential. There, I then used the result for the second moment of the latter, Equation (7.60), to compute the average power output, which defines

the upper bound to the average extractable work in this regime. Remarkably, the same correspondence can be exploited to relate the fourth moment of the particle position,

$$\mathbb{E}_x[x^4] = \frac{3D_x^2}{\kappa^2} + \frac{6D_x\nu^2}{\kappa^2(\kappa + 2\alpha)} + \frac{3\nu^4}{\kappa^2(\kappa + 2\alpha)(3\kappa + 2\alpha)}, \quad (7.61)$$

to the second moment of the power output distribution upon application of the optimal protocol F_{ext}^* , which is found to be

$$\frac{\mathbb{E}_{\xi,w}[\dot{W}_{\text{RnT}}^2(F_{\text{ext}}^*)]}{(\nu^2/4)^2} \simeq \frac{\mathbb{E}_{\xi,w}[(Q[\{x\}_0^T])^4]}{16} = \frac{3}{64}\text{Pe}^2 + \mathcal{O}(\text{Pe}^3) \quad (7.62)$$

to leading order in small Pe . Correspondingly, the coefficient of variation in this regime is

$$C_{\text{RnT}}^W = \frac{\sqrt{\mathbb{E}_{\xi,w}[\dot{W}_{\text{RnT}}^2(F_{\text{ext}}^*)] - (\mathbb{E}_{\xi,w}[\dot{W}_{\text{RnT}}(F_{\text{ext}}^*)])^2}}{\mathbb{E}_{\xi,w}[\dot{W}_{\text{RnT}}(F_{\text{ext}}^*)]} = \sqrt{2} \approx 1.414 \quad (7.63)$$

indicating that, even under optimal control, fluctuations often lead to transients of negative power extraction. Equation (7.61) reduces to the Gaussian kurtosis $\mathbb{E}_x[x^4]/(\mathbb{E}_x[x^2])^2 = 3$ in the limit $\alpha \rightarrow \infty$, where the self-propulsion becomes dynamically (although not thermodynamically [38, 226]) irrelevant.

7.C.b Active Ornstein-Uhlenbeck particle

I now provide the derivation of the moments of the positional probability density for an active Ornstein-Uhlenbeck process in a harmonic potential. First, I calculate the second moment of the particle position $x(t)$, which is used in Appendix 7.D below to derive an upper bound to the average extractable work in the asymptotic regime $\text{Pe} \ll 1$, Equation (7.78). I start from the Fokker-Planck equation for the joint probability density $\mathcal{P}(x, w, t)$ that the particle is at position x exhibiting an instantaneous self-propulsion velocity $w(t)$ at time t ,

$$\partial_t \mathcal{P} = D_x \partial_x^2 \mathcal{P} + \kappa \partial_x (x \mathcal{P}) - w \partial_x \mathcal{P} + D_w \partial_w^2 \mathcal{P} + \mu \partial_w (w \mathcal{P}), \quad (7.64)$$

where κ denotes the stiffness of the harmonic potential acting on the position x and μ that of the harmonic potential acting on the self-propulsion velocity $w(t)$. At steady state, $\partial_t \mathcal{P}(x, w, t) = 0$. Then, multiplying the right-hand side of Equation (7.64) separately by x^2 and xw , and then integrating with respect to both x and w yields, respectively,

$$0 = D_x - \kappa \mathbb{E}_{x,w}[x^2] + \mathbb{E}_{x,w}[xw], \quad (7.65a)$$

$$0 = -(\kappa + \mu) \mathbb{E}_{x,w}[xw] + \mathbb{E}_{x,w}[w^2]. \quad (7.65b)$$

Combining the equations above with the known second moment of the standard Ornstein-Uhlenbeck process [57], $\mathbb{E}_{x,w}[w^2] = D_w/\mu$, one eventually arrives at the desired result

$$\mathbb{E}_{x,w}[x^2] = \frac{D_x}{\kappa} + \frac{D_w}{\mu\kappa(\mu + \kappa)}. \quad (7.66)$$

Equation (7.66) is consistent with the variance of x reducing to that of a standard OU process in the equilibrium limit $D_w \rightarrow 0$, where $\mathbb{E}_{x,w}[x^2] = D_x/\kappa$. A similar procedure can be followed to calculate the higher-order positional moments given that the moments $\mathbb{E}_{x,w}[w^k]$ are known from the literature on the OU process [57], i.e.

$$\mathbb{E}_{x,w}[w^k] = \begin{cases} 0 & \text{if } k \text{ is odd} \\ (k-1)!!(D_w/\mu)^{\frac{k}{2}} & \text{if } k \text{ is even} \end{cases}. \quad (7.67)$$

Again, starting from the Fokker-Planck equation (7.64) at steady state and multiplying by $x^n w^m$ ($n, m \in \mathbb{N}$) before integrating with respect to both variables, gives

$$\begin{aligned} 0 = & D_x(n)_2 \mathbb{E}_{x,w}[x^{n-2}w^m] - (\kappa n + \mu m) \mathbb{E}_{x,w}[x^n w^m] + n \mathbb{E}_{x,w}[x^{n-1}w^{m+1}] \\ & + D_w(m)_2 \mathbb{E}_{x,w}[x^n w^{m-2}], \end{aligned} \quad (7.68)$$

for $n, m \geq 0$, defining the falling factorial $(k)_2 = k(k-1)$ for compactness. Together with Equation (7.65), Equation (7.68) can be solved to compute any desired moment $\mathbb{E}_{x,w}[x^n]$. Here, only even moments are non-trivial since $\mathbb{E}_{x,w}[x^{2k+1}] = 0$ for all $k \in \mathbb{N}$ by symmetry. Similarly, $\mathbb{E}_{x,w}[x^{2k+1}w^{2\ell}] = \mathbb{E}_{x,w}[x^{2k}w^{2\ell+1}] = 0$ for $\ell \in \mathbb{N}$. Combining the expressions of the type (7.68)—obtained from all choices of n and m such that $n+m=4$ —with Equations (7.65)–(7.67), eventually gives the Gaussian kurtosis

$$\mathbb{E}_{x,w}[x^4] = 3 (\mathbb{E}_{x,w}[x^2])^2. \quad (7.69)$$

As shown in Appendix 7.D below, in the asymptotic regime $\text{Pe} \ll 1$, the dynamics of the fluctuating power extracted from an AOU process with hidden self-propulsion state $w(t)$ subject to the optimal protocol F_{ext}^* are identical to those of the square of the position of an AOU particle in a harmonic potential. There, I use the result for the second moment of the latter, Equation (7.66), to compute the average power output, which defines the upper bound to the average extractable work in this regime, Equation (7.78). The same correspondence allows computation of the second moment of the power output through Equation (7.69) to leading order in small Pe ,

$$\frac{\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}^2(F_{\text{ext}}^*)]}{(\sigma_w^2/4)^2} \simeq \mathbb{E}_{\xi,w}[(\mathcal{L}^{(1)}[\{x\}_0^T])^4] = \frac{3}{2^{10}} \text{Pe}^2 + \mathcal{O}(\text{Pe}^3). \quad (7.70)$$

The coefficient of variation in this regime is thus

$$C_{\text{AOU}}^W = \frac{\sqrt{\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}^2(F_{\text{ext}}^*)] - (\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}(F_{\text{ext}}^*)])^2}}{\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}(F_{\text{ext}}^*)]} = \sqrt{2} \approx 1.414 \quad (7.71)$$

i.e. the same as for the RnT case in the previous section, Equation (7.63).

7.D Optimal protocol for an active Ornstein-Uhlenbeck particle at low Péclet number

In this appendix, I illustrate the general result for the optimal protocol at low Péclet number obtained in the main text, Equation (7.30), by applying it to the specific case of a one-dimensional AOU process, the simplest canonical active particle model with a continuous self-propulsion state [73]. The dynamics of the self-propulsion velocity $w(t)$ are captured by the equilibrium linear Langevin equation

$$\dot{w}(t) = -\mu w(t) + \sqrt{2D_w}\eta(t), \quad (7.72)$$

with $\eta(t)$ a zero-mean, unit-variance white noise with associated diffusivity D_w . The prior probability density is thus Boltzmann $\mathbb{P}(w) \propto \exp(-\mu w^2/(2D_w))$, see Chapter 2, whence $\sigma_w^2 = D_w/\mu$. Due to $w(t)$ being a Gaussian process, $\mathcal{L}[\{x\}_0^T, v] = \mathcal{L}^{(0)}[\{x\}_0^T] + (v/\sigma_w)\mathcal{L}^{(1)}[\{x\}_0^T]$, i.e. conditional cumulants are, at most, linear in v [57]. Equation (7.28) thus reduces to

$$\mathbb{E}_w[w(T)|\{x\}_0^T] = \left. \frac{\partial \mathcal{H}_{\text{AOU}}(z)}{\partial z} \right|_{z=\mathcal{L}^{(1)}/\sigma_w}, \quad (7.73)$$

where $\mathcal{H}_{\text{AOU}}(z) = \log \mathbb{E}_w[e^{wz}] = \sigma_w^2 z^2/2$ is the known cumulant-generating function of the fluctuating self-propulsion velocity prior probability density $\mathbb{P}(w)$. Combining Equations (7.5) and (7.73) reveals the optimal protocol to be

$$F_{\text{ext}}^*(t) = -\frac{\sigma_w}{2}\mathcal{L}^{(1)}[\{x\}_0^T] \quad (7.74)$$

and thus

$$\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}(F_{\text{ext}}^*)] = \frac{\sigma_w^2}{4}\mathbb{E}_{\xi,w}[\mathcal{L}^{(1)}[\{x\}_0^T]^2]. \quad (7.75)$$

At this point, the only outstanding challenge is to compute the dimensionless functional $\mathcal{L}^{(1)}[\{x\}_0^T]$. To leading order in $\text{Pe} \ll 1$,

$$\mathcal{L}^{(1)}[\{x\}_0^T] = \frac{\text{Pe}}{4} \int_0^T dt \left(\frac{\mu \dot{x}_c(t)}{\sigma_w} \right) e^{-\mu(T-t)} + \mathcal{O}(\text{Pe}^2), \quad (7.76)$$

where I have used $\overline{w(t)}^{(v),c} = v \exp(-\mu(T-t))$. The same result can be obtained starting from Equation (7.30), noticing the second conditional cumulant of the OU process, $\overline{w^2(t)}^{(v),c}$, is independent of v . By rescaling $T' = \mu T$ as in the RnT case, Equation (7.20), and taking $\dot{x}_c(t) = 0$ for $t < 0$, Equation (7.76) can be recast into a differential equation

for $\mathcal{L}^{(1)}(T')$ mirroring that of an AOU particle in a harmonic potential,

$$\frac{d\mathcal{L}^{(1)}(T')}{dT'} = \frac{\text{Pe}}{4} \cdot \frac{w(T')}{\sigma_w} - \mathcal{L}^{(1)}(T') + \sqrt{\frac{\text{Pe}}{8}} \cdot \eta(T'). \quad (7.77)$$

This mapping allows extraction of a tight upper bound to the average extractable power from an AOU particle with hidden self-propulsion velocity in the low-Pe asymptote, i.e.

$$\frac{\mathbb{E}_{\xi,w}[\dot{W}_{\text{AOU}}(F_{\text{ext}}^*)]}{\sigma_w^2/4} = \frac{\text{Pe}}{16} + \mathcal{O}(\text{Pe}^2), \quad (7.78)$$

as reported in Equation (7.31) of the main text.

7.E Conditional expectations from empirical measurements

Consider the overdamped Langevin equation for a generic active particle, $\dot{x}(t) = w(t) + \xi(t)$ with $\langle \xi(t)\xi(t') \rangle = 2D_x\delta(t-t')$, where $w(t)$ represents a hidden self-propulsion velocity governed by an unknown Langevin or master equation. In this appendix, I outline a procedure to relate expectations of any function of the net velocity *conditioned on a particular final net velocity* $\dot{x}(T)$, to correlation functions of the same observable *conditioned on a particular final value* $w(T)$ *of the hidden self-propulsion velocity*. While the first type of expectation is empirically accessible, it is the second which appears in the definition of the generic optimal protocol at low Pe, Equation (7.30) in the main text. The ability to derive the latter from the former is thus key to achieving maximum power output even when the Langevin/master equation governing the self-propulsion velocity is not known *a priori*. Importantly, the statistics of the additive noise (here, the value of the diffusivity D_x) are assumed to be known, e.g. by characterising the dynamics of the particle in an experimental setup where activity is inhibited, or by considering a passive probe which otherwise has the same physical properties as the active particle.

I first introduce the notation for the two types of conditional expectations,

$$\bar{\bullet}^{(v)} := \int \mathcal{D}w \bullet \mathbb{P}_w[\{w(t)\}_0^T | w(T) = v] \quad (7.79)$$

$$\bar{\bar{\bullet}}^{(v)} := \int \mathcal{D}x \bullet \mathbb{P}_x[\{\dot{x}(t)\}_0^T | \dot{x}(T) = v]. \quad (7.80)$$

Here, I use $\delta(\cdot)$ and $\delta[\cdot]$ to denote Dirac delta functions and functionals, respectively. Similarly, I distinguish between the steady-state probability density function and path probability density for a given stochastic process y by denoting them as $P_y(\cdot)$ and $\mathbb{P}_y[\cdot]$ respectively. With this notation in place, conditional correlations of the type (7.80) can

be related to those of the type (7.79) as follows,

$$\overline{\bullet}^{(v)} = \frac{1}{P_{\dot{x}}(v)} \int \mathcal{D}x \bullet \mathbb{P}_{\dot{x}}[\{\dot{x}\}_0^T] \delta(\dot{x}(T) - v) \quad (7.81a)$$

$$= \frac{1}{P_{\dot{x}}(v)} \int \mathcal{D}x \bullet \delta(\dot{x}(T) - v) \int \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \mathbb{P}_w[\{\dot{x} - \xi\}_0^T] \quad (7.81b)$$

$$= \frac{1}{P_{\dot{x}}(v)} \int \mathcal{D}x \bullet \delta(\dot{x}(T) - v) \int \mathcal{D}\xi \mathcal{D}w \mathbb{P}_{\xi}[\{\xi\}_0^T] \mathbb{P}_w[\{w\}_0^T] \delta[w + \xi - \dot{x}] \quad (7.81c)$$

$$= \frac{1}{P_{\dot{x}}(v)} \int \mathcal{D}w \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \mathbb{P}_w[\{w\}_0^T] \int \mathcal{D}x \bullet \delta(\dot{x}(T) - v) \delta[w + \xi - \dot{x}] \quad (7.81d)$$

$$= \frac{1}{P_{\dot{x}}(v)} \int \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \int \mathcal{D}w \mathbb{P}_w[\{w\}_0^T] \bullet|_{\dot{x}=w+\xi} \delta(w(T) + \xi(T) - v) \quad (7.81e)$$

$$= \frac{1}{P_{\dot{x}}(v)} \int \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \overline{\bullet}^{(v-\xi(T))} P_w(v - \xi(T)), \quad (7.81f)$$

where in going from (7.81a) to (7.81b) I used that the path probability of $\dot{x}(t) = w(t) + \xi(t)$ is the convolution of the path probabilities of the summands,

$$\mathbb{P}_{\dot{x}}[\{\dot{x} = w + \xi\}_0^T] = \int \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \mathbb{P}_w[\{\dot{x} - \xi\}_0^T], \quad (7.82)$$

while in going from (7.81b) to (7.81c) I used the property of the Dirac delta functional,

$$\mathbb{P}_w[\{\dot{x} - \xi\}_0^T] = \int \mathcal{D}w \mathbb{P}_w[\{w\}_0^T] \delta[w + \xi - \dot{x}]. \quad (7.83)$$

Finally, in going from (7.81e) to (7.81f) I used (7.79) to write the functional integral over the self-propulsion velocity path $w(t)$ in terms of the expectation conditioned on a particular final value. The probability densities $P_{\dot{x}}$ and P_w appearing in (7.81f) can both be extracted from observable trajectories: the first by simply constructing empirical histograms of the net velocity $\dot{x}$ and the second by deconvolution of the relation $P_{\dot{x}}(v) = \int d\xi P_{\xi}(\xi) P_w(v - \xi)$ originating from the additive nature of the noise, where again I assume P_{ξ} to be known. Note the definition of P_{ξ} for the case of white noise requires a suitable time discretisation of the trajectories, as discussed below.

Once again, the aim is to express the conditional correlations $\overline{w(t)}^{(v)}$ and $\overline{w^2(t)}^{(v)}$ appearing in the definition (7.30) of the generic optimal protocol at low-Peclet number in terms of correlations that can be measured empirically. Equipped with Equation (7.81f), one can then consider particular choices for the observable $\bullet(\dot{x})$. Firstly, let $\bullet = \dot{x}(t)$ with $t < T$,

$$\begin{aligned} \overline{\dot{x}(t)}^{(v)} P_{\dot{x}}(v) &= \int \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \left[\overline{w(t) + \xi(t)}^{(v-\xi(T))} \right] P_w(v - \xi(T)) \\ &= \int \mathcal{D}\xi \mathbb{P}_{\xi}[\{\xi\}_0^T] \overline{w(t)}^{(v-\xi(T))} P_w(v - \xi(T)), \end{aligned} \quad (7.84)$$

where I have used linearity of the conditional expectation together with the fact that ξ is

zero-mean. Secondly, let $\bullet = \dot{x}^2(t)$ with $t < T$,

$$\begin{aligned} \overline{\dot{x}^2(t)}^{(v)} P_{\dot{x}}(v) &= \int \mathcal{D}\xi \, \mathbb{P}_{\xi}[\{\xi\}_0^T] \left[\overline{w^2(t) + \xi^2(t) + 2\xi(t)w(t)}^{(v-\xi(T))} \right] P_w(v - \xi(T)) \\ &= \int \mathcal{D}\xi \, \mathbb{P}_{\xi}[\{\xi\}_0^T] \overline{w^2(t)}^{(v-\xi(T))} P_w(v - \xi(T)) \\ &\quad + \int \mathcal{D}\xi \, \mathbb{P}_{\xi}[\{\xi\}_0^T] \xi^2(t) P_w(v - \xi(T)), \end{aligned} \quad (7.85)$$

where, again, I have used that ξ is zero mean to remove the cross term. For the last step, and in order to regularise the high-frequency behaviour of the white noise ξ , I introduce a time discretisation of the empirical trajectories with timestep $\tau = T/N$, which is taken to be small compared to all other characteristic timescales of the problem. Functional integrals over noise realisations are thus expressed as products of regular integrals,

$$\int \mathcal{D}\xi \, \mathbb{P}_{\xi}[\{\xi\}_0^T] = \int \prod_{i=0}^N d\xi_i P_{\xi}(\xi_i), \quad (7.86)$$

where the subscript $i = 0, \dots, N$ denotes the timestep index, such that $\xi_0 = \tau^{-1} \int_0^{\tau} dt \, \xi(t)$ and $\xi_N = \tau^{-1} \int_{T-\tau}^T dt \, \xi(t)$. Using (7.86), Equations (7.84) and (7.85) reduce to

$$\overline{\dot{x}(t)}^{(v)} P_{\dot{x}}(v) = \int d\xi_N \, P_{\xi}(\xi_N) \overline{w(t)}^{(v-\xi_N)} P_w(v - \xi_N) \quad (7.87)$$

$$\left(\overline{\dot{x}^2(t)}^{(v)} - \frac{2D_x}{\tau} \right) P_{\dot{x}}(v) = \int d\xi_N \, P_{\xi}(\xi_N) \overline{w^2(t)}^{(v-\xi_N)} P_w(v - \xi_N), \quad (7.88)$$

which can be rearranged, via straightforward deconvolution, into expressions for the desired first- and second-order conditional moments of the hidden self-propulsion velocity $w(t)$. Note that, while the above shows such indirect measurement is possible, practical difficulties may arise, particularly when the state space of $w(t)$ is discrete. For example, deconvolution in Fourier space requires a suitable representation on the whole real line $v \in \mathbb{R}$ for the left-hand sides of Equations (7.87) and (7.88), which are obtained empirically and thus have finite support by definition. Similar problems prevent one from naively “dividing through” by the empirical probability P_w . The treatment of such technical difficulties constitutes an interesting problem in itself [227]. However, this lies beyond the scope of this chapter.

7.E.a Numerical verification of Equations (7.87) and (7.88) for an active Ornstein-Uhlenbeck particle

Here, I verify Equations (7.87) and (7.88) in the case of an AOU particle, as described in Appendix 7.D, for which the first and second conditional moments are available in closed form. The integral appearing on the right-hand side of each equation can be performed

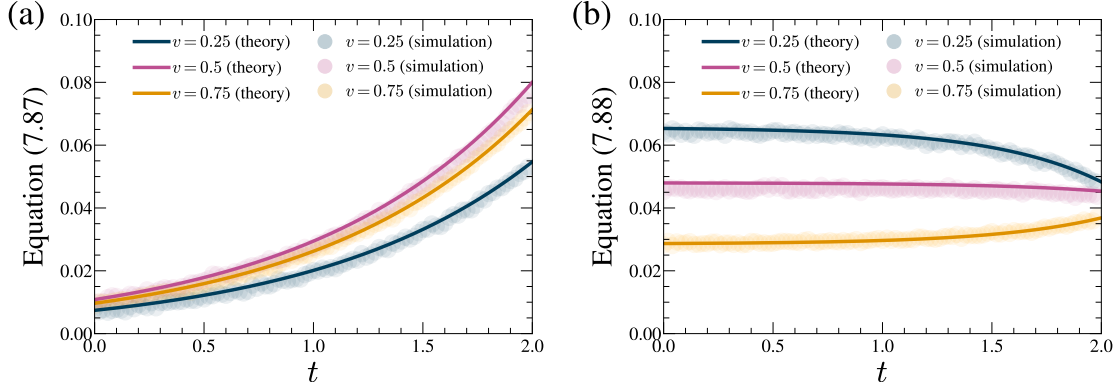


Figure 7.4: Numerical verification of (a) Equation (7.87) and (b) Equation (7.88) for the particular case of an AOU particle with $\mu = 1$, $D_w = 0.1$, $D_x = 10^{-4}$. Solid curves indicate the analytical evaluation of the right-hand sides, as written in Equations (7.89) and (7.92) respectively. Markers indicate empirical values of the left-hand sides of Equations (7.87) and (7.88), obtained from numerical simulations of AOU dynamics in one dimension. The timestep of the numerical integration was $\Delta t = 10^{-4}$, the timestep of the empirical trajectory was $\tau = 10^{-3}$, and the total time was $T = 2$.

explicitly, giving

$$\overline{\dot{x}(t)}^{(v)} P_x(v) = \left(\frac{\mu \tau^3 D_w^2 v^2}{2\pi(2\mu D_x + \tau D_w)} \right)^{\frac{1}{2}} \exp \left(-\mu \left[(T - t) + \frac{v^2 \tau}{2D_w \tau + 4\mu D_x} \right] \right), \quad (7.89)$$

$$\left(\overline{\dot{x}^2(t)}^{(v)} - \frac{2D_x}{\tau} \right) P_x(v) = \left(\frac{\mu \tau}{2\pi(2\mu D_x + \tau D_w)} \right)^{\frac{1}{2}} \left[\frac{D_w}{\mu} (1 - \exp(-2\mu(T - t))) \right] \quad (7.90)$$

$$\times \exp \left(-\frac{\mu v^2 \tau}{2D_w \tau + 4\mu D_x} \right) + \left(\left(\frac{v \tau D_w}{2\mu D_x + \tau D_w} \right)^2 + \frac{2D_x D_w}{2\mu D_x + \tau D_w} \right) \quad (7.91)$$

$$\times \exp \left(-\mu \left[2(T - t) + \frac{v^2 \tau}{2D_w \tau + 4\mu D_x} \right] \right). \quad (7.92)$$

The comparison of these predictions to data from numerical experiments is shown in Figure 7.4, where the right-hand sides of Equations (7.87) and (7.88), given explicitly by Equations (7.89) and (7.92), are plotted against numerical estimates of the left-hand sides. Good agreement between the theoretical results and simulations is observed in all cases.

7.F Boundary-update protocol

7.F.a Derivation of conditional splitting probabilities for a run-and-tumble particle

In this section, I derive the conditional splitting probabilities that form the basis of the numerical “boundary-update” protocol conjectured to achieve optimal power extraction

from a RnT particle for all Pe. These generalise the known results for the (unconditional) splitting probabilities for a run-and-tumble particle [27].

Consider a run-and-tumble process governed by the Langevin equation

$$\dot{x}(t) = \nu w(t) + \sqrt{2D_x} \xi(t), \quad (7.93)$$

where the normalised self-propulsion state $w \in \{-1, 1\}$ follows a symmetric telegraph process with switching rate α . I define the particle to be in a right-moving (respectively, left-moving) state at time t if $w(t) = +1$ (respectively, $w(t) = -1$). Let $\Pi_{s_1 L/2}^{s_2}(x_0, s_3)$ with $s_{1,2,3} \in \{-, +\}$ denote the probability for a particle to exit through the boundary at $x = s_1 L/2$ in the $w = s_2$ state given it was initialised at position $x_0 \in [-L/2, L/2]$ in the $w = s_3$ state. For example, $\Pi_{-L/2}^-(x_0, +)$ denotes the probability for a particle to exit through the left-hand boundary at $x = -L/2$ in the left-moving state given it was initialised at position $x_0 \in [-L/2, L/2]$ in the right-moving state. Four of the eight combinations of $s_{1,2,3}$ can be readily obtained from the remaining ones by exploiting the symmetries $\Pi_{L/2}^\pm(x_0, +) = \Pi_{-L/2}^\mp(-x_0, -)$ and $\Pi_{L/2}^\pm(x_0, -) = \Pi_{-L/2}^\mp(-x_0, +)$. As such, I will calculate only the splitting probabilities to exit at the left-hand boundary, $x = -L/2$. To ease notation, I define $\pi^\pm(x_0, \pm) := \Pi_{-L/2}^\pm(x_0, \pm)$.

I first derive the governing ODEs for the splitting probabilities by starting from the microscopic description on a lattice and taking the continuum limit [56]. On a lattice of spacing δ , a particle undergoes one of three processes at each time step,

1. hopping to the right-adjacent site, $x + \delta$, with rate h_r ,
2. hopping to the left-adjacent site, $x - \delta$, with rate h_ℓ ,
3. switching internal state with rate α , while remaining at the current site, x .

Whence, for a particle leaving through $x = -L/2$ in the $w = -1$ state, the corresponding conditional splitting probabilities obey the following identities

$$\begin{aligned} \pi^-(x, +) &= \frac{h_r^+}{h_r^+ + h_\ell^+ + \alpha} \pi^-(x + \delta, +) + \frac{h_\ell^+}{h_r^+ + h_\ell^+ + \alpha} \pi^-(x - \delta, +) \\ &\quad + \frac{\alpha}{h_r^+ + h_\ell^+ + \alpha} \pi^-(x, -), \end{aligned} \quad (7.94a)$$

$$\begin{aligned} \pi^-(x, -) &= \frac{h_r^-}{h_r^- + h_\ell^- + \alpha} \pi^-(x + \delta, -) + \frac{h_\ell^-}{h_r^- + h_\ell^- + \alpha} \pi^-(x - \delta, -) \\ &\quad + \frac{\alpha}{h_r^- + h_\ell^- + \alpha} \pi^-(x, +), \end{aligned} \quad (7.94b)$$

where, for instance, h_ℓ^+ is the rate for a right-moving particle to hop to the left such that $h_\ell^+/(h_r^+ + h_\ell^+ + \alpha)$ is the transition probability for a right-moving particle to hop to the left. Expanding each term on the right-hand side of Equation (7.94) in small δ , e.g.

$$\pi^-(x - \delta, -) = \pi^-(x, -) - \delta \frac{d\pi^-(x, -)}{dx} + \frac{1}{2} \delta^2 \frac{d^2 \pi^-(x, -)}{dx^2} + \mathcal{O}(\delta^3), \quad (7.95)$$

produces, after rearrangement and up to second order in δ ,

$$0 = \delta (h_r^+ - h_\ell^+) \frac{d\pi^-(x, +)}{dx} + \frac{1}{2}\delta^2 (h_r^+ + h_\ell^+) \frac{d^2\pi^-(x, +)}{dx^2} + \alpha (\pi^-(x, -) - \pi^-(x, +)), \quad (7.96a)$$

$$0 = \delta (h_r^- - h_\ell^-) \frac{d\pi^-(x, -)}{dx} + \frac{1}{2}\delta^2 (h_r^- + h_\ell^-) \frac{d^2\pi^-(x, -)}{dx^2} + \alpha (\pi^-(x, +) - \pi^-(x, -)). \quad (7.96b)$$

Finally, taking $\delta \rightarrow 0$ while keeping $\nu = \delta(h_r^+ - h_\ell^+) = \delta(h_\ell^- - h_r^-)$ and $D_x = \delta^2(h_r^+ + h_\ell^+)/2 = \delta^2(h_r^- + h_\ell^-)/2$ finite results in the following coupled backward equations,

$$0 = \nu \frac{d\pi^-(x, +)}{dx} + D_x \frac{d^2\pi^-(x, +)}{dx^2} + \alpha (\pi^-(x, -) - \pi^-(x, +)), \quad (7.97a)$$

$$0 = -\nu \frac{d\pi^-(x, -)}{dx} + D_x \frac{d^2\pi^-(x, -)}{dx^2} + \alpha (\pi^-(x, +) - \pi^-(x, -)). \quad (7.97b)$$

By a similar procedure, the backward equations for the particle exiting the interval at $x = -L/2$ as a right mover can be shown to satisfy

$$0 = \nu \frac{d\pi^+(x, +)}{dx} + D_x \frac{d^2\pi^+(x, +)}{dx^2} + \alpha (\pi^+(x, -) - \pi^+(x, +)), \quad (7.98a)$$

$$0 = -\nu \frac{d\pi^+(x, -)}{dx} + D_x \frac{d^2\pi^+(x, -)}{dx^2} + \alpha (\pi^+(x, +) - \pi^+(x, -)). \quad (7.98b)$$

Since $\pi^-(x, \pm)$ and $\pi^+(x, \pm)$ are governed by the same ODEs, I proceed to solve Equations (7.97) and (7.98) simultaneously up till the point of applying the different boundary conditions for each case, which are

$$\pi^\pm(-L/2, \pm) = 1, \quad \pi^\mp(-L/2, \pm) = 0, \quad \pi^\pm(L/2, \pm) = 0, \quad \pi^\mp(L/2, \pm) = 0, \quad (7.99)$$

i.e. only one boundary condition for each statistic is non-vanishing due to the added constraint on the internal state as the particle exits the interval.

I define $\rho^\pm(x) := \pi^\pm(x, -) + \pi^\pm(x, +)$ and $\sigma^\pm(x) := \pi^\pm(x, -) - \pi^\pm(x, +)$ such that, after adding and subtracting Equations (7.97a) and (7.97b) (or, equivalently, Equations (7.98a) and (7.98b)), I obtain

$$0 = \frac{d^2\rho^\pm(x)}{dx^2} - \frac{\nu}{D_x} \frac{d\sigma^\pm(x)}{dx}, \quad (7.100a)$$

$$0 = \frac{d^2\sigma^\pm(x)}{dx^2} - \frac{\nu}{D_x} \frac{d\rho^\pm(x)}{dx} - \frac{2\alpha}{D_x} \sigma^\pm(x), \quad (7.100b)$$

with updated boundary conditions

$$\rho^\pm(-L/2) = 1, \quad \sigma^\pm(-L/2) = \mp 1, \quad \rho^\pm(L/2) = 0, \quad \sigma^\pm(L/2) = 0. \quad (7.101)$$

Integrating Equation (7.100a),

$$\frac{d\rho^\pm(x)}{dx} = \frac{\nu}{D_x}\sigma^\pm(x) - \frac{D_x}{\nu}k^2c_1^\pm, \quad (7.102)$$

and substituting the right-hand side of Equation (7.102) in place of $\rho'(x)$ in Equation (7.100b), yields

$$\frac{d^2\sigma^\pm(x)}{dx^2} = k^2(\sigma^\pm(x) - c_1^\pm), \quad (7.103)$$

which has the general solution

$$\sigma^\pm(x) = c_3^\pm e^{kx} + c_2^\pm e^{-kx} + c_1^\pm, \quad (7.104)$$

where $k = \sqrt{\nu^2/D_x^2 + 2\alpha/D_x} > 0$ and the $c_i^\pm$ are constants to be fixed. Substituting the solution for $\sigma^\pm(x)$, Equation (7.104), into Equation (7.102) and integrating leads to

$$\rho^\pm(x) = \frac{\nu}{D_x k} \left(c_4^\pm + c_3^\pm e^{kx} - c_2^\pm e^{-kx} \right) - \frac{2\alpha}{\nu} c_1^\pm x. \quad (7.105)$$

Now, applying the boundary conditions for the separate $w = \pm 1$ cases, Equation (7.101), to Equations (7.104) and (7.105) fixes the constants as

$$c_1^\pm = \frac{1}{2} \frac{\cosh(\frac{kL}{2}) \mp \frac{\nu}{D_x k} \sinh(\frac{kL}{2})}{\frac{\alpha L}{\nu} \cosh(\frac{kL}{2}) + \frac{\nu}{D_x k} \sinh(\frac{kL}{2})}, \quad (7.106a)$$

$$c_2^\pm = \mp \frac{1}{4} \left(\frac{\frac{\alpha L}{\nu} \pm 1}{\frac{\alpha L}{\nu} \cosh(\frac{kL}{2}) + \frac{\nu}{D_x k} \sinh(\frac{kL}{2})} + \operatorname{csch}\left(\frac{kL}{2}\right) \right), \quad (7.106b)$$

$$c_3^\pm = \mp \frac{1}{4} \left(\frac{\frac{\alpha L}{\nu} \pm 1}{\frac{\alpha L}{\nu} \cosh(\frac{kL}{2}) + \frac{\nu}{D_x k} \sinh(\frac{kL}{2})} - \operatorname{csch}\left(\frac{kL}{2}\right) \right), \quad (7.106c)$$

$$c_4^\pm = \frac{1}{2} \left(\frac{D_x k}{\nu} \mp \coth\left(\frac{kL}{2}\right) \right), \quad (7.106d)$$

such that $\pi^\pm(x_0, -) = (\rho^\pm(x_0) + \sigma^\pm(x_0))/2$ and $\pi^\pm(x_0, +) = (\rho^\pm(x_0) - \sigma^\pm(x_0))/2$ are now fully determined by Equations (7.104)–(7.106).

The conditional splitting probabilities, which I verified with Monte-Carlo simulations, are plotted in Figure 7.5. Interestingly, there can be a higher likelihood to observe a right mover at the left-hand boundary if it is first initialised as a left mover (as seen in Figure 7.5b for $x_0 \gtrsim -L/4$). Such a phenomenon can be studied only through the conditional splitting probabilities derived here. By summing suitable combinations of the conditional splitting probabilities, i.e. $\pi(x_0, \pm) = \pi^-(x_0, \pm) + \pi^+(x_0, \pm)$, where $\pi(x_0, \pm)$ is the probability to observe *any* particle at the left-hand boundary given initialisation at x_0 in the $w = \pm 1$ state, one can verify the results against the (unconditional) splitting probabilities derived in Ref. [27], see Figure 7.5c.

Finally, to establish the foundation of the boundary-update protocol mentioned in the main text, Bayes' theorem can be used in combination with the splitting probabilities

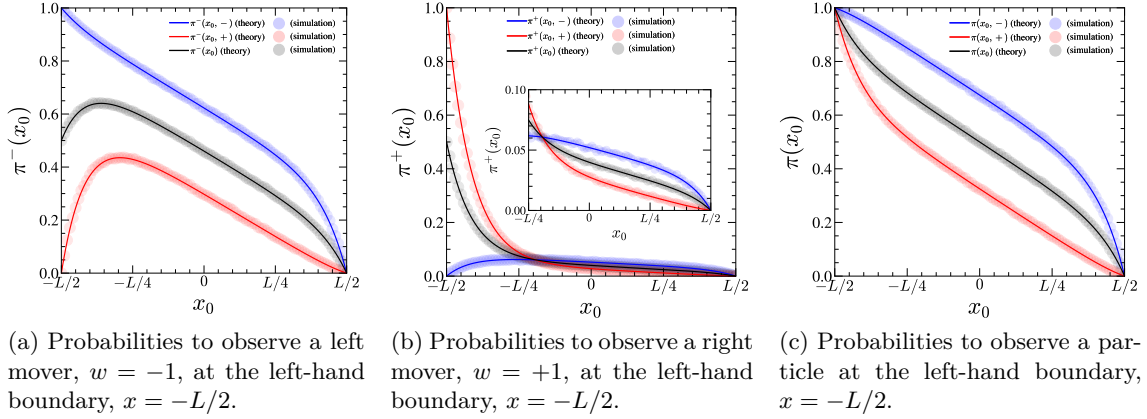


Figure 7.5: Conditional splitting probabilities, as a function of initialisation position x_0 , for a RnT particle with $\nu = 1$, $D_x = 0.1$ and $\alpha = 2$, to cross the left-hand boundary at $x = -L/2$, before crossing the right-hand boundary at $x = L/2$, if it exits as (a) a left mover, (b) a right mover, or (c) either a left mover or a right mover. In each subfigure, red (respectively, blue/black) lines indicate the initialisation of a right mover (respectively, left mover/equal superposition of a left mover and a right mover). Subfigure (c) corresponds to the (unconditional) splitting probabilities derived in Ref. [27]. Monte-Carlo simulations (markers) were performed by numerically integrating the Langevin equation, $\dot{x} = \nu w(t) + \sqrt{2D_x}\xi(t)$, in timesteps of $\Delta t = 10^{-5}$ to determine the proportion of times the particle exits through the left-hand boundary for 10^5 realisations at each $x_0/L = 0, 0.01, \dots, 1$. The theoretical results are in good agreement with simulations.

derived above to determine the posterior likelihood of a particle's internal state, $w(T) = \pm 1$, *given* it has crossed a particular boundary at time $t = T$. For instance, the probability of a particle being a left mover given it was initialised at $x_0 = 0$ and has crossed the left-hand boundary at $x = -L/2$ is

$$\begin{aligned}
 \mathbb{P}[w(T) = -1 | \text{left exit}, x_0 = 0] &= \frac{\mathbb{P}[w(T) = -1 \cap \text{left exit}]}{\mathbb{P}[\text{left exit}]} \\
 &= \frac{\pi^-(0, -)\mathbb{P}[w(0) = -1] + \pi^-(0, +)\mathbb{P}[w(0) = +1]}{\pi(0, -)\mathbb{P}[w(0) = -1] + \pi(0, +)\mathbb{P}[w(0) = +1]}, \tag{7.107a}
 \end{aligned}$$

where $\mathbb{P}[w(0) = \pm 1]$ denotes the prior probability of the self-propulsion state at initialisa-

tion. Similarly,

$$\mathbb{P}[w(T) = -1 | \text{right exit}, x_0 = 0] = \frac{\Pi_{L/2}^-(0, -)\mathbb{P}[w(0) = -1] + \Pi_{L/2}^-(0, +)\mathbb{P}[w(0) = +1]}{(1 - \pi(0, -))\mathbb{P}[w(0) = -1] + (1 - \pi(0, +))\mathbb{P}[w(0) = +1]}, \quad (7.107b)$$

$$\mathbb{P}[w(T) = +1 | \text{left exit}, x_0 = 0] = \frac{\pi^+(0, -)\mathbb{P}[w(0) = -1] + \pi^+(0, +)\mathbb{P}[w(0) = +1]}{\pi(0, -)\mathbb{P}[w(0) = -1] + \pi(0, +)\mathbb{P}[w(0) = +1]}, \quad (7.107c)$$

$$\mathbb{P}[w(T) = +1 | \text{right exit}, x_0 = 0] = \frac{\Pi_{L/2}^+(0, -)\mathbb{P}[w(0) = -1] + \Pi_{L/2}^+(0, +)\mathbb{P}[w(0) = +1]}{(1 - \pi(0, -))\mathbb{P}[w(0) = -1] + (1 - \pi(0, +))\mathbb{P}[w(0) = +1]}. \quad (7.107d)$$

7.F.b Numerical implementation of boundary-update protocol

In this section, I describe the numerical implementation of the boundary-update protocol for the RnT dynamics discussed in the main text. The boundary-update protocol draws on Equation (7.5) in the main text, which states that the optimal protocol $F_{\text{ext}}^*(t)$ is proportional to the instantaneous posterior expectation of the hidden self-propulsion velocity at time t given the entire observed trajectory of the net velocity, $\dot{x}(t')$ for $t' \in [0, t]$. In this scheme, the posterior expectation is updated on the fly upon the RnT particle exiting an interval of interest using the conditional splitting probabilities in Equation (7.107).

In the following, $p_{\text{prior}}(t)$ and $p_{\text{post}}(t)$ denote the Bayesian prior and posterior probability respectively (with respect to the observation that the particle has exited the interval) that the particle is currently a right-mover. Whilst the particle is in the bulk of the interval, no additional information is collected to improve the Bayesian inference of the hidden self-propulsion velocity and the posterior probability evolves in accordance to the Markov master equation

$$\begin{aligned} \frac{d\mathbb{P}_w[w(t) = +1]}{dt} &= \alpha(\mathbb{P}_w[w(t) = -1] - \mathbb{P}_w[w(t) = +1]) \\ &= \alpha(1 - 2\mathbb{P}_w[w(t) = +1]), \end{aligned} \quad (7.108)$$

which describes self-propulsion velocity reversal with Poisson rate α . Accordingly, $\dot{p}_{\text{post}}(t) = \alpha(1 - 2p_{\text{post}}(t))$, which has $p_{\text{post}} = 1/2$ as an attractive fixed point, reflecting the gradual loss of knowledge of the particle's internal state as time progresses. The following pseudocode summarises the numerical implementation of the boundary-update protocol:

Initialise:

- Set $t = 0$, $x(0) = 0$, $F_{\text{ext}}(0) = 0$;
- Set $p_{\text{prior}}(0) = p_{\text{post}}(0) = \mathbb{P}_w[w(0) = +1] = \frac{1}{2}$ and $[x_-, x_+] = [-L/2, L/2]$;

```

1 while  $t < T$  do
2     • Increment particle position according to the forward Euler scheme, i.e.
       $x(t + \Delta t) = x(t) + \Delta t(\nu w(t) + F_{\text{ext}}(t)) + \sqrt{2D_x \Delta t} \Delta \xi$ , where  $\Delta \xi$  represents a
      unit variance Gaussian random variable drawn at each time step;
3     • Increment the extracted work by
       $W(t + \Delta t) = W(t) - F_{\text{ext}}(t + \Delta t) \cdot (x(t + \Delta t) - x(t))$ ;
4     • Increment the posterior probability according to
       $p_{\text{post}}(t + \Delta t) = p_{\text{post}}(t) + \Delta t \cdot \alpha(1 - 2p_{\text{post}}(t))$ ;
5     • Update  $F_{\text{ext}}(t + \Delta t) = -\nu p_{\text{post}}(t + \Delta t)/2$  in accordance with Equation (7.5);
6     if  $x(t + \Delta t) > x_+$  then
7         • Set posterior probability  $p_{\text{post}}(t + \Delta t) = \mathbb{P}_w[w(t + \Delta t) = +1 | \text{right exit}]$ 
          from Equation (7.107d), with  $\mathbb{P}[w(0) = +1] = p_{\text{prior}}$  and correspondingly
           $\mathbb{P}[w(0) = -1] = 1 - p_{\text{prior}}$  ;
8         • Update  $F_{\text{ext}}(t + \Delta t)$  according to Equation (7.5);
9         • Update the prior probability  $p_{\text{prior}}(t + \Delta t) = p_{\text{post}}(t + \Delta t)$ ;
10        • Reset boundaries to  $[x_-, x_+] = [x(t + \Delta t) - L/2, x(t + \Delta t) + L/2]$ ;
11    else if  $x(t + \Delta t) < x_-$  then
12        • Set posterior probability  $p_{\text{post}}(t + \Delta t) = \mathbb{P}_w[w(t + \Delta t) = +1 | \text{left exit}]$ 
          from Equation (7.107c), with  $\mathbb{P}[w(0) = +1] = p_{\text{prior}}$  and correspondingly
           $\mathbb{P}[w(0) = -1] = 1 - p_{\text{prior}}$  ;
13        • Update  $F_{\text{ext}}(t + \Delta t)$  according to Equation (7.5);
14        • Update the prior probability  $p_{\text{prior}}(t + \Delta t) = p_{\text{post}}(t + \Delta t)$ ;
15        • Reset boundaries to  $[x_-, x_+] = [x(t + \Delta t) - L/2, x(t + \Delta t) + L/2]$ ;
16    • Increment the simulation time,  $t = t + \Delta t$ 
    
```

This protocol was simulated for 400 values of $\text{Pe} = \nu^2/(\alpha D_x)$, evenly distributed in logarithmic space in the range $10^{-3} < \text{Pe} < 10^4$, and for a run duration of $T = 3 \times 10^5$ with $\Delta t = 10^{-4}$. Without loss of generality, the parameters were set as $\nu = 1$, $D_x = 1$, such that $\text{Pe} = \alpha^{-1}$, and then α was varied in the range $10^{-4} < \alpha < 10^3$. Although optimal work extraction is conjectured to be achieved only in the limit $L \rightarrow 0$, i.e. $\lim_{L \rightarrow 0} p_{\text{post}}(t) = \mathbb{P}[w(t) | \{x\}_0^t]$, in practice the restriction of a finite simulation timestep Δt prevents access to this limit. Instead, it was found numerically that, for given Δt , the power output is maximal at a small but finite interval size $L_{\text{opt}}(\Delta t)$, that depended on Pe . To account for this effect, the boundary-update protocol was executed for 60 evenly spaced values of L in the range $L \in [0.02, 1.2]$ to identify L_{opt} . Figure 7.6 illustrates the variation in time-averaged extractable power $\langle \dot{W} \rangle$ as a function of L for different values of Pe and demonstrates that optimal work extraction cannot be attained from a single choice of interval length L for all values of Pe .

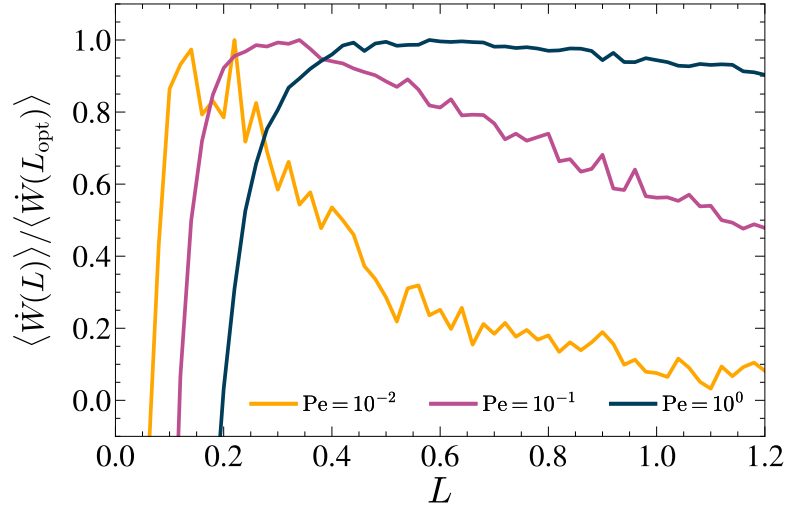


Figure 7.6: Time-averaged extractable power $\langle \dot{W}(L) \rangle$ as a function of interval length L for different values of Pe . The notation $\langle \bullet \rangle$ denotes a time-average over an entire simulated trajectory of duration $T = 3 \times 10^5$. The power is normalised by that attained using the optimal interval length L_{opt} at each Pe value. Since maximum power is attained at different interval lengths L_{opt} for each value of Pe , no single choice of L can be used for the entire range of values of Pe .

The numerical results for this protocol, which are shown in Figure 2 of the main text, are in excellent agreement with the theoretical asymptotes derived in Equations (7.3) and (7.25). Extending this approach to continuous-state self-propulsion dynamics, such as the AOU process, remains an open challenge.

~ Part 3 ~

Extension to dense active matter
systems

8

Active crystals

This chapter is based on a manuscript in preparation with Gunnar Pruessner under the working title ‘Exact treatment of two-dimensional harmonic active crystals’.

Author contributions to original manuscript: GP supervised the project. I derived the bulk of the analytical results and produced all figures. GP and I interpreted the results and wrote the manuscript.

Chapter summary

The purpose of this chapter is to lay the foundations for the study of dense active matter in the context of active engines. To do so, I examine one such class of dense active matter known as “active crystals”. An active crystal is a regularly arranged lattice of interacting active particles that emerges through motility induced phase separation. Here, I provide a thorough analysis of both one- and two-dimensional *harmonic* active crystals by performing exact calculations of their key thermodynamic properties, such as fluctuations, instantaneous energy, and entropy production. These results inform our understanding of how energy is dissipated in these systems, which is particularly relevant to the efficiency of active engines operating on ensembles of active particles. This chapter also addresses more foundational principles regarding crystalline order. More specifically, by appealing to Mermin’s original criterion [52], this chapter gives a definitive answer as to whether activity supports or undermines long-range translational order.

8.1 Introduction

One of the most striking phenomena in active matter is the formation of a condensed phase from active particles that interact only through repulsive forces [31]. When these condensates are densely packed in two dimensions, they form an almost perfect triangular lattice or “active crystal” [228–235]. Much of the understanding of the condensed phase in the literature is based on the much simpler analysis of the one-dimensional counterpart [236–247]. As a result, there is relatively little quantitative understanding of these crystals in higher dimensions as well as apparent or supposed clashes with established concepts such as the Mermin-Wagner theorem [52, 248–251]. Hence, to address these issues, this chapter will characterise such active crystals in two dimensions.

Starting from a setup of dense, non-linearly repulsively interacting active particles, I show in the appendix how a Langevin description of a *harmonic* active crystal is derived. In this description, the equations of motion are exactly solvable, so that correlation functions can be determined in exact form. These can then be used to quantify observables that are

physically more relevant, such as the entropy production [38, 44] and fluctuations [70]. The results relate the macroscopic properties of the active crystal directly to the underlying microscopic interactions. Crucially, I avoid entirely the commonly adopted approach of casting the dynamics as an effective one-dimensional equation (as used in Refs. [229–231] and originally derived in Refs. [32, 252]), characterised by a single effective coupling, whose interpretation hinges on the assumption that dimensionality has little to no bearing on the *average* behaviour of the system. Instead, I show in which sense crystalline order is or is not sustained in two dimensions. Such a quantitative characterisation of active crystals can also inform our understanding of more complex biological processes, such as extrusion events in cell monolayers [253].

The remainder of this chapter is structured as follows: in Section 8.2, I present a detailed overview of the model and highlight the features that have been ignored or unnecessarily approximated in the literature. Much of the technical details of the derivation are relegated to Appendix 8.B. In Section 8.3, I state the main results of the derivation, such as whether crystalline order exists according to Mermin’s criterion [52], Equation (8.8), the mean squared particle separation (i.e. the variance of the lattice spacing), Equation (8.12), the absence of equipartition, Equation (8.15), and finally the entropy production, Equation (8.20). The contribution to the entropy production from each normal mode is found to have the same form as that of non-interacting active particles moving in a harmonic potential [41, 42], suggesting the derived expression is generally applicable to any system of active particles subject to linear forces. Again, the details of the derivation can be found in the extensive appendix, in particular at the end of Appendix 8.A.a. I finally conclude this chapter in Section 8.4.

8.2 Model

In the following, I study the bulk-properties of a triangular lattice composed of active particles, Figure 8.1. Aside from motility induced phase separation [31], this can occur when active particles are confined to a finite volume by suitable boundaries. In contrast to passive systems, particles in the bulk may be subject to very significant pressures—either from the bath or the boundaries—so that their rest positions are determined by the balancing of all forces exerted by neighbouring particles, rather than those forces all vanishing. Hence, the pair potentials between any neighbouring particles residing at their rest positions are generally not at a minimum, Figure 8.1a, but rather the forces sum to zero. In other words, the particles are “hemmed in”.

The active particles are indexed by $\mathbf{n} = (n^1, n^2) \in \{1, 2, \dots, N_1\} \otimes \{1, 2, \dots, N_2\}$ and are described in terms of their displacement $\mathbf{u}_{\mathbf{n}}(t)$ from lattice positions $\mathbf{R}_{\mathbf{n}} = (\mathbf{a}_1 n^1 + \mathbf{a}_2 n^2)\ell$, where the primitive lattice vectors are dimensionless, i.e. $|\mathbf{a}_{1,2}| = 1$, and ℓ represents the physical lattice spacing. The setup is illustrated in Figure 8.1b. Throughout this chapter, superscripts will generally denote components of two-dimensional vectors, while subscripts will typically represent lattice indices.

I assume there is exactly one particle associated with each lattice site and therefore

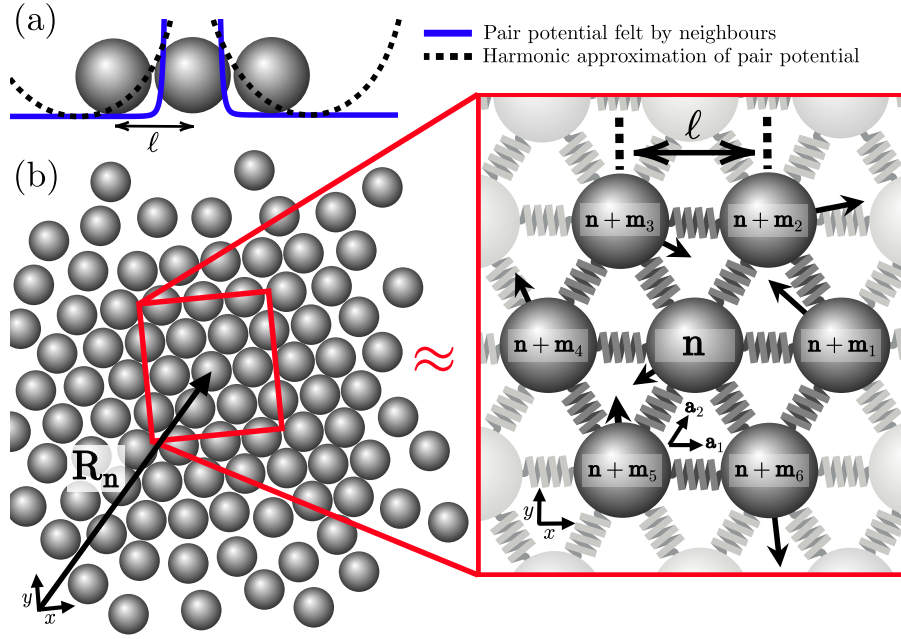


Figure 8.1: Schematic representation of how the bulk of a condensate of densely packed active particles, interacting through repulsive pair potentials, can be approximated by that of a harmonic active crystal. (a) Illustration of the repulsive pair potential felt by nearest neighbours of the central particle. To leading order, the neighbours are subject to a harmonic pair potential. (b) In the bulk of the condensate, particles form an ordered lattice. Harmonic particle interactions are illustrated by springs. Arrows indicate the direction and magnitude of each particle's self-propulsion $\mathbf{w}_{\mathbf{n}'}(t)$.

$V = N_1 N_2$ particles in total. For finite N_1 and N_2 , I assume periodic (Born-von Karman) boundary conditions, such that (n_1, n_2) refers to the same particle (and rest position) as $(n_1 + N_1, n_2)$ and $(n_1, n_2 + N_2)$. I further assume that every particle indexed by $\mathbf{n}$ interacts with 6 nearest neighbouring particles indexed by $\mathbf{n}' = \mathbf{n} + \mathbf{m}_q$ for $q = 1, 2, \dots, 6$, where $\mathbf{m}_q$ represents the allowed index “displacements”, as in Figure 8.1 and Appendix 8.A.a.

In order to keep displacements well-defined, I assume particles are initially located at $\mathbf{R}_{\mathbf{n}}$, so that $\mathbf{u}_{\mathbf{n}}(t = 0) = \mathbf{0}$. Given the periodic boundary conditions, there might be a rigid global translation

$$\bar{\mathbf{u}}(t) = \frac{1}{V} \sum_{\mathbf{n}} \mathbf{u}_{\mathbf{n}}(t) \quad (8.1)$$

of all particles, so that the $\mathbf{u}_{\mathbf{n}}(t)$ become much larger than the lattice spacing ℓ . Most of the relevant physics is thus captured by the *relative* displacement,

$$\mathbf{v}_{\mathbf{n}}(t) = \mathbf{u}_{\mathbf{n}}(t) - \bar{\mathbf{u}}(t). \quad (8.2)$$

The stochastic equation of motion in the harmonic approximation, Appendix 8.B, for the

triangular lattice is

$$\dot{\mathbf{u}}_{\mathbf{n}}(t) = - \sum_{\mathbf{n}'} \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'}(t) + \boldsymbol{\xi}_{\mathbf{n}}(t) + \mathbf{w}_{\mathbf{n}}(t), \quad (8.3)$$

with dynamical matrix $\mathbf{D}_{\mathbf{nn}'}$ as defined in Appendix 8.A.a [254], thermal noise characterised by the correlator matrix

$$\langle \boldsymbol{\xi}_{\mathbf{n}}(t) \boldsymbol{\xi}_{\mathbf{n}'}^{\top}(t') \rangle = \Gamma^2 \mathbb{1}_2 \delta_{\mathbf{n},\mathbf{n}'} \delta(t - t'), \quad (8.4)$$

where $\mathbb{1}_2$ is the 2×2 identity matrix, and active noise $\mathbf{w}_{\mathbf{n}}(t)$ with correlator

$$\langle \mathbf{w}_{\mathbf{n}}(t) \mathbf{w}_{\mathbf{n}'}^{\top}(t') \rangle = w^2 \mathbb{1}_2 \delta_{\mathbf{n},\mathbf{n}'} e^{-\mu|t-t'|}, \quad (8.5)$$

implementing the self-propulsion of speed w and correlation time $1/\mu$. Equation (8.5) represents a general active-noise correlator satisfied by the three canonical active particle models: active Ornstein-Uhlenbeck, run-and-tumble, and active Brownian (see Chapter 2). More complicated active noises can be considered and implemented by adjusting the derivation in Appendix 8.A.a. The identity matrix $\mathbb{1}_2$ in Equations (8.5) means activity in the x -direction does not affect activity in the y -direction, and vice versa, which arises from the mirror and rotation symmetry of the statistics of $\mathbf{w}(t)$.

As I assume nearest-neighbour interactions only, $\mathbf{D}_{\mathbf{nn}'}$ vanishes for all $\mathbf{n}'$ except for $\mathbf{n}' = \mathbf{n}$ and for the six nearest neighbours $\mathbf{n}' = \mathbf{n} + \mathbf{m}_q$. This renders Equation (8.3) amenable to a significant simplification by Fourier transform. However, $\mathbf{D}_{\mathbf{nn}'}$ is generally not diagonal for any of the six nearest neighbours $\mathbf{n}' = \mathbf{n} + \mathbf{m}_q$. Till now, this has been ignored in the literature by effectively replacing $\mathbf{D}_{\mathbf{nn}'}$ with $\sum_q \mathbf{D}_{\mathbf{n},\mathbf{n}+\mathbf{m}_q} = \mathbb{1}_2 \text{Tr } \mathbf{D}_{\mathbf{nn}}/2$ [229–231, 255], which amounts to an effective interaction averaged over the nearest neighbours. In this chapter, I will calculate the displacement-correlator without resorting to this effective one-dimensional approximation. I will then use the resulting framework to derive some key properties of active crystals in closed form.

8.3 Results and discussion

The relative displacements $\mathbf{v}_{\mathbf{n}}(t)$ can be described in terms of wavevectors located in the first Brillouin zone, i.e. $\mathbf{k}_{\mathbf{p}} = (2\pi p^1/N_1, 2\pi p^2/N_2)$, where $\mathbf{p} = (p^1, p^2) \in \{0, 1, \dots, N_1 - 1\} \otimes \{0, 1, \dots, N_2 - 1\} = \mathbb{P}$. The wavevectors can be seen as an arbitrary local degree of freedom displaying collective excitations, resulting in wave-like $\mathbf{v}_{\mathbf{n}}(t)$ varying between lattice sites $\mathbf{n}$. They are also the Fourier modes of functions of $\mathbf{n}$, which become arbitrarily dense in the thermodynamic limit. In physical space, where $\mathbf{n}$ corresponds to $\mathbf{R}_{\mathbf{n}}$, the largest component of such a Fourier mode has magnitude $2\pi/\ell$, the smallest has magnitude $2\pi/L_{1,2}$, with $L_{1,2} = N_{1,2}\ell$ the physical extent of the lattice.

While I will present the results in terms of these Fourier modes, Mermin instead used the reciprocal lattice vectors in his seminal paper to characterise crystallinity [52]. In that work, Mermin focused on the properties of the expectation of the instantaneous density

$\sum_{\mathbf{n}} \delta(\mathbf{R}_{\mathbf{n}} + \mathbf{u}_{\mathbf{n}}(t) - \mathbf{x})$ and its Fourier-modes. Since there may be a global rigid displacement $\bar{\mathbf{u}}(t)$ in the present setup—in contrast to Mermin’s original setup—one may instead define the density as $\rho(\mathbf{x}; t) = \sum_{\mathbf{n}} \delta(\mathbf{R}_{\mathbf{n}} + \mathbf{v}_{\mathbf{n}}(t) - \mathbf{x})$ in the present case.

All $\mathbf{v}_{\mathbf{n}}(t)$ follow the same statistics for different $\mathbf{n}$, so the density $\langle \rho(\mathbf{x}; t) \rangle$ is invariant under changing the fixed $\mathbf{n}'$ in

$$\langle \rho(\mathbf{x}; t) \rangle = \sum_{\mathbf{n}} \langle \delta(\mathbf{R}_{\mathbf{n}} + \mathbf{v}_{\mathbf{n}'}(t) - \mathbf{x}) \rangle, \quad (8.6)$$

with the sum solely implementing the translational invariance $\langle \rho(\mathbf{x}; t) \rangle = \langle \rho(\mathbf{x} + \mathbf{R}_{\mathbf{n}}; t) \rangle$ for *any* lattice vector $\mathbf{R}_{\mathbf{n}}$. With this periodicity, the Fourier transform

$$\langle \hat{\rho}(\mathbf{q}; t) \rangle = \int d^d x e^{-i\mathbf{x} \cdot \mathbf{q}} \langle \rho(\mathbf{x}; t) \rangle = V \left\langle e^{-i\mathbf{q} \cdot \mathbf{v}_{\mathbf{n}'}(t)} \right\rangle, \quad (8.7)$$

taken over the entire physical space, draws on the physical reciprocal lattice vectors $\mathbf{q}$ such that $\mathbf{q} \cdot \mathbf{R}_{\mathbf{n}}$ is an integer multiple of 2π for every $\mathbf{n}$. The smallest, non-vanishing reciprocal lattice vector has magnitude $2\pi/\ell$, while there is no largest, reflecting that the $\mathbf{v}_{\mathbf{n}}(t)$ are continuous, so that $\rho(\mathbf{x}; t)$ may be evaluated for any $\mathbf{x}$ within the unit cell.

Crystallinity—according to Mermin [52]—depends on finding a non-vanishing *non-trivial* mode $\langle \hat{\rho}(\mathbf{q}; t) \rangle$, Equation (8.7), i.e. a non-zero reciprocal lattice vector for which $\langle \hat{\rho}(\mathbf{q}; t) \rangle$ is non-zero. Equation (8.7) renders $\langle \hat{\rho}(\mathbf{q}; t) \rangle$ proportional to the characteristic function of the local displacements $\mathbf{v}_{\mathbf{n}}(t)$. In the harmonic approximation used in this chapter, the characteristic function is Gaussian—provided the noises are also Gaussian—whence

$$\frac{1}{V} \langle \hat{\rho}(\mathbf{q}; t) \rangle = \left\langle e^{-i\mathbf{q} \cdot \mathbf{v}_{\mathbf{n}'}(t)} \right\rangle = e^{-\frac{1}{2} \mathbf{q} \cdot \langle \mathbf{v}_{\mathbf{n}'}(t) \mathbf{v}_{\mathbf{n}'}^T(t) \rangle \mathbf{q}}, \quad (8.8)$$

which does indeed vanish in the thermodynamic limit, for all non-vanishing $\mathbf{q}$, if all eigenvalues of the correlation matrix $\langle \mathbf{v}_{\mathbf{n}'}(t) \mathbf{v}_{\mathbf{n}'}^T(t) \rangle$ diverge in the thermodynamic limit. In general, however, the active noises might not be Gaussian. In that case, one might resort to the easier task of verifying only whether the correlator $\langle \mathbf{v}_{\mathbf{n}'}(t) \cdot \mathbf{v}_{\mathbf{n}'}(t) \rangle$ diverges.

Based on the detailed calculation in Appendix 8.A.a, the correlation matrix in the steady state behaves like Equation (8.57) reproduced here,

$$\lim_{t \rightarrow \infty} \left\langle \mathbf{v}_{\mathbf{n}}(t) \mathbf{v}_{\mathbf{n}}^T(t) \right\rangle = \frac{1}{V} \sum_{\mathbf{p}}^* \left(\mathbf{E}_{\mathbf{p}}^- \left[\frac{w^2}{\lambda_{\mathbf{p}}^-(\lambda_{\mathbf{p}}^- + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^-} \right] + \mathbf{E}_{\mathbf{p}}^+ \left[\frac{w^2}{\lambda_{\mathbf{p}}^+(\lambda_{\mathbf{p}}^+ + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^+} \right] \right), \quad (8.9)$$

where the starred sum $\sum_{\mathbf{p}}^*$ runs over $\mathbf{p} \in \mathbb{P} \setminus \{(0, 0)\}$, i.e. it omits $\mathbf{p} = (0, 0)$, and $\mathbf{E}_{\mathbf{p}}^{\pm}$ are matrices formed from the eigenvectors of the dynamical matrix, Equation (8.54), which has corresponding eigenvalues $\lambda_{\mathbf{p}}^{\pm}$. In large V , the right-hand side of Equation (8.9) is logarithmically divergent. A harmonic active crystal in two dimensions therefore does not display crystalline order according to Mermin’s criterion above. In fact, Equation (8.9) would suggest activity undermines crystalline order more so than in its absence.

A similar result is obtained for a one-dimensional active crystal, for which the steady-state variance of the relative displacement is found to be

$$\lim_{t \rightarrow \infty} \langle v_n(t) v_n(t) \rangle = \frac{1}{N} \sum_{p=1}^{N-1} \left(\frac{w^2}{\hat{D}_p(\hat{D}_p + \mu)} + \frac{\Gamma^2}{2\hat{D}_p} \right), \quad (8.10)$$

as given in Equation (8.88), where $\hat{D}_p$ are the Fourier modes of the equivalent dynamical interaction in one dimension. However, the divergence of the variance for the one-dimensional crystal is linear in the total particle number N , and one can indeed show that

$$\lim_{t \rightarrow \infty} \langle v_n(t) v_n(t) \rangle \approx \frac{N}{12U''(\ell)} \left(\frac{w^2}{\mu} + \frac{\Gamma^2}{2} \right), \quad \text{for } N \gg 1, \quad (8.11)$$

where $U(|\mathbf{u}_n(t) - \mathbf{u}_{n+\mathbf{m}_q}(t) - \ell \mathbf{a}_q|)$ is the pair potential between neighbouring particles.

Arguably, the expected particle separation is of greater physical relevance than Mermin's criterion for crystallinity. This is because a finite particle separation is required to maintain, firstly, the harmonic approximation of the potential, Appendix 8.B, and, secondly, the local neighbourhood of any given lattice site. In other words, if the average particle separation becomes large with respect to ℓ and particles start slipping past each other, then the notion of a lattice of active particles breaks down. While the divergences encountered in the correlation matrix of the two-dimensional crystal, Equation (8.9), may be read as the small- k behaviour of the integral $\int_{2\pi/L}^{2\pi/\ell} d^2k k^{-2}$, unsurprisingly, these divergences do not occur for the mean squared particle separation, which goes as $\int_{2\pi/L}^{2\pi/\ell} d^2k k^0$. As a result, one could alternatively define crystalline *integrity* as finite average particle separation even in the absence of crystallinity according to Mermin's criterion. In two dimensions, the steady-state mean squared particle separation is (up to a shift of ℓ^2),

$$\begin{aligned} \lim_{t \rightarrow \infty} \langle |\mathbf{u}_n(t) - \mathbf{u}_{n+\mathbf{m}_q}(t)|^2 \rangle &= \frac{1}{V} \sum_{\mathbf{p}}^* 2(1 - \cos(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{m}_q)) \left(\frac{w^2}{\lambda_{\mathbf{p}}^-(\lambda_{\mathbf{p}}^- + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^-} \right. \\ &\quad \left. + \frac{w^2}{\lambda_{\mathbf{p}}^+(\lambda_{\mathbf{p}}^+ + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^+} \right), \end{aligned} \quad (8.12)$$

which is finite as $(1 - \cos(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{m}_q))/\lambda_{\mathbf{p}}^{\pm}$ is bounded. In comparison, the steady-state mean squared particle separation for a one-dimensional crystal is

$$\lim_{t \rightarrow \infty} \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle = \frac{1}{N} \sum_{p=1}^{N-1} 2(1 - \cos(k_p)) \left(\frac{w^2}{\hat{D}_p(\hat{D}_p + \mu)} + \frac{\Gamma^2}{2\hat{D}_p} \right), \quad (8.13)$$

which is always independent of q . Once again, a compact expression for the one-dimensional case is obtained in the thermodynamic limit, i.e.

$$\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle = \frac{1}{U''(\ell)} \left(\frac{w^2}{\mu \sqrt{1 + 4 \frac{U''(\ell)}{\mu}}} + \frac{\Gamma^2}{2} \right), \quad (8.14)$$

clearly indicating that the average particle separation remains finite. More generally, the finiteness of Equations (8.12) and (8.13) guarantees crystalline integrity in the sense that the local neighbourhood of a particle is maintained, even when the squared relative displacement of individual sites diverges.

I will now consider more global features of the crystal, namely energy and entropy production. Within the harmonic approximation, the energy is readily expressed in terms of the dynamical matrix, Equation (8.108), whence

$$\lim_{t \rightarrow \infty} \langle \mathcal{E}_{\text{harm.}}(t) \rangle = \frac{1}{4} \Gamma^2 d(V-1) + \frac{1}{2} w^2 \sum_{\mathbf{p}}^* \left(\frac{1}{\lambda_{\mathbf{p}}^+ + \mu} + \frac{1}{\lambda_{\mathbf{p}}^- + \mu} \right). \quad (8.15)$$

up to an irrelevant constant offset $3VU(\ell)$, as in Equation (8.63). The first term on the right-hand side of Equation (8.15) is solely due to the thermal noise, with Γ^2 , Equation (8.4), playing the role of (twice) a diffusion constant or (twice) the thermal energy $k_B T$. Hence, $\Gamma^2 d(V-1)/4$ apportions an energy of $k_B T/2$ to each of the $d(V-1)$ degrees of freedom, with the total number of modes V being reduced by one due to the divergent zero-mode not contributing. The second term on the right-hand side of Equation (8.15) is solely due to the self-propulsion/activity w . If the pair potential between particles is very soft, so that both U'' and U'/ℓ are small compared to μ , then the summands in Equation (8.15) depend only weakly on $\mathbf{p}$ via $\lambda_{\mathbf{p}}$, Equation (8.34). Thus, the total contribution due to the sum may be approximated in this case by $w^2 d(V-1)/(2\mu)$. Comparing to the first term in Equation (8.15) would suggest that for μ large compared to the pair potential U , the activity plays the role of a diffusion constant w^2/μ , see Chapter 2.

If, on the other hand, the pair-potential is stiff compared to the characteristic frequency μ , then the contributions to the overall energy of the active crystal from different modes becomes dependent on $\mathbf{p}$, signifying the breakdown of equipartition, with both very small $\mathbf{p}$ and very large $\mathbf{p}$ making the most significant contributions to the energy as these correspond to small $\lambda_{\mathbf{p}}$.

Unlike the two-dimensional case above, the energy of the one-dimensional crystal can be readily expressed in terms of the mean squared separation, Equation (8.13), explicitly

$$\langle \mathcal{E}_{\text{harm.}}(t) \rangle = \frac{1}{2} \sum_{n=1}^N \sum_{q=1}^2 \frac{1}{2} U''(\ell) \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle, \quad (8.16)$$

up to an irrelevant constant offset $NU(\ell)$, where the factor $1/2$ accounts for double counting of the pair potentials in the double sum, as $|u_n(t) - u_{n+m_q}(t)|$ is the same for either n with $q=1$, or $n+1$ with $q=2$. Then, using Equation (8.14), the steady-state energy per particle in the thermodynamic limit is

$$\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} \frac{\langle \mathcal{E}_{\text{harm.}}(t) \rangle}{N} = \frac{1}{2} \left(\frac{w^2}{\mu \sqrt{1 + 4 \frac{U''(\ell)}{\mu}}} + \frac{\Gamma^2}{2} \right). \quad (8.17)$$

This illustrates that the energy of a crystal depends on the interactions between its constituents *only* if those constituents are active. Otherwise, the energy is the same as that of an ensemble of non-interacting particles.

Finally, the entropy production of the crystal can be derived on the basis of the framework in Ref. [106], in particular Equation (8.68) reproduced in the appendix, which has two contributions: one from the effective velocity squared over the thermal diffusion constant, $\Gamma^2/2$, and one from the second derivative of the pair-potential, which is readily expressed in terms of the trace of the dynamical matrix, Equation (8.69). After rewriting in terms of Fourier modes, one ultimately obtains the following expression for the entropy production per particle

$$\langle \dot{\sigma}_{\mathbf{n}} \rangle = \frac{1}{V} \sum_{\mathbf{p}} \frac{2w^2}{\Gamma^2} \frac{2 + \mu^{-1}(\lambda_{\mathbf{p}}^+ + \lambda_{\mathbf{p}}^-)}{(1 + \mu^{-1}\lambda_{\mathbf{p}}^+)(1 + \mu^{-1}\lambda_{\mathbf{p}}^-)}, \quad (8.18)$$

as found in Equation (8.74). Similarly, the entropy production per particle for the one-dimensional crystal is

$$\langle \dot{\sigma}_n \rangle = \frac{1}{N} \sum_{p=0}^{N-1} \frac{2w^2}{\Gamma^2} \frac{\mu}{\mu + \hat{D}_p}. \quad (8.19)$$

Equation (8.18) is seen to be of the same form as Equation (8.19) by setting the eigenvalues $\lambda_{\mathbf{p}}^{\pm}$ equal to each other (which would correspond to that of a two-dimensional square crystal, or two independent one-dimensional crystals in the harmonic case) and then halving the result. In the absence of interactions, or for $\mu \rightarrow \infty$, the entropy production in both cases reduces to that of a free active particle $2w^2/\Gamma^2$, as calculated in Chapter 2.

Finally, note that the entropy production per particle of the two-dimensional crystal can be rewritten in the highly compact form

$$\langle \dot{\sigma}_{\mathbf{n}} \rangle = \frac{1}{V} \sum_{\mathbf{p}} \frac{2w^2}{\Gamma^2} \frac{\text{Tr}(\mathbb{1}_2 + \mu^{-1}\hat{\mathbf{D}}_{\mathbf{p}})}{\det(\mathbb{1}_2 + \mu^{-1}\hat{\mathbf{D}}_{\mathbf{p}})}. \quad (8.20)$$

The derivation of the entropy production constitutes a key result of this chapter and is made more remarkable by the fact that its derivation assumes nothing other than translational invariance and that the dynamics of the two-dimensional system in question satisfy the Langevin equation (8.3) for *any* symmetric $\mathbf{D}_{\mathbf{n}\mathbf{n}'}$. In particular, any two-dimensional system of active particles subject to harmonic interactions, whether external or interparticle, has an entropy production given by Equation (8.20). Since the motion about the minimum of any potential is often approximated as harmonic, this makes Equation (8.20) extremely general. Indeed, one can recover the entropy production rate of a generic active particle in a harmonic potential of strength κ , as derived in Refs. [41, 42], by choosing $\mathbf{D}_{\mathbf{n}\mathbf{n}'} = \kappa \mathbb{1}_2$ for $\mathbf{n}' = \mathbf{n}$ and 0 for all other $\mathbf{n}'$.

8.4 Conclusion

In this chapter, I derived exact analytical expressions for the key thermodynamic properties of harmonic active crystals, including their fluctuations, Equations (8.9) and (8.14), energy, Equations (8.15)–(8.17), and entropy production, Equations (8.18)–(8.20). Importantly, the approach avoided casting the dynamics as an effective one-dimensional description [229–231, 255], and therefore provided a more accurate description of an active crystal.

The divergence of the displacement correlation function, Equations (8.9), suggests that active crystals do not display long-range translational order according to Mermin’s original criterion [52]. However, I demonstrated that—despite these diverging fluctuations—crystalline *integrity* is maintained in the sense that the average particle separation remains constant in the thermodynamic limit, see Equations (8.12) and (8.14). This suggests that both one- and two-dimensional active crystals sustain their ordered structure in infinitely large systems, while also validating the use of the harmonic approximation in Appendix 8.B.

In the context of the wider thesis, this chapter contributed to the broader understanding of entropy production in active matter systems. By leveraging the exact results mentioned above, I derived a highly general expression for the entropy production that paves the way for the study of energy dissipation in ensembles of active particles. Furthermore, by thoroughly analysing the properties of active crystals, this chapter lays the groundwork for understanding how work can be extracted from dense active matter. The exact calculations presented here are essential for future research aimed at designing efficient active engines. Future extensions to this work could include exploring higher-dimensional crystals, alternative boundary conditions, and the impact of defects, all of which would further our understanding of active matter and its potential practical applications.

CHAPTER 8 APPENDICES

8.A Notation and derivation

In this appendix, I introduce the notation used in the main text and provide detailed derivations of many of this chapter's exact results. I begin with that of the more illustrative two-dimensional active crystal, before doing the same for its simpler one-dimensional counterpart.

8.A.a Two-dimensional crystals

Fluctuations and energy

The notation used in this chapter obeys the following conventions: vectors are bold lower-case roman characters, whilst matrices are upper-case bold sans-serif characters. Components are indexed by superscripts, using α as their index when needed. Positions on the real lattice are indexed by $\mathbf{n} \in \mathbb{Z}^2$, and displacements, i.e. differences between any such indices, by $\mathbf{m}$. This notation is essentially that of Ashcroft and Mermin's *Solid State Physics* [254, Ch. 22, Equation (22.45)], while being stricter about parameter dependencies as well as the use of lower-case and upper-case bold characters. For example, Ashcroft and Mermin use $\mathbf{R}$ to indicate the position of a site on the regular lattice, when I write $\mathbf{R}_{\mathbf{n}}$, and they write the dynamical matrix as a function $\mathbf{D}(\mathbf{R} - \mathbf{R}')$ whereas I write $\mathbf{D}_{\mathbf{nn}'}$.

Under the harmonic approximation outlined in Appendix 8.B, the stochastic equation of motion is

$$\dot{\mathbf{u}}_{\mathbf{n}}(t) = - \sum_{\mathbf{n}'} \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'}(t) + \boldsymbol{\xi}_{\mathbf{n}}(t) + \mathbf{w}_{\mathbf{n}}(t), \quad (8.21)$$

where $\mathbf{u}_{\mathbf{n}}(t) \in \mathbb{R}^2$ is the local displacement vector at a site $\mathbf{R}_{\mathbf{n}}$ indexed by the vector $\mathbf{n} \in \{1, 2, \dots, N_1\} \otimes \{1, 2, \dots, N_2\} = \mathbb{S}$, so that the total number of sites is $V = N_1 N_2$. There are two independent vectorial noises acting at each site. Firstly, the thermal noise $\boldsymbol{\xi}_{\mathbf{n}}(t)$ with correlation matrix

$$\langle \boldsymbol{\xi}_{\mathbf{n}}(t) \boldsymbol{\xi}_{\mathbf{n}'}^T(t') \rangle = \Gamma^2 \mathbb{1}_2 \delta_{\mathbf{n}, \mathbf{n}'} \delta(t - t'), \quad (8.22)$$

where $\mathbb{1}_2$ denotes the 2×2 identity matrix. The expectation on the left-hand side of Equation (8.22) is taken over an outer product so that the correlator may equivalently be written in terms of components indexed by $\alpha, \alpha' \in \{1, 2\}$,

$$\langle \xi_{\mathbf{n}}^{\alpha}(t) \xi_{\mathbf{n}'}^{\alpha'}(t') \rangle = \Gamma^2 \delta^{\alpha, \alpha'} \delta_{\mathbf{n}, \mathbf{n}'} \delta(t - t'). \quad (8.23)$$

There is also the active noise $\mathbf{w}_{\mathbf{n}}(t)$ with correlator

$$\langle \mathbf{w}_{\mathbf{n}}(t) \mathbf{w}_{\mathbf{n}'}^T(t') \rangle = w^2 \mathbb{1}_2 \delta_{\mathbf{n}, \mathbf{n}'} e^{-\mu |t - t'|}, \quad (8.24)$$

which renders the evolution of $\mathbf{u}_{\mathbf{n}}(t)$ by itself, i.e. without explicit knowledge of $\mathbf{w}_{\mathbf{n}}(t)$, non-Markovian, except in the limiting case where the noise amplitude $w \propto \mu$ and $\mu \rightarrow \infty$.

The active noise being diagonal in the components, i.e. proportional to $\mathbb{1}_2$, simplifies the calculations below. This arises from the mirror and rotation symmetry of the statistics of $\mathbf{w}(t)$.

The sum on the right-hand side of Equation (8.21) runs over all sites $\mathbf{n}' \in \mathbb{S}$, but the dynamical matrix $\mathbf{D}_{\mathbf{n}\mathbf{n}'}$ is defined such that it vanishes for $\mathbf{n}'$ that are not nearest neighbours of $\mathbf{n}$. It is further chosen to be translationally invariant, specifically

$$\mathbf{D}_{\mathbf{n}\mathbf{n}'} = \begin{cases} -\frac{U'(\ell)}{\ell} \mathbb{1}_2 - \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) (\mathbf{a}_q \mathbf{a}_q^\top), & \text{for } \mathbf{n}' = \mathbf{n} + \mathbf{m}_q, \\ 3 \left(U''(\ell) + \frac{U'(\ell)}{\ell} \right) \mathbb{1}_2, & \text{for } \mathbf{n}' = \mathbf{n}, \\ 0, & \text{otherwise,} \end{cases} \quad (8.25)$$

based on the harmonic approximation in Appendix 8.B. Here, $\mathbf{a}_q \mathbf{a}_q^\top$ denotes an outer product, with all $\mathbf{a}_q$ normalised, i.e. $|\mathbf{a}_q|^2 = 1$, and the physical distance between sites given by ℓ .

The definition (8.25) of $\mathbf{D}_{\mathbf{n}\mathbf{n}'}$ spells out that the dynamical matrix is non-zero only when $\mathbf{n}'$ is either $\mathbf{n}$ or a nearest neighbouring site, with periodic boundary conditions applied such that, say, $(0, n_2)$ and (N, n_2) refer to the same site. In what direction on the lattice a site is a nearest neighbour is encoded by q as $\mathbf{n}' = \mathbf{n} + \mathbf{m}_q$. The set of “allowed” differences in the indices $\{\mathbf{m}_1, \dots, \mathbf{m}_6\} = \{(1, 0)^\top, (0, 1)^\top, (-1, 1)^\top, (-1, 0)^\top, (0, -1)^\top, (1, -1)^\top\}$ has, associated with it, a corresponding set of lattice vectors $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_6\}$, which can all be written as linear combinations of the primitive lattice vectors $\mathbf{a}_1 = (1, 0)^\top$ and $\mathbf{a}_2 = (1/2, \sqrt{3}/2)^\top$,

$$\mathbf{a}_q = m_q^1 \mathbf{a}_1 + m_q^2 \mathbf{a}_2 = \mathbf{A} \mathbf{m}_q, \quad (8.26)$$

where $\mathbf{m}_q = (m_q^1, m_q^2)^\top$ and $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2)$ is the matrix composed of the column vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. The entry $\mathbf{D}_{\mathbf{n}\mathbf{n}}$ is the negative of the total sum of the entries for the nearest neighbours,

$$\mathbf{D}_{\mathbf{n}\mathbf{n}} = - \sum_{q=1}^6 \mathbf{D}_{\mathbf{n}, \mathbf{n} + \mathbf{m}_q} = 3 \left(U''(\ell) + \frac{U'(\ell)}{\ell} \right) \mathbb{1}_2. \quad (8.27)$$

As $\mathbf{D}_{\mathbf{n}\mathbf{n}'}$ is translationally invariant, the Fourier transform

$$\hat{\mathbf{u}}_{\mathbf{p}}(t) = \sum_{\mathbf{n}} e^{-i\mathbf{k}_{\mathbf{p}} \cdot \mathbf{n}} \mathbf{u}_{\mathbf{n}}(t), \quad (8.28a)$$

$$\mathbf{u}_{\mathbf{n}}(t) = \frac{1}{V} \sum_{\mathbf{p}} e^{i\mathbf{k}_{\mathbf{p}} \cdot \mathbf{n}} \hat{\mathbf{u}}_{\mathbf{p}}(t), \quad (8.28b)$$

diagonalises the equation of motion (8.21).

Henceforth, $\mathbf{n} \in \mathbb{S}$ is reserved to index a lattice site and $\mathbf{p} \in \{0, 1, \dots, N_1 - 1\} \otimes \{0, 1, \dots, N_2 - 1\} = \mathbb{P}$ to index wavevectors. The wavevector is determined from $\mathbf{p} = (p^1, p^2)^\top$ by $\mathbf{k}_{\mathbf{p}} = (2\pi p^1/N_1, 2\pi p^2/N_2)^\top$, where superscripts are used here to denote components, but will occasionally also be used elsewhere to denote exponents. Whichever convention is being used will be clear from context.

Performing a similar transform on the dynamical matrix,

$$\hat{\mathbf{D}}_{\mathbf{p}\mathbf{p}'} = \sum_{\mathbf{n}, \mathbf{n}'} e^{-i(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{n} + \mathbf{k}_{\mathbf{p}'} \cdot \mathbf{n}')} \mathbf{D}_{\mathbf{n}\mathbf{n}'}, \quad (8.29a)$$

$$\mathbf{D}_{\mathbf{n}\mathbf{n}'} = \frac{1}{V^2} \sum_{\mathbf{p}, \mathbf{p}'} e^{i(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{n} + \mathbf{k}_{\mathbf{p}'} \cdot \mathbf{n}')} \hat{\mathbf{D}}_{\mathbf{p}\mathbf{p}'}, \quad (8.29b)$$

and correspondingly for the thermal and active noise, with correlators

$$\langle \hat{\xi}_{\mathbf{p}}^{\alpha}(t) \hat{\xi}_{\mathbf{p}'}^{\alpha'}(t') \rangle = \Gamma^2 V \delta_{\mathbf{p}+\mathbf{p}', 0} \delta^{\alpha, \alpha'} \delta(t - t'), \quad (8.30a)$$

$$\langle \hat{w}_{\mathbf{p}}^{\alpha}(t) \hat{w}_{\mathbf{p}'}^{\alpha'}(t') \rangle = w^2 V \delta_{\mathbf{p}+\mathbf{p}', 0} \delta^{\alpha, \alpha'} e^{-\mu|t-t'|}, \quad (8.30b)$$

results in the Langevin Equation (8.21) simplifying to

$$\dot{\hat{\mathbf{u}}}_{\mathbf{p}}(t) = -\hat{\mathbf{D}}_{\mathbf{p}} \hat{\mathbf{u}}_{\mathbf{p}}(t) + \hat{\xi}_{\mathbf{p}}(t) + \hat{\mathbf{w}}_{\mathbf{p}}(t). \quad (8.31)$$

Above, I introduced the Fourier-transformed dynamical 2×2 matrix depending on only a single wavevector index $\mathbf{p}$,

$$\hat{\mathbf{D}}_{\mathbf{p}\mathbf{p}'} = V \delta_{\mathbf{p}+\mathbf{p}', 0} \hat{\mathbf{D}}_{\mathbf{p}} = V \delta_{\mathbf{p}+\mathbf{p}', 0} \sum_{q=1}^3 2[1 - \cos(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{m}_q)] \left\{ \frac{U'(\ell)}{\ell} \mathbb{1}_2 + \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \mathbf{a}_q \mathbf{a}_q^{\top} \right\}, \quad (8.32)$$

where I used that $\mathbf{D}_{\mathbf{n}\mathbf{n}'}$ is translational invariant, as well as $\mathbf{m}_q = -\mathbf{m}_{q+3}$ and $\mathbf{a}_q \mathbf{a}_q^{\top} = \mathbf{a}_{q+3} \mathbf{a}_{q+3}^{\top}$ for $q \in \{1, 2, 3\}$. As the elements of $\hat{\mathbf{D}}_{\mathbf{p}} = \begin{pmatrix} \hat{\mathbf{D}}_{\mathbf{p}}^{1,1} & \hat{\mathbf{D}}_{\mathbf{p}}^{1,2} \\ \hat{\mathbf{D}}_{\mathbf{p}}^{2,1} & \hat{\mathbf{D}}_{\mathbf{p}}^{2,2} \end{pmatrix}$ will appear in what follows, I spell out their explicit form here,

$$\begin{aligned} \hat{\mathbf{D}}_{\mathbf{p}}^{1,1} &= \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \left\{ 3 - 2 \cos\left(\frac{2\pi p^1}{N_1}\right) - \frac{1}{2} \left[\cos\left(\frac{2\pi p^1}{N_1} - \frac{2\pi p^2}{N_2}\right) + \cos\left(\frac{2\pi p^2}{N_2}\right) \right] \right\} \\ &\quad + \frac{U'(\ell)}{\ell} \left[6 - 2 \cos\left(\frac{2\pi p^1}{N_1}\right) - 2 \cos\left(\frac{2\pi p^1}{N_1} - \frac{2\pi p^2}{N_2}\right) - 2 \cos\left(\frac{2\pi p^2}{N_2}\right) \right], \end{aligned} \quad (8.33a)$$

$$\hat{\mathbf{D}}_{\mathbf{p}}^{1,2} = \hat{\mathbf{D}}_{\mathbf{p}}^{2,1} = \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \frac{\sqrt{3}}{2} \left[\cos\left(\frac{2\pi p^1}{N_1} - \frac{2\pi p^2}{N_2}\right) - \cos\left(\frac{2\pi p^2}{N_2}\right) \right], \quad (8.33b)$$

$$\begin{aligned} \hat{\mathbf{D}}_{\mathbf{p}}^{2,2} &= \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \left\{ 3 - \frac{3}{2} \left[\cos\left(\frac{2\pi p^1}{N_1} - \frac{2\pi p^2}{N_2}\right) + \cos\left(\frac{2\pi p^2}{N_2}\right) \right] \right\} \\ &\quad + \frac{U'(\ell)}{\ell} \left[6 - 2 \cos\left(\frac{2\pi p^1}{N_1}\right) - 2 \cos\left(\frac{2\pi p^1}{N_1} - \frac{2\pi p^2}{N_2}\right) - 2 \cos\left(\frac{2\pi p^2}{N_2}\right) \right]. \end{aligned} \quad (8.33c)$$

In the form of Equation (8.31), the Langevin equation has a simple, exponential, formal solution. Making the solution explicit requires finding the eigensystem of the 2×2 matrix

$\hat{\mathbf{D}}_{\mathbf{p}}$. The two eigenvalues for each $\mathbf{p}$ are

$$\lambda_{\mathbf{p}}^{\pm} = \frac{1}{2} \left(\hat{\mathbf{D}}_{\mathbf{p}}^{1,1} + \hat{\mathbf{D}}_{\mathbf{p}}^{2,2} \pm \sqrt{\left(\hat{\mathbf{D}}_{\mathbf{p}}^{1,1} - \hat{\mathbf{D}}_{\mathbf{p}}^{2,2} \right)^2 + 4 \left(\hat{\mathbf{D}}_{\mathbf{p}}^{1,2} \right)^2} \right), \quad (8.34)$$

which are even in $\mathbf{p}$ and all positive except for the $\mathbf{0}$ -mode $\mathbf{p} = \mathbf{0}$, in which case both eigenvalues vanish.

To see that the eigenvalues are non-negative, first note that

$$\begin{aligned} \lambda_{\mathbf{p}}^+ + \lambda_{\mathbf{p}}^- &= \text{Tr}(\hat{\mathbf{D}}_{\mathbf{p}}) \\ &= \left(U''(\ell) + \frac{U'(\ell)}{\ell} \right) \left[6 - 2 \cos \left(\frac{2\pi p^1}{N_1} \right) - 2 \cos \left(\frac{2\pi p^2}{N_2} \right) - \cos \left(\frac{2\pi p^1}{N_1} - \frac{2\pi p^2}{N_2} \right) \right], \end{aligned} \quad (8.35)$$

which is non-negative for all p^1 and p^2 provided $U''(\ell) + U'(\ell)/\ell \geq 0$, which is generally the case for a purely repulsive pair potential. It then remains to show that $\lambda_{\mathbf{p}}^+ \lambda_{\mathbf{p}}^- = \det(\hat{\mathbf{D}}_{\mathbf{p}}) \geq 0$. To show that the determinant of the dynamical matrix is always non-negative, it is instructive to rewrite the dynamical matrix in the form

$$\hat{\mathbf{D}}_{\mathbf{p}} = \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \mathbf{S}_{\mathbf{p}} + \frac{U'(\ell)}{\ell} \text{Tr}(\mathbf{S}_{\mathbf{p}}) \mathbb{1}_2, \quad (8.36)$$

by inspection of Equation (8.33), where $\text{Tr}(\mathbf{S}_{\mathbf{p}}) = 6 - 2 \cos(2\pi p^1/N_1) - 2 \cos(2\pi p^2/N_2) - 2 \cos(2\pi p^1/N_1 - 2\pi p^2/N_2)$. Next, one can use the general result $\det(\mathbf{B} + \mathbf{C}) = \det(\mathbf{C}) + \det(\mathbf{B}) + \text{Tr}(\mathbf{C}^{-1}\mathbf{B}) \det(\mathbf{C})$ for any 2×2 matrices $\mathbf{B}$ and $\mathbf{C}$, to eventually obtain

$$\det(\hat{\mathbf{D}}_{\mathbf{p}}) = U''(\ell) \frac{U'(\ell)}{\ell} [\text{Tr}(\mathbf{S}_{\mathbf{p}})]^2 + \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right)^2 \det(\mathbf{S}_{\mathbf{p}}). \quad (8.37)$$

Since $\mathbf{S}_{\mathbf{p}}$ is independent of any parameters, one can readily show (using Mathematica for instance) that $\det(\mathbf{S}_{\mathbf{p}}) \geq 0$ for all $\mathbf{p}$. Hence, if $U''(\ell)$ and $U'(\ell)$ have the same sign (which is typically the case for a repulsive pair potential), then Equation (8.37) would suggest $\det(\hat{\mathbf{D}}_{\mathbf{p}}) \geq 0$ for all $\mathbf{p}$. Hence, since both $\lambda_{\mathbf{p}}^+ + \lambda_{\mathbf{p}}^- \geq 0$, Equation (8.35), and $\lambda_{\mathbf{p}}^+ \lambda_{\mathbf{p}}^- \geq 0$, Equation (8.37), then both $\lambda_{\mathbf{p}}^+ \geq 0$ and $\lambda_{\mathbf{p}}^- \geq 0$ for all $\mathbf{p}$.

Since $\hat{\mathbf{D}}_{\mathbf{p}}$ is symmetric, its normalised eigenvectors $\mathbf{e}_{\mathbf{p}}^{\pm}$ are orthogonal,

$$\mathbf{e}_{\mathbf{p}}^{\pm} = \frac{1}{\sqrt{(\epsilon_{\mathbf{p}}^{\pm})^2 + 1}} \begin{pmatrix} \epsilon_{\mathbf{p}}^{\pm} \\ 1 \end{pmatrix}, \quad (8.38)$$

where

$$\epsilon_{\mathbf{p}}^{\pm} = \frac{1}{2\hat{\mathbf{D}}_{\mathbf{p}}^{1,2}} \left(\hat{\mathbf{D}}_{\mathbf{p}}^{1,1} - \hat{\mathbf{D}}_{\mathbf{p}}^{2,2} \pm \sqrt{\left(\hat{\mathbf{D}}_{\mathbf{p}}^{1,1} - \hat{\mathbf{D}}_{\mathbf{p}}^{2,2} \right)^2 + 4 \left(\hat{\mathbf{D}}_{\mathbf{p}}^{1,2} \right)^2} \right). \quad (8.39)$$

This allows $\hat{\mathbf{u}}_{\mathbf{p}}(t)$ to be written succinctly in terms of the two components

$$\hat{\mathbf{u}}_{\mathbf{p}}(t) = \hat{u}_{\mathbf{p}}^+(t)\mathbf{e}_{\mathbf{p}}^+ + \hat{u}_{\mathbf{p}}^-(t)\mathbf{e}_{\mathbf{p}}^-, \quad (8.40)$$

and similarly for the noises,

$$\hat{\boldsymbol{\xi}}_{\mathbf{p}}(t) = \hat{\xi}_{\mathbf{p}}^+(t)\mathbf{e}_{\mathbf{p}}^+ + \hat{\xi}_{\mathbf{p}}^-(t)\mathbf{e}_{\mathbf{p}}^-, \quad (8.41)$$

where

$$\left\langle \begin{pmatrix} \hat{\xi}_{\mathbf{p}}^+(t)\hat{\xi}_{\mathbf{p}'}^+(t') & \hat{\xi}_{\mathbf{p}}^+(t)\hat{\xi}_{\mathbf{p}'}^-(t') \\ \hat{\xi}_{\mathbf{p}}^-(t)\hat{\xi}_{\mathbf{p}'}^+(t') & \hat{\xi}_{\mathbf{p}}^-(t)\hat{\xi}_{\mathbf{p}'}^-(t') \end{pmatrix} \right\rangle = \Gamma^2 V \delta_{\mathbf{p}+\mathbf{p}',\mathbf{0}} \mathbb{1}_2 \delta(t-t'), \quad (8.42)$$

and

$$\hat{\mathbf{w}}_{\mathbf{p}}(t) = \hat{w}_{\mathbf{p}}^+(t)\mathbf{e}_{\mathbf{p}}^+ + \hat{w}_{\mathbf{p}}^-(t)\mathbf{e}_{\mathbf{p}}^-, \quad (8.43)$$

where

$$\left\langle \begin{pmatrix} \hat{w}_{\mathbf{p}}^+(t)\hat{w}_{\mathbf{p}'}^+(t') & \hat{w}_{\mathbf{p}}^+(t)\hat{w}_{\mathbf{p}'}^-(t') \\ \hat{w}_{\mathbf{p}}^-(t)\hat{w}_{\mathbf{p}'}^+(t') & \hat{w}_{\mathbf{p}}^-(t)\hat{w}_{\mathbf{p}'}^-(t') \end{pmatrix} \right\rangle = w^2 V \delta_{\mathbf{p}+\mathbf{p}',\mathbf{0}} \mathbb{1}_2 e^{-\mu|t-t'|}. \quad (8.44)$$

Hence, Equation (8.31) reduces to two decoupled scalar differential equations

$$\dot{\hat{u}}_{\mathbf{p}}^{\pm}(t) = -\lambda_{\mathbf{p}}^{\pm} \hat{u}_{\mathbf{p}}^{\pm}(t) + \hat{\xi}_{\mathbf{p}}^{\pm}(t) + \hat{w}_{\mathbf{p}}^{\pm}(t), \quad (8.45)$$

with solution

$$\hat{u}_{\mathbf{p}}^{\pm}(t) = \int_0^t dt' e^{-\lambda_{\mathbf{p}}^{\pm}(t-t')} \left\{ \hat{\xi}_{\mathbf{p}}^{\pm}(t') + \hat{w}_{\mathbf{p}}^{\pm}(t') \right\}, \quad (8.46)$$

and initial condition $\hat{u}_{\mathbf{p}}^{\pm}(t=0) = 0$. Based on this solution, it is straightforward but cumbersome to evaluate the correlator

$$\langle \hat{u}_{\mathbf{p}}^{\pm}(t_1) \hat{u}_{-\mathbf{p}}^{\pm}(t_2) \rangle = V \mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2) + V \Xi_{\mathbf{p}}^{\pm}(t_1, t_2), \quad (8.47)$$

which separates into independent active $\mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2)$ and thermal $\Xi_{\mathbf{p}}^{\pm}(t_1, t_2)$ components, to be specified below, and is the fundamental ingredient in all calculations to come. Here, if the active noise is Gaussian, this correlator is, given that the system is harmonic, also that of a Gaussian and hence all that needs to be determined to characterise the system fully.

The correlator of the active noise being diagonal, as mentioned after Equation (8.24), renders the correlator Equation (8.44) diagonal. This is an important simplification. If the noise were originally not diagonal in Equation (8.24), say

$$\langle \mathbf{w}_{\mathbf{n}}(t) \mathbf{w}_{\mathbf{n}'}^{\mathsf{T}}(t') \rangle = \mathbf{W} \delta_{\mathbf{n},\mathbf{n}'} e^{-\mu|t-t'|}, \quad (8.48)$$

this would result in mixed components $+$ and $-$ in the correlator (8.44), as the off-diagonal (in $\pm$) elements $\sum_{\alpha,\alpha'} e_{\mathbf{p}}^{+,\alpha} \mathbf{W}^{\alpha,\alpha'} e_{\mathbf{p}}^{-,\alpha'}$ with eigenvectors $\mathbf{e}_{\mathbf{p}}^{\pm} = (e_{\mathbf{p}}^{\pm,1}, e_{\mathbf{p}}^{\pm,1})$ generally would not vanish, even when $\mathbf{e}_{\mathbf{p}}^{\pm}$ are orthogonal, $\sum_{\alpha} e_{\mathbf{p}}^{+,\alpha} e_{\mathbf{p}}^{-,\alpha} = 0$.

Returning to the displacement correlator, Equation (8.47), the reason why it is cum-

bersome are the double integrals

$$\begin{aligned} V\mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2) &:= \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\lambda_{\mathbf{p}}^{\pm}(t_1-t')} e^{-\lambda_{-\mathbf{p}}^{\pm}(t_2-t'')} \langle \hat{w}_{\mathbf{p}}^{\pm}(t') \hat{w}_{-\mathbf{p}}^{\pm}(t'') \rangle \\ &= \int_0^{t_1} dt' \int_0^{t_2} dt'' V e^{-\lambda_{\mathbf{p}}^{\pm}(t_1-t'+t_2-t'')} w^2 e^{-\mu|t'-t''|}, \end{aligned} \quad (8.49a)$$

$$\begin{aligned} V\Xi_{\mathbf{p}}^{\pm}(t_1, t_2) &:= \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\lambda_{\mathbf{p}}^{\pm}(t_1-t')} e^{-\lambda_{-\mathbf{p}}^{\pm}(t_2-t'')} \langle \hat{\xi}_{\mathbf{p}}^{\pm}(t') \hat{\xi}_{-\mathbf{p}}^{\pm}(t'') \rangle \\ &= \int_0^{t_1} dt' \int_0^{t_2} dt'' V e^{-\lambda_{\mathbf{p}}^{\pm}(t_1-t'+t_2-t'')} \Gamma^2 \delta(t' - t''), \end{aligned} \quad (8.49b)$$

which, of course, can be evaluated in closed form, as in Appendix 8.C, but are too unwieldy for the analysis that follows. To simplify the expressions, I focus on large times t . Strictly speaking, there is never a stationary state, as the whole lattice diffuses. A stationary state would require $t_{1,2} \gg 1/\mu$ and $t_{1,2} \gg 1/\lambda_{\mathbf{p}}^{\pm}$. However, the latter can never be achieved for $\mathbf{p} = \mathbf{0}$, as $\lambda_{\mathbf{0}}^{\pm}$ vanishes, resulting in the equal-time correlators behaving for large t like

$$\mathcal{W}_{\mathbf{p}}^{\pm}(t, t) = \begin{cases} \frac{2w^2}{\mu} t, & \text{for } \mathbf{p} = \mathbf{0} \text{ and } t \gg 1/\mu, \\ \frac{w^2}{\lambda_{\mathbf{p}}^{\pm}(\lambda_{\mathbf{p}}^{\pm} + \mu)}, & \text{for } \mathbf{p} \neq \mathbf{0}, t \gg 1/\mu \text{ and } t \gg 1/\lambda_{\mathbf{p}}^{\pm}, \end{cases} \quad (8.50a)$$

$$\quad (8.50b)$$

and similarly

$$\Xi_{\mathbf{p}}^{\pm}(t, t) = \begin{cases} \Gamma^2 t, & \text{for } \mathbf{p} = \mathbf{0}, \\ \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^{\pm}}, & \text{for } \mathbf{p} \neq \mathbf{0} \text{ and } t \gg 1/\lambda_{\mathbf{p}}^{\pm}. \end{cases} \quad (8.51a)$$

$$\quad (8.51b)$$

The exceptional nature of the $\mathbf{0}$ -mode has its physical origin in the diffusion of the lattice as a whole. As the interaction ties the displaced sites together, the resulting net displacement decreases with the number of sites V . The resulting correlator is, component-by-component,

$$\begin{aligned} \langle u_{\mathbf{n}}^{\alpha}(t) u_{\mathbf{n}'}^{\alpha'}(t) \rangle &= \frac{1}{V} \sum_{\mathbf{p}} e^{i\mathbf{k}_{\mathbf{p}} \cdot (\mathbf{n} - \mathbf{n}')} \left(e^{+, \alpha} e^{+, \alpha'} [\mathcal{W}_{\mathbf{p}}^{+}(t, t) + \Xi_{\mathbf{p}}^{+}(t, t)] \right. \\ &\quad \left. + e^{-, \alpha} e^{-, \alpha'} [\mathcal{W}_{\mathbf{p}}^{-}(t, t) + \Xi_{\mathbf{p}}^{-}(t, t)] \right), \end{aligned} \quad (8.52)$$

using Equations (8.28b), (8.40), and (8.47), with $e^{\pm, \alpha}$ denoting the α component of the eigenvector $\mathbf{e}^{\pm}$, Equation (8.38). This can be written more succinctly using outer products,

$$\begin{aligned} \langle \mathbf{u}_{\mathbf{n}}(t) \mathbf{u}_{\mathbf{n}'}^{\top}(t) \rangle &= \frac{1}{V} \mathbb{1}_2 \left(\Gamma^2 + \frac{2w^2}{\mu} \right) t \\ &\quad + \frac{1}{V} \sum_{\mathbf{p}}^{*} e^{i\mathbf{k}_{\mathbf{p}} \cdot (\mathbf{n} - \mathbf{n}')} \left(\mathbf{E}_{\mathbf{p}}^{+} [\mathcal{W}_{\mathbf{p}}^{+}(t, t) + \Xi_{\mathbf{p}}^{+}(t, t)] + \mathbf{E}_{\mathbf{p}}^{-} [\mathcal{W}_{\mathbf{p}}^{-}(t, t) + \Xi_{\mathbf{p}}^{-}(t, t)] \right), \end{aligned} \quad (8.53)$$

assuming $t \gg 1/\mu$ in order to use the result for $\mathcal{W}_{\mathbf{p}}^{\pm}(t, t)$ for $\mathbf{p} = \mathbf{0}$, as stated in Equation (8.50a), and the 2×2 matrices

$$\mathbf{E}_{\mathbf{p}}^{\pm} = \mathbf{e}_{\mathbf{p}}^{\pm} (\mathbf{e}_{\mathbf{p}}^{\pm})^{\top} \quad (8.54)$$

are the outer products of the eigenvectors in Equation (8.38). In Equation (8.53), the starred sum denotes the summation over all $\mathbf{p}$ except $\mathbf{p} = \mathbf{0}$. Keeping $\mathcal{W}_{\mathbf{p}}^{\pm}(t, t)$ and $\Xi_{\mathbf{p}}^{\pm}(t, t)$ in their closed forms, as derived in Appendix 8.C, the second line of Equation (8.53) is exact. Approximations enter when the integrals of the correlators are replaced by their large- t approximations, Equations (8.50) and (8.51), as done for $\mathbf{p} = \mathbf{0}$ in the first line of Equation (8.53).

Taking $V \rightarrow \infty$ in Equation (8.53) would appear to suppress the large- t divergence due to the $\mathbf{0}$ -mode. However, as V gets large, the $\lambda_{\mathbf{p}}^{\pm}$ become arbitrarily small, thereby spoiling the assumptions in Equations (8.50) and (8.51) that allowed the easy evaluation of the integrals. In fact, as $V \rightarrow \infty$, the integrals for any given $\mathbf{p}$ approach the integrals for $\mathbf{p} = \mathbf{0}$ as $\lim_{V \rightarrow \infty} \mathbf{k}_{\mathbf{p}} = \mathbf{0}$ for any $\mathbf{p}$. In other words, taking the limit $V \rightarrow \infty$ at finite t resolves the problem posed by $\mathbf{p} = \mathbf{0}$, while introducing plenty of new ones. In essence, the large- t divergence cannot be avoided by simply taking $V \rightarrow \infty$.

However, as large t is necessary to make use of the approximations in Equations (8.50) and (8.51), the $\mathbf{0}$ -mode therefore needs to be deducted explicitly. This amounts to subtracting from the displacement the global rigid translation

$$\bar{\mathbf{u}}(t) = \frac{1}{V} \sum_{\mathbf{n}} \mathbf{u}_{\mathbf{n}}(t) = \frac{1}{V} \hat{\mathbf{u}}_{\mathbf{p}=\mathbf{0}}(t) \quad (8.55)$$

of the lattice as a whole. The $\mathbf{0}$ -mode, given by setting $\mathbf{p} = \mathbf{0}$ in Equation (8.28a), is thus in fact the displacement of the centre of mass. Deducting the $\mathbf{0}$ -mode from the displacement gives

$$\mathbf{v}_{\mathbf{n}}(t) = \mathbf{u}_{\mathbf{n}}(t) - \bar{\mathbf{u}}(t) = \frac{1}{V} \sum_{\mathbf{p}}^* e^{i\mathbf{k}_{\mathbf{p}} \cdot \mathbf{n}} \hat{\mathbf{u}}_{\mathbf{p}}(t), \quad (8.56)$$

with the sum replaced by the starred sum compared to Equation (8.28b). With this adjustment, the first term on the right-hand side of Equation (8.53) disappears from the equal-time two-point correlator of the relative displacements so that, in the steady-state limit and in terms of components,

$$\begin{aligned} \lim_{t \rightarrow \infty} \langle v_{\mathbf{n}}^{\alpha}(t) v_{\mathbf{n}'}^{\alpha'}(t) \rangle &= \frac{1}{V} \sum_{\mathbf{p}}^* e^{i\mathbf{k}_{\mathbf{p}} \cdot (\mathbf{n} - \mathbf{n}')} \left(\mathbf{e}_{\mathbf{p}}^{-, \alpha} \mathbf{e}_{\mathbf{p}}^{-, \alpha'} \left[\frac{w^2}{\lambda_{\mathbf{p}}^{-} (\lambda_{\mathbf{p}}^{-} + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^{-}} \right] \right. \\ &\quad \left. + \mathbf{e}_{\mathbf{p}}^{+, \alpha} \mathbf{e}_{\mathbf{p}}^{+, \alpha'} \left[\frac{w^2}{\lambda_{\mathbf{p}}^{+} (\lambda_{\mathbf{p}}^{+} + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^{+}} \right] \right). \end{aligned} \quad (8.57)$$

While Equation (8.57) is the full correlation matrix, its trace, the sum over $\alpha = \alpha'$, is the more standard two-point correlator. In the particular case of $\mathbf{n} = \mathbf{n}'$, Equation (8.57) simplifies in the obvious way that the exponential from the Fourier transform disappears

from the expression.

To address the question of the existence of an ordered state, one may investigate the behaviour of the variance in large V ,

$$\lim_{t \rightarrow \infty} \langle \mathbf{v}_{\mathbf{n}}(t) \cdot \mathbf{v}_{\mathbf{n}}(t) \rangle = \frac{1}{V} \sum_{\mathbf{p}}^* \left(\left[\frac{w^2}{\lambda_{\mathbf{p}}^-(\lambda_{\mathbf{p}}^- + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^-} \right] + \left[\frac{w^2}{\lambda_{\mathbf{p}}^+(\lambda_{\mathbf{p}}^+ + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^+} \right] \right), \quad (8.58)$$

using that $\sum_{\alpha} \mathbf{e}^{\pm, \alpha} \mathbf{e}^{\pm, \alpha} = \text{Tr } \mathbf{E}^{\pm} = \mathbf{e}^{\pm} \cdot \mathbf{e}^{\pm} = 1$. By inspection, Equation (8.58) diverges logarithmically in large V , as $\lambda_{\mathbf{p}}^{\pm}$ vanishes like $|\mathbf{p}|^2$ for fixed $\mathbf{p}$ as $V \rightarrow \infty$, Equation (8.34). As indicated in the main text, in the case of a harmonic pair potential, the divergence of the variance of the relative displacement indicates the absence of crystalline order according to Mermin's original criterion [52].

However, the crystalline *integrity* is much better probed via the steady-state mean squared particle separation. From Equations (8.53) and (8.57), this is, up to a shift by ℓ^2 ,

$$\begin{aligned} \lim_{t \rightarrow \infty} \langle |\mathbf{u}_{\mathbf{n}}(t) - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q}(t)|^2 \rangle &= \frac{1}{V} \sum_{\mathbf{p}}^* 2(1 - \cos(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{m}_q)) \left(\left[\frac{w^2}{\lambda_{\mathbf{p}}^-(\lambda_{\mathbf{p}}^- + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^-} \right] \right. \\ &\quad \left. + \left[\frac{w^2}{\lambda_{\mathbf{p}}^+(\lambda_{\mathbf{p}}^+ + \mu)} + \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^+} \right] \right), \end{aligned} \quad (8.59)$$

which is generally not independent of q because of the lattice having different extent in different directions, even when it is square, $N_1 = N_2$. Mirror symmetry results in, for example, $q = 1$ and $q = 4$ having the same mean squared separation, as do all of $q = 2, 3, 5, 6$, see Figure 8.1. From Equation (8.34), it is clear that $\lambda_{\mathbf{p}}^{\pm}$ vanishes for fixed $\mathbf{p}$ in large V as fast as $1 - \cos(\mathbf{k}_{\mathbf{p}} \cdot \mathbf{m}_q)$. Hence, the large- V limit of the summands in Equation (8.59) converges, meaning that the sum diverges only as fast as V , which is compensated by the prefactor $1/V$ in front of the sum. Overall, Equation (8.59) has a finite asymptote in the limit $V \rightarrow \infty$. Because of the complicated dependence on $\mathbf{p}$ through $\lambda_{\mathbf{p}}^{\pm}$, Equation (8.34), an analytical form of the asymptote is hard to come by, but a numerical summation in the case $N_1 = N_2 \rightarrow \infty$ and $U''(\ell) \gg U'(\ell)/\ell$ allows one to determine the contribution from the thermal noise exactly up to a numerical factor, in particular

$$\langle |\mathbf{u}_{\mathbf{n}}(t) - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q}(t)|^2 \rangle \approx \frac{1}{U''(\ell)} \left(\frac{w^2}{\mu} F(U''(\ell)/\mu) + 0.812 \Gamma^2 \right), \quad (8.60)$$

where $F(x)$ is a function whose dependence on x proved too difficult to determine.

Equation (8.59) is a meaningful measure as far as the lattice geometry is concerned, but it does not capture the energetics of the crystal well. In the harmonic approximation, the different modes decouple and are, in equilibrium, expected to each carry energy $k_B T/2$, corresponding to $\Gamma^2/4$ according to Equation (8.22). As discussed in Appendix 8.B, the

total instantaneous energy of the entire crystal is

$$\mathcal{E}(t) = \frac{1}{2} \sum_{\mathbf{n}} \sum_{q=1}^6 U(|\mathbf{u}_{\mathbf{n}}(t) - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q}(t) - \ell \mathbf{a}_q|), \quad (8.61)$$

where the factor of $1/2$ corrects for the double counting of each pair potential from the double sum. Even in the harmonic approximation, when $U(z)$ is assumed to be (at most) quadratic, because of the modulus in its argument, this does not mean that the energy can be approximated by terms of the form $(\mathbf{u}_{\mathbf{n}}(t) - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q}(t) - \ell \mathbf{a}_q)^2$. As a result, the expected energy is not easily expressed in terms of the mean squared separation, Equation (8.59).

However, given the (harmonic) force in Equation (8.21), the instantaneous energy of the entire system can be approximated by

$$\mathcal{E}_{\text{harm.}}(t) = \frac{1}{2} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \mathbf{u}_{\mathbf{n}}(t) \cdot \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'}(t), \quad (8.62)$$

up to a constant (irrelevant) offset $3VU(\ell)$, see Appendix 8.B. After taking the Fourier transform of Equation (8.62), and using the orthogonal eigensystem $\hat{\mathbf{D}}_{\mathbf{p}} \mathbf{e}_{\mathbf{p}}^{\pm} = \lambda_{\mathbf{p}}^{\pm} \mathbf{e}_{\mathbf{p}}^{\pm}$, the expected total energy in the harmonic approximation at stationarity simplifies much better than the mean squared separation, Equation (8.59), and turns out to be

$$\lim_{t \rightarrow \infty} \langle \mathcal{E}_{\text{harm.}}(t) \rangle = \frac{1}{4} \Gamma^2 d(V-1) + \frac{1}{2} w^2 \sum_{\mathbf{p}}^* \left(\frac{1}{\lambda_{\mathbf{p}}^+ + \mu} + \frac{1}{\lambda_{\mathbf{p}}^- + \mu} \right), \quad (8.63)$$

where $d = 2$ is the dimension of the system, so that $d(V-1)$ is the total number of excitable degrees of freedom. The modes that are energetically most affected by the presence of the activity are the very small and the very large $\mathbf{p}$, namely any $\mathbf{p}$ such that $\lambda_{\mathbf{p}}^{\pm} \ll \mu$. If $\lambda_{\mathbf{p}}^{\pm} \ll \mu$, then the contribution to the total energy due to the activity is approximately proportional to $2w^2/\mu$. The number of modes that have this property grows linearly in V for $N_1 \propto N_2$, so that generally in large V the expected total energy scales like $\langle \mathcal{E}_{\text{harm.}} \rangle \propto V(\Gamma^2/2 + \mathcal{C}w^2/\mu)$ for some constant $\mathcal{C}$.

As a sanity check of Equation (8.63), one may consider $w^2 = \tilde{\Gamma}^2 \mu/2$, so that the active noise Equation (8.24) becomes thermal with amplitude $\tilde{\Gamma}$ in the limit of large μ and indeed in this case $\langle \mathcal{E}_{\text{harm.}} \rangle = \Gamma^2(V-1)/2 + \tilde{\Gamma}^2(V-1)/2$.

Steady-state entropy production

Before calculating the entropy production of the active crystal, one final ingredient is the cross correlator,

$$\begin{aligned} \langle \hat{w}_{\mathbf{p}}^{\pm}(t_1) \hat{w}_{-\mathbf{p}}^{\pm}(t_2) \rangle &= \int_0^{t_2} dt'' e^{-\lambda_{-\mathbf{p}}^{\pm}(t_2-t'')} \langle \hat{w}_{\mathbf{p}}^{\pm}(t_1) \hat{w}_{-\mathbf{p}}^{\pm}(t'') \rangle \\ &= \int_0^{t_2} dt'' V e^{-\lambda_{\mathbf{p}}^{\pm}(t_2-t'')} w^2 e^{-\mu|t_1-t''|}, \end{aligned} \quad (8.64)$$

where I inserted the solution for $\hat{u}_{-\mathbf{p}}^\pm(t_2)$ from Equation (8.46), and have used that $\lambda_{-\mathbf{p}}^\pm = \lambda_{\mathbf{p}}^\pm$, Equation (8.34). Performing the integration in Equation (8.64), the following expression is obtained

$$\langle \hat{w}_{\mathbf{p}}^\pm(t_1) \hat{u}_{-\mathbf{p}}^\pm(t_2) \rangle = \begin{cases} V \frac{w^2}{\lambda_{\mathbf{p}}^\pm + \mu} \left(e^{-\mu(t_1-t_2)} - e^{-\lambda_{\mathbf{p}}^\pm t_2} e^{-\mu t_1} \right), & \text{for } t_1 \geq t_2, \\ V \frac{w^2}{\lambda_{\mathbf{p}}^\pm + \mu} \left(e^{-\lambda_{\mathbf{p}}^\pm(t_1-t_2)} - e^{-\lambda_{\mathbf{p}}^\pm t_2} e^{-\mu t_1} \right) \\ + V \frac{w^2}{\lambda_{\mathbf{p}}^\pm - \mu} \left(e^{-\mu(t_2-t_1)} - e^{-\lambda_{\mathbf{p}}^\pm(t_2-t_1)} \right), & \text{for } t_2 \geq t_1, \end{cases} \quad (8.65)$$

noting that, in contrast to the $\langle \hat{u}_{\mathbf{p}}^\pm(t_1) \hat{u}_{-\mathbf{p}}^\pm(t_2) \rangle$ correlator, Equation (8.47), there is no exceptional case for $\mathbf{p} = \mathbf{0}$. In the equal-time steady-state limit $t_1 = t_2 \rightarrow \infty$, the cross-correlation, Equation (8.65), becomes

$$\lim_{t \rightarrow \infty} \langle \hat{w}_{\mathbf{p}}^\pm(t) \hat{u}_{-\mathbf{p}}^\pm(t) \rangle = V \frac{w^2}{\lambda_{\mathbf{p}}^\pm + \mu}. \quad (8.66)$$

By comparing to the explicit expression for $\mathcal{W}_{\mathbf{p}}^\pm(t, t)$ at large times $t \gg \lambda_{\mathbf{p}}^\pm$, Equation (8.50), one can write

$$\lim_{t \rightarrow \infty} \lambda_{\mathbf{p}}^\pm \langle \hat{w}_{\mathbf{p}}^\pm(t) \hat{u}_{-\mathbf{p}}^\pm(t) \rangle = \begin{cases} 0, & \text{for } \mathbf{p} = \mathbf{0}, \\ (\lambda_{\mathbf{p}}^\pm)^2 \lim_{t \rightarrow \infty} V \mathcal{W}_{\mathbf{p}}^\pm(t, t) = (\lambda_{\mathbf{p}}^\pm)^2 V \mathcal{W}_{\mathbf{p}}^\pm, & \text{otherwise,} \end{cases} \quad (8.67)$$

which is precisely the term that arises in the calculation of the steady-state entropy production below.

The entropy production of an active crystal is most easily determined using the framework outlined in Ref. [106], which introduces a notion of instantaneous, internal, *local* entropy production rate in the steady-state limit,

$$\langle \dot{\sigma}_{\mathbf{n}} \rangle = \frac{2}{\Gamma^2} \left(\mathbf{w}_{\mathbf{n}} - \sum_{q=1}^6 \nabla_{\mathbf{u}_{\mathbf{n}}} U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) \right)^2 - \sum_{q=1}^6 \nabla_{\mathbf{u}_{\mathbf{n}}}^2 U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|). \quad (8.68)$$

Under the harmonic approximation derived in Appendix 8.B, the force from the neighbouring particles can be written in terms of the dynamical matrix, Equation (8.25), i.e. $-\sum_q \nabla_{\mathbf{u}_{\mathbf{n}}} U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) = -\sum_{\mathbf{n}'} \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'}$, see Equation (8.103). The Laplacian is then given by $\sum_q \nabla_{\mathbf{u}_{\mathbf{n}}}^2 U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) = \text{Tr } \mathbf{D}_{\mathbf{nn}}$, Equation (8.107). Replacing the gradient and Laplacian of the potential in Equation (8.68) with these expressions, followed by expanding the brackets and taking the expectation of Equation (8.68), yields

$$\langle \dot{\sigma}_{\mathbf{n}} \rangle = \frac{2}{\Gamma^2} \left(\langle \mathbf{w}_{\mathbf{n}} \cdot \mathbf{w}_{\mathbf{n}} \rangle - \sum_{\mathbf{n}'} 2 \langle \mathbf{w}_{\mathbf{n}} \cdot \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'} \rangle + \sum_{\mathbf{n}'} \sum_{\mathbf{n}''} \langle \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'} \cdot \mathbf{D}_{\mathbf{nn}''} \mathbf{u}_{\mathbf{n}''} \rangle \right) - \text{Tr } \mathbf{D}_{\mathbf{nn}}. \quad (8.69)$$

To obtain a closed-form expression for $\langle \dot{\sigma}_{\mathbf{n}} \rangle$, the most straightforward way to proceed is to consider its Fourier representation. To simplify the subsequent calculations, one can

consider the average local entropy production of the particle residing at site $\mathbf{n} = \mathbf{0}$, i.e. $\langle \dot{\sigma}_0 \rangle$. This comes at no penalty to the generality of the final result, since translational invariance of the active crystal ensures the local entropy production rate is the same for each particle, i.e. $\langle \dot{\sigma}_{\mathbf{n}} \rangle = \langle \dot{\sigma}_0 \rangle$ for all $\mathbf{n}$. However, this has the advantage of simplifying the subsequent Fourier transforms, since the Fourier factors $\exp(i\mathbf{k}_{\mathbf{p}} \cdot \mathbf{n})$ (and its inverse) are trivially unity, resulting in conversion between real-space and Fourier quantities reducing to plain sums over all modes or lattice sites, respectively, e.g. $\langle \dot{\sigma}_0 \rangle = \sum_{\mathbf{p}} \langle \dot{\sigma}_{\mathbf{p}} \rangle / V$, where the average entropy production rate in Fourier space is given by

$$\langle \dot{\sigma}_{\mathbf{p}} \rangle = \frac{2}{V\Gamma^2} \left(\langle \hat{\mathbf{w}}_{\mathbf{p}} \cdot \hat{\mathbf{w}}_{-\mathbf{p}} \rangle - 2 \langle \hat{\mathbf{w}}_{\mathbf{p}} \cdot \hat{\mathbf{D}}_{-\mathbf{p}} \hat{\mathbf{u}}_{-\mathbf{p}} \rangle + \langle \hat{\mathbf{D}}_{\mathbf{p}} \hat{\mathbf{u}}_{\mathbf{p}} \cdot \hat{\mathbf{D}}_{-\mathbf{p}} \hat{\mathbf{u}}_{-\mathbf{p}} \rangle \right) - \text{Tr } \mathbf{D}_{\mathbf{nn}}. \quad (8.70)$$

One can now use that the action of the dynamical matrix on the displacement vector is

$$\hat{\mathbf{D}}_{-\mathbf{p}} \hat{\mathbf{u}}_{-\mathbf{p}} = \lambda_{\mathbf{p}}^+ \hat{u}_{-\mathbf{p}}^+ \mathbf{e}_{-\mathbf{p}}^+ + \lambda_{\mathbf{p}}^- \hat{u}_{-\mathbf{p}}^- \mathbf{e}_{-\mathbf{p}}^-, \quad (8.71)$$

using that $\lambda_{-\mathbf{p}}^{\pm} = \lambda_{\mathbf{p}}^{\pm}$, to obtain

$$\begin{aligned} \langle \dot{\sigma}_{\mathbf{p}} \rangle &= \frac{2}{V\Gamma^2} \left(2w^2V - 2 \left(\lambda_{\mathbf{p}}^+ \langle \hat{u}_{\mathbf{p}}^+ \hat{u}_{-\mathbf{p}}^+ \rangle + \lambda_{\mathbf{p}}^- \langle \hat{u}_{\mathbf{p}}^- \hat{u}_{-\mathbf{p}}^- \rangle \right) \right. \\ &\quad \left. + (\lambda_{\mathbf{p}}^+)^2 \langle \hat{u}_{\mathbf{p}}^+ \hat{u}_{-\mathbf{p}}^+ \rangle + (\lambda_{\mathbf{p}}^-)^2 \langle \hat{u}_{\mathbf{p}}^- \hat{u}_{-\mathbf{p}}^- \rangle \right) - \text{Tr } \mathbf{D}_{\mathbf{nn}}, \end{aligned} \quad (8.72)$$

where I also used that $\langle \hat{\mathbf{w}}_{\mathbf{p}} \cdot \hat{\mathbf{w}}_{\mathbf{p}} \rangle = 2w^2V$, see Equation (8.30b). Next, one can insert the exact expressions for the correlators derived previously, namely $\langle \hat{u}_{\mathbf{p}}^{\pm} \hat{u}_{-\mathbf{p}}^{\pm} \rangle = V(\mathcal{W}_{\mathbf{p}}^{\pm} + \Xi_{\mathbf{p}}^{\pm})$, Equation (8.47), and $\lambda_{\mathbf{p}}^{\pm} \langle \hat{u}_{\mathbf{p}}^{\pm} \hat{u}_{-\mathbf{p}}^{\pm} \rangle = (\lambda_{\mathbf{p}}^{\pm})^2 V \mathcal{W}_{\mathbf{p}}^{\pm}$, Equation (8.67). Inserting these expressions into Equation (8.72) yields

$$\langle \dot{\sigma}_{\mathbf{p}} \rangle = \frac{2}{\Gamma^2} \left[2w^2 - (\lambda_{\mathbf{p}}^+)^2 \mathcal{W}_{\mathbf{p}}^+ - (\lambda_{\mathbf{p}}^-)^2 \mathcal{W}_{\mathbf{p}}^- + (\lambda_{\mathbf{p}}^+)^2 \Xi_{\mathbf{p}}^+ + (\lambda_{\mathbf{p}}^-)^2 \Xi_{\mathbf{p}}^- \right] - \text{Tr } \mathbf{D}_{\mathbf{nn}}. \quad (8.73)$$

Then, the explicit large- t expressions for $\mathcal{W}_{\mathbf{p}}^{\pm}$, Equation (8.50), and $\Xi_{\mathbf{p}}^{\pm}$, Equation (8.51), can be inserted into Equation (8.73), noting that the divergent $\mathbf{p} = \mathbf{0}$ modes of $\mathcal{W}_{\mathbf{p}}^{\pm}$ and $\Xi_{\mathbf{p}}^{\pm}$ are suppressed by the factors $(\lambda_0^{\pm})^2 = 0$ and so these expressions can simply be replaced by their $\mathbf{p} \neq \mathbf{0}$ modes. Inserting these expressions and rearranging gives

$$\langle \dot{\sigma}_{\mathbf{p}} \rangle = \frac{2w^2}{\Gamma^2} \frac{2 + \mu^{-1}(\lambda_{\mathbf{p}}^+ + \lambda_{\mathbf{p}}^-)}{(1 + \mu^{-1}\lambda_{\mathbf{p}}^+)(1 + \mu^{-1}\lambda_{\mathbf{p}}^-)} + \text{Tr } \hat{\mathbf{D}}_{\mathbf{p}} - \text{Tr } \mathbf{D}_{\mathbf{nn}}, \quad (8.74)$$

where I used that $\lambda_{\mathbf{p}}^+ + \lambda_{\mathbf{p}}^- = \text{Tr } \hat{\mathbf{D}}_{\mathbf{p}}$. On performing the backwards transform, $\langle \dot{\sigma}_0 \rangle = \sum_{\mathbf{p}} \langle \dot{\sigma}_{\mathbf{p}} \rangle / V$, the terms $\text{Tr } \hat{\mathbf{D}}_{\mathbf{p}}$ and $\text{Tr } \hat{\mathbf{D}}_{\mathbf{nn}}$ cancel since $\sum_{\mathbf{p}} \text{Tr } \hat{\mathbf{D}}_{\mathbf{p}} = V \text{Tr } \mathbf{D}_{\mathbf{nn}}$. Using this result, and that $\langle \dot{\sigma}_{\mathbf{n}} \rangle = \langle \dot{\sigma}_0 \rangle$ for any $\mathbf{n}$, the real-space average entropy production rate for a single particle can be written in the highly compact form

$$\langle \dot{\sigma}_{\mathbf{n}} \rangle = \frac{1}{V} \sum_{\mathbf{p}} \frac{2w^2}{\Gamma^2} \frac{\text{Tr}(\mathbb{1}_2 + \mu^{-1} \hat{\mathbf{D}}_{\mathbf{p}})}{\det(\mathbb{1}_2 + \mu^{-1} \hat{\mathbf{D}}_{\mathbf{p}})}. \quad (8.75)$$

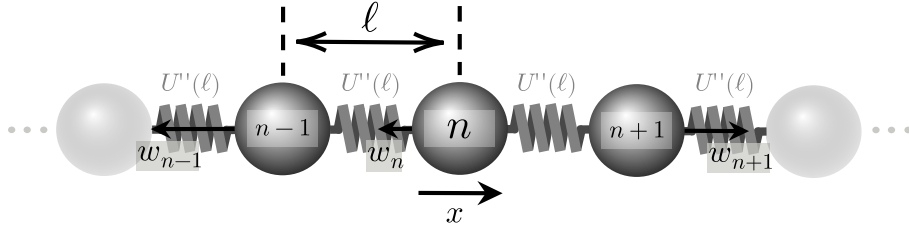


Figure 8.2: Schematic of the one-dimensional harmonic active chain.

As pointed out in the main text, Equation (8.75) is in fact a very general expression for that of active particles in two dimensions.

8.A.b One-dimensional crystals

I will now perform the analogous derivation for the case of a one-dimensional harmonic active crystal, i.e. a harmonic active chain, as illustrated in Fig. 8.2. To limit repetition, I will omit much of the detail in the following since most of the mathematical machinery was already introduced for the two-dimensional case above.

Under the harmonic approximation, Appendix 8.B, the stochastic equation of motion is

$$\dot{u}_n(t) = - \sum_{n'=1}^N D_{nn'} u_{n'}(t) + \xi_n(t) + w_n(t), \quad (8.76)$$

where $u_n(t) \in \mathbb{R}$ represents the local displacement of the particle at a site indexed by $n \in \{1, 2, \dots, N\}$. As for the two-dimensional crystal, the zero-mean thermal and active noise have autocorrelation functions given by, respectively,

$$\langle \xi_n(t) \xi_{n'}(t') \rangle = \Gamma^2 \delta_{n,n'} \delta(t - t'), \quad (8.77a)$$

$$\langle w_n(t) w_{n'}(t') \rangle = w^2 \delta_{n,n'} e^{-\mu|t-t'|}. \quad (8.77b)$$

The sum $\sum_{n'}$ in Equation (8.76) is over the set $\{1, 2, \dots, N\}$ of all sites. However, the dynamical interaction kernel selects only those n' that are nearest neighbours of n , explicitly,

$$D_{nn'} = \begin{cases} -U''(\ell), & \text{for } n' = n + m_q, \\ 2U''(\ell), & \text{for } n' = n, \\ 0, & \text{otherwise,} \end{cases} \quad (8.78)$$

based on the harmonic approximation in Appendix 8.B, where the set of allowed differences in the indices is now simply $\{m_1, m_2\} = \{1, -1\}$, with an associated set of displacements $\{\ell, -\ell\}$.

As for the two-dimensional case, I solve the system by first introducing the Fourier

transforms for the displacements,

$$\hat{u}_p(t) = \sum_{n=1}^N e^{-ik_p n} u_n(t), \quad (8.79a)$$

$$u_n(t) = \frac{1}{N} \sum_{p=0}^{N-1} e^{ik_p n} \hat{u}_p(t), \quad (8.79b)$$

the dynamical interaction kernel,

$$\hat{D}_{pp'} = \sum_{n=1}^N \sum_{n'=1}^N e^{-i(k_p n + k_{p'} n')} D_{nn'}, \quad (8.80a)$$

$$D_{nn'} = \frac{1}{N} \sum_{p=0}^{N-1} \frac{1}{N} \sum_{p'=0}^{N-1} e^{i(k_p n + k_{p'} n')} \hat{D}_{pp'}, \quad (8.80b)$$

and the autocorrelation functions of the noises,

$$\langle \hat{\xi}_p(t) \hat{\xi}_{p'}(t') \rangle = \Gamma^2 N \delta_{p+p',0} \delta(t - t'), \quad (8.81a)$$

$$\langle \hat{w}_p(t) \hat{w}_{p'}(t') \rangle = w^2 N \delta_{p+p',0} e^{-\mu|t-t'|}, \quad (8.81b)$$

where the wavenumber is $k_p = 2\pi p/N$ and is indexed by $p \in \{0, 1, \dots, N-1\}$. After taking the above Fourier transforms, the Langevin Equation (8.76) simplifies to

$$\dot{\hat{u}}_p(t) = -\hat{D}_p \hat{u}_p(t) + \hat{\xi}_p(t) + \hat{w}_p(t), \quad (8.82)$$

where I introduced

$$\hat{D}_{pp'} = N \delta_{p+p',0} \hat{D}_p = N \delta_{p+p',0} 2U''(\ell) [1 - \cos(k_p)]. \quad (8.83)$$

The solution to Equation (8.82) is thus

$$\hat{u}_p(t) = \int_0^t dt' e^{-\hat{D}_p(t-t')} \{ \hat{\xi}_p(t') + \hat{w}_p(t') \}, \quad (8.84)$$

with initial condition $\hat{u}_p(t=0) = 0$. By analogy to Equation (8.46), it is clear the correlator is given by

$$\langle \hat{u}_p(t_1) \hat{u}_{-p}(t_2) \rangle = N \mathcal{W}_p^{1D}(t_1, t_2) + N \Xi_p^{1D}(t_1, t_2), \quad (8.85)$$

where $\mathcal{W}_p^{1D}(t_1, t_2)$ and $\Xi_p^{1D}(t_1, t_2)$ are given by the same expressions for $\mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2)$ and $\Xi_{\mathbf{p}}^{\pm}(t_1, t_2)$ in Equation (8.49), after replacing all instances of $\lambda_{\mathbf{p}}^{\pm}$, Equation (8.34), with $\hat{D}_p$, Equation (8.83). Furthermore, the correlator in real space is given by

$$\langle u_n(t_1) u_{n'}(t_2) \rangle = \frac{1}{N} \sum_{p=0}^{N-1} e^{ik_p(n-n')} (\mathcal{W}_p^{1D}(t_1, t_2) + \Xi_p^{1D}(t_1, t_2)). \quad (8.86)$$

The relative displacements are also defined by subtracting the average displacement $\bar{u}(t) = \hat{u}_{p=0}(t)/N$, i.e.

$$v_n(t) = u_n(t) - \bar{u}(t) = \frac{1}{N} \sum_{p=1}^{N-1} e^{ik_p n} \hat{u}_p(t). \quad (8.87)$$

This now permits an exact expression for the steady-state variance that does not *trivially* diverge,

$$\lim_{t \rightarrow \infty} \langle v_n(t) v_n(t) \rangle = \frac{1}{N} \sum_{p=1}^{N-1} \left(\frac{w^2}{\hat{D}_p(\hat{D}_p + \mu)} + \frac{\Gamma^2}{2\hat{D}_p} \right). \quad (8.88)$$

Furthermore, a more compact expression can now be obtained for $N \gg 1$. From the expression for $\hat{D}_p$, Equation (8.83), the modes that will dominate the sum in Equation (8.88) for large N are the small- and large- p modes in equal measure. Hence, for large N and finite p , one may approximate $\hat{D}_p \approx U''(\ell) k_p^2 \ll 1/\mu$, whence

$$\lim_{t \rightarrow \infty} \langle v_n(t) v_n(t) \rangle \approx \frac{1}{U''(\ell)} \left(\frac{w^2}{\mu} + \frac{\Gamma^2}{2} \right) \frac{2}{N} \sum_{p=1}^{(N-1)/2} \frac{1}{k_p^2}, \quad \text{for } N \gg 1. \quad (8.89)$$

The summands $1/k_p^2$ decay sufficiently fast with increasing p that the upper limit of the sum in Equation (8.89) can be safely extended to ∞ . Then, using that $\sum_{p=1}^{\infty} 1/k_p^2 = N^2/24$,

$$\lim_{t \rightarrow \infty} \langle v_n(t) v_n(t) \rangle \approx \frac{N}{12U''(\ell)} \left(\frac{w^2}{\mu} + \frac{\Gamma^2}{2} \right), \quad \text{for } N \gg 1. \quad (8.90)$$

Hence, the variance of the relative displacement diverges linearly with the number of particles for the one-dimensional crystal, in contrast to the logarithmic divergence found for that of the two-dimensional crystal, Equation (8.58).

The crystalline integrity for the one-dimensional crystal is better probed by the steady-state mean squared particle separation, which is, up to a shift by ℓ^2 ,

$$\lim_{t \rightarrow \infty} \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle = \frac{1}{N} \sum_{p=1}^{N-1} 2(1 - \cos(k_p)) \left(\frac{w^2}{\hat{D}_p(\hat{D}_p + \mu)} + \frac{\Gamma^2}{2\hat{D}_p} \right), \quad (8.91)$$

which, in contrast to the two-dimensional case, is observed to be independent of q . After inserting the explicit expression for $\hat{D}_p$, Equation (8.83), the resulting sum

$$\lim_{t \rightarrow \infty} \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle = \frac{1}{NU''(\ell)} \left\{ \frac{N-1}{2} \Gamma^2 + \sum_{p=1}^{N-1} \frac{w^2}{\hat{D}_p + \mu} \right\} \quad (8.92)$$

has a closed form in the limit $N \rightarrow \infty$. In particular, using that $\lim_{N \rightarrow \infty} (1/N) \sum_{p=1}^N 1/(c -$

$\cos(k_p) = 1/\sqrt{c^2 - 1}$ for $c > 1$,

$$\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle = \frac{1}{U''(\ell)} \left(\frac{w^2}{\mu \sqrt{1 + 4 \frac{U''(\ell)}{\mu}}} + \frac{\Gamma^2}{2} \right). \quad (8.93)$$

Next, the total instantaneous energy of the one-dimensional crystal is given by

$$\mathcal{E}(t) = \frac{1}{2} \sum_{n=1}^N \sum_{q=1}^2 U(|u_n(t) - u_{n+m_q}(t) - \ell m_q|), \quad (8.94)$$

with the factor $1/2$ accounting for the double counting of the pair potentials in the double sum, since $|u_n(t) - u_{n+m_q}(t) - \ell m_q|$ is the same for either n with $q = 1$, or $n+1$ with $q = 2$. Unlike the two-dimensional crystal, the average energy can be expressed in terms of the mean squared separation, Equation (8.91), using the harmonic approximation derived in Appendix 8.B, i.e.

$$\langle \mathcal{E}_{\text{harm.}}(t) \rangle = \frac{1}{2} \sum_{n=1}^N \sum_{q=1}^2 \frac{1}{2} U''(\ell) \langle |u_n(t) - u_{n+m_q}(t)|^2 \rangle, \quad (8.95)$$

up to an irrelevant constant offset $NU(\ell)$. Using Equations (8.83) and (8.92), one arrives at

$$\lim_{t \rightarrow \infty} \langle \mathcal{E}_{\text{harm.}}(t) \rangle = \frac{1}{4} \Gamma^2 (N-1) + \frac{1}{2} \sum_{p=1}^{N-1} \frac{w^2}{\hat{D}_p + \mu}, \quad (8.96)$$

which is structurally identical to Equation (8.63). Using Equation (8.93) and the translational invariance in Equation (8.95), one can read-off the steady-state average energy per particle in the thermodynamic limit using Equation (8.93), yielding

$$\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} \frac{\langle \mathcal{E}_{\text{harm.}}(t) \rangle}{N} = \frac{1}{2} \left(\frac{w^2}{\mu \sqrt{1 + 4 \frac{U''(\ell)}{\mu}}} + \frac{\Gamma^2}{2} \right). \quad (8.97)$$

Lastly, I will calculate the entropy production of the one-dimensional crystal. Starting from the general expression for the steady-state entropy production of an active crystal, Equation (8.68), the entropy production specialised to the one-dimensional case is

$$\dot{\sigma}_n = \frac{2}{\Gamma^2} \left(w_n - \sum_{n'=1}^N D_{nn'} u_{n'} \right)^2 - 2U''(\ell). \quad (8.98)$$

The derivation of a closed-form expression for the average entropy production of the one-dimensional crystal proceeds analogously to the two-dimensional case in Appendix 8.A.a.

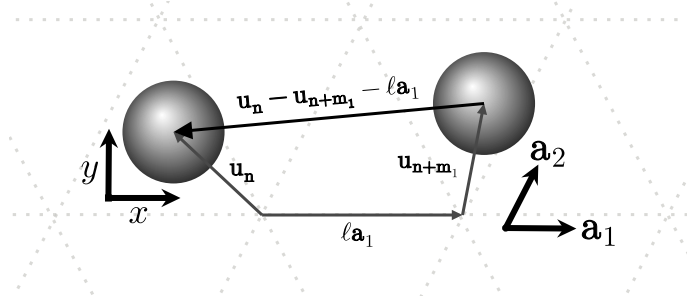


Figure 8.3: Illustration of the distance vector $\mathbf{u}_n(t) - \mathbf{u}_{n+m_q}(t) - \ell \mathbf{a}_q$ between two particles that have been displaced away from their equilibrium lattice positions.

Skipping over this repetitive detail, one ultimately obtains

$$\langle \dot{\sigma}_n \rangle = \frac{1}{N} \sum_{p=0}^{N-1} \frac{2w^2}{\Gamma^2} \frac{\mu}{\mu + \hat{D}_p}, \quad (8.99)$$

which strongly resembles the entropy production of an active particle in a harmonic potential [41, 42].

8.B Harmonic approximation of a general pair potential

As introduced in Appendix 8.A, a particle indexed by site $\mathbf{n}$ is subject to repulsive forces from its nearest neighbours at sites indexed by $\mathbf{m}_q$, which, in turn, are encoded in q as $\{\mathbf{m}_1, \dots, \mathbf{m}_6\} = \{(1, 0), (0, 1), (-1, 1), (-1, 0), (0, -1), (1, -1)\}$. The interparticle forces hail from a short-ranged pair potential $U(|\mathbf{u}_n(t) - \mathbf{u}_{n+m_q}(t) - \ell \mathbf{a}_q|)$ depending only on the distance between particles, Figure 8.3. To render the model exactly solvable, here I approximate the pair potential to second order in the particle separation vector $\mathbf{u}_n(t) - \mathbf{u}_{n+m_q}(t)$, equivalent to leading order for the interparticle force as I show below. For the sake of brevity, I omit the displacement vectors' explicit dependence on time t in the following. Firstly, I use that

$$\begin{aligned} |\mathbf{u}_n - \mathbf{u}_{n+m_q} - \ell \mathbf{a}_q| &= \sqrt{(\mathbf{u}_n - \mathbf{u}_{n+m_q})^2 - 2(\mathbf{u}_n - \mathbf{u}_{n+m_q}) \cdot \ell \mathbf{a}_q + \ell^2} \\ &= \ell - (\mathbf{u}_n - \mathbf{u}_{n+m_q}) \cdot \mathbf{a}_q \\ &\quad + \frac{1}{2\ell} \left((\mathbf{u}_n - \mathbf{u}_{n+m_q})^2 - [(\mathbf{u}_n - \mathbf{u}_{n+m_q}) \cdot \mathbf{a}_q]^2 \right) \\ &\quad + \mathcal{O} \left((\mathbf{u}_n - \mathbf{u}_{n+m_q})^3 \right) \end{aligned} \quad (8.100)$$

to show the pair potential approximated to second order in the relative displacements is

$$\begin{aligned} U(|\mathbf{u}_n - \mathbf{u}_{n+m_q} - \ell \mathbf{a}_q|) &= U(\ell) - (\mathbf{u}_n - \mathbf{u}_{n+m_q}) \cdot \mathbf{a}_q U'(\ell) \\ &\quad + \frac{1}{2\ell} \left((\mathbf{u}_n - \mathbf{u}_{n+m_q})^2 - [(\mathbf{u}_n - \mathbf{u}_{n+m_q}) \cdot \mathbf{a}_q]^2 \right) U'(\ell) \\ &\quad + \frac{1}{2} \left((\mathbf{u}_n - \mathbf{u}_{n+m_q}) \cdot \mathbf{a}_q \right)^2 U''(\ell) + \mathcal{O} \left((\mathbf{u}_n - \mathbf{u}_{n+m_q})^3 \right), \end{aligned} \quad (8.101)$$

where I assumed $U'(\ell) \neq 0$ in order to model a tightly packed system where particles are unable to relax to their equilibrium separations. Said another way, if the pairwise interactions are thought of as being mediated by springs, then this amounts to the springs being under constant tension. If the original pair potential started out as harmonic, e.g. $U(|z - \ell|) = a + bz + cz^2$, then the $\mathcal{O}((\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q})^3)$ term would drop out of Equation (8.101). Henceforth, I will neglect the $\mathcal{O}((\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q})^3)$ term, and refer to the resulting calculations as that of the *harmonic approximation*.

Using that the pair potential is short-ranged and so only nearest neighbours contribute significantly, the total force acting on the particle indexed by site $\mathbf{n}$, under the harmonic approximation, is given by

$$\begin{aligned} -\sum_{q=1}^6 \nabla_{\mathbf{u}_{\mathbf{n}}} U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) &= -\frac{U'(\ell)}{\ell} \sum_{q=1}^6 (\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q}) \\ &\quad - \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \sum_{q=1}^6 \mathbf{a}_q \mathbf{a}_q \cdot (\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q}), \end{aligned} \quad (8.102)$$

where the linear term from Equation (8.101) vanishes in Equation (8.102) due to the force-balance condition, $-\sum_q \nabla_{\mathbf{u}_{\mathbf{n}}} U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|)|_{\mathbf{u}_{\mathbf{n}}=\mathbf{u}_{\mathbf{n}+\mathbf{m}_q}} = \mathbf{0}$, equivalently $U'(\ell) \sum_q \mathbf{a}_q = \mathbf{0}$ due to the mirror symmetry of the lattice vectors. The force on the particle indexed by $\mathbf{n}$, Equation (8.102), can be expressed equivalently in terms of the dynamical matrix $\mathbf{D}_{\mathbf{nn}'}$,

$$-\sum_{q=1}^6 \nabla_{\mathbf{u}_{\mathbf{n}}} U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) = -\sum_{\mathbf{n}'} \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'}, \quad (8.103)$$

where

$$\mathbf{D}_{\mathbf{nn}'} = \begin{cases} -\frac{U'(\ell)}{\ell} \mathbb{1}_2 - \left(U''(\ell) - \frac{U'(\ell)}{\ell} \right) \mathbf{a}_q \mathbf{a}_q^{\top}, & \text{for } \mathbf{n}' = \mathbf{n} + \mathbf{m}_q, \\ 3 \left(U''(\ell) + \frac{U'(\ell)}{\ell} \right) \mathbb{1}_2, & \text{for } \mathbf{n}' = \mathbf{n}, \\ 0, & \text{otherwise,} \end{cases} \quad (8.104)$$

as deduced by comparing Equations (8.102) and (8.103), and using that $\sum_q \mathbf{a}_q \mathbf{a}_q^{\top} = 3\mathbb{1}_2$.

The above suggests the total instantaneous energy of the system can be expressed as

$$\begin{aligned} \mathcal{E} &= \frac{1}{2} \sum_{\mathbf{n}} \sum_{q=1}^6 U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) = 3VU(\ell) + \frac{1}{2} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \mathbf{u}_{\mathbf{n}} \cdot \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'} \\ &\quad + \mathcal{O}((\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q})^3), \end{aligned} \quad (8.105)$$

where the factors of 1/2 correct for the double counting of each pair potential from the double sums, and the linear term from Equation (8.101) vanishes due to the mirror symmetry of the lattice vectors, e.g. $\mathbf{a}_1 = -\mathbf{a}_4$, resulting in $\sum_{\mathbf{n}} \sum_q \mathbf{u}_{\mathbf{n}} \cdot \mathbf{a}_q = \sum_{\mathbf{n}} \sum_q \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} \cdot \mathbf{a}_q$.

Under the harmonic approximation, the instantaneous energy can be written as

$$\mathcal{E}_{\text{harm.}} = \frac{1}{2} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \mathbf{u}_{\mathbf{n}} \cdot \mathbf{D}_{\mathbf{nn}'} \mathbf{u}_{\mathbf{n}'}, \quad (8.106)$$

up to an irrelevant constant offset $3VU(\ell)$. Equation (8.106) is of the same form as the expressions used to calculate the energy in Refs. [232, 254]. Even under the harmonic approximation, the instantaneous energy is not simply composed of terms like the squared separation $(\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}'})^2$, but, due to the modulus in the argument of the pair potential $U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|)$, the energy contains projections along the lattice vectors as dictated by Equation (8.104).

Finally, note that taking a further derivative of Equation (8.103) produces

$$\sum_{q=1}^6 \nabla_{\mathbf{u}_{\mathbf{n}}}^2 U(|\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}+\mathbf{m}_q} - \ell \mathbf{a}_q|) = \text{Tr } \mathbf{D}_{\mathbf{nn}} = 6 \left(U''(\ell) + \frac{U'(\ell)}{\ell} \right). \quad (8.107)$$

8.C Exact expressions for components of fully time-dependent displacement correlator, Equation (8.47)

Here, I derive exact expressions for the active $\mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2)$ and thermal $\Xi_{\mathbf{p}}^{\pm}(t_1, t_2)$ components of the displacement correlator, Equation (8.47).

First, the integral arising from the thermal noise correlator,

$$V\Xi_{\mathbf{p}}^{\pm}(t_1, t_2) := \int_0^{t_2} dt'' \int_0^{t_1} dt' e^{-\lambda_{\mathbf{p}}^{\pm}(t_1-t')} e^{-\lambda_{-\mathbf{p}}^{\pm}(t_2-t'')} \left\langle \hat{\xi}_{\mathbf{p}}^{\pm}(t') \hat{\xi}_{-\mathbf{p}}^{\pm}(t'') \right\rangle. \quad (8.108)$$

In the case $\lambda_{\mathbf{p}}^{\pm} > 0$, after inserting the explicit expression for the thermal noise correlation, Equation (8.42), one obtains

$$\begin{aligned} \Xi_{\mathbf{p}}^{\pm}(t_1, t_2) &= \Gamma^2 e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \int_0^{t_2} dt'' \int_0^{t_1} dt' e^{\lambda_{\mathbf{p}}^{\pm}(t'+t'')} \delta(t'' - t') \\ &= \Gamma^2 e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \int_0^{t_2} dt'' e^{2\lambda_{\mathbf{p}}^{\pm} t''} \Theta(t_1 - t'') \\ &= \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^{\pm}} e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \left(e^{2\lambda_{\mathbf{p}}^{\pm} \min(t_1, t_2)} - 1 \right) \\ &= \frac{\Gamma^2}{2\lambda_{\mathbf{p}}^{\pm}} \left(e^{-\lambda_{\mathbf{p}}^{\pm}|t_2-t_1|} - e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \right), \end{aligned} \quad (8.109)$$

where $\Theta(t)$ is the Heaviside function, defined to be 1 for $t \geq 0$ and 0 otherwise. For the case $\lambda_{\mathbf{p}}^{\pm} = 0$, corresponding to the $\mathbf{0}$ -mode, one finds instead

$$\Xi_{\mathbf{0}}^{\pm}(t_1, t_2) = \Gamma^2 \min(t_1, t_2). \quad (8.110)$$

By considering the long-time $t \gg \lambda_{\mathbf{p}}^{\pm}$ behaviour of Equations (8.109) and (8.110), one recovers Equation (8.51) in Appendix 8.A.

Next, the integral arising from the active noise is

$$V\mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2) := \int_0^{t_2} dt'' \int_0^{t_1} dt' e^{-\lambda_{\mathbf{p}}^{\pm}(t_1-t')} e^{-\lambda_{-\mathbf{p}}^{\pm}(t_2-t'')} \langle \hat{w}_{\mathbf{p}}^{\pm}(t') \hat{w}_{-\mathbf{p}}^{\pm}(t'') \rangle. \quad (8.111)$$

To proceed, I separate the double integral into three components depending on whether $t'' > t'$ or $t' > t''$. Generally,

$$\begin{aligned} \int_0^{t_2} dt'' \int_0^{t_1} dt' f(t', t'') &= \int_0^{t_1} dt'' \int_{t''}^{t_1} dt' f(t', t'') \Theta(t' - t'') \\ &\quad + \int_0^{t_1} dt' \int_{t'}^{t_1} dt'' f(t', t'') \Theta(t'' - t') \\ &\quad + \int_0^{t_1} dt' \int_{t_1}^{t_2} dt'' f(t', t'') \Theta(t'' - t') \\ &= 2 \int_0^{t_1} dt'' \int_{t''}^{t_1} dt' f(t', t'') \Theta(t' - t'') \\ &\quad + \int_0^{t_1} dt' \int_{t_1}^{t_2} dt'' f(t', t'') \Theta(t'' - t'), \end{aligned} \quad (8.112)$$

for a function $f(t', t'')$, where I used that the first two terms on the right-hand side of the first equality evaluate to the same expression and I assumed, without loss of generality, $t_2 \geq t_1$. Inserting the explicit expression for the active noise correlation, Equation (8.44), the double integral in the case $\lambda_{\mathbf{p}}^{\pm} > 0$ is

$$\begin{aligned} \mathcal{W}_{\mathbf{p}}^{\pm}(t_1, t_2) &= w^2 e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \int_0^{t_2} dt'' \int_0^{t_1} dt' e^{\lambda_{\mathbf{p}}^{\pm}(t'+t'')} e^{-\mu|t''-t'|} \\ &= 2w^2 e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \int_0^{t_1} dt'' e^{t''(\lambda_{\mathbf{p}}^{\pm}+\mu)} \int_{t''}^{t_1} dt' e^{t'(\lambda_{\mathbf{p}}^{\pm}-\mu)} \\ &\quad + w^2 e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \int_0^{t_1} dt' e^{t'(\lambda_{\mathbf{p}}^{\pm}+\mu)} \int_{t_1}^{t_2} dt'' e^{t''(\lambda_{\mathbf{p}}^{\pm}-\mu)} \\ &= w^2 \frac{\mu}{(\lambda_{\mathbf{p}}^{\pm})^2 - \mu^2} \left(\frac{e^{-\mu|t_2-t_1|}}{\mu} - \frac{e^{-\lambda_{\mathbf{p}}^{\pm}|t_2-t_1|}}{\lambda_{\mathbf{p}}^{\pm}} - \frac{e^{-\mu t_1} e^{-\lambda_{\mathbf{p}}^{\pm} t_2} + e^{-\mu t_2} e^{-\lambda_{\mathbf{p}}^{\pm} t_1}}{\mu} \right. \\ &\quad \left. + \frac{\lambda_{\mathbf{p}}^{\pm} + \mu}{\lambda_{\mathbf{p}}^{\pm} \mu} e^{-\lambda_{\mathbf{p}}^{\pm}(t_1+t_2)} \right), \end{aligned} \quad (8.113)$$

and similarly for $\lambda_{\mathbf{p}}^{\pm} = 0$,

$$\mathcal{W}_{\mathbf{0}}^{\pm}(t_1, t_2) = \frac{w^2}{\mu^2} \left(e^{-\mu t_1} + e^{-\mu t_2} - e^{-\mu|t_2-t_1|} - 1 + 2\mu \min(t_1, t_2) \right). \quad (8.114)$$

As above, considering $t \gg \lambda_{\mathbf{p}}^{\pm}$ and $t \gg 1/\mu$ in Equations (8.113) and (8.114) recovers Equation (8.50) in Appendix 8.A.

~ Part 4 ~

Outlook

9

Conclusion

The ability to spontaneously produce useful work is a phenomenon that is unique to non-equilibrium systems. Arguably, work extraction from *microscopic* active matter, a subclass of non-equilibrium systems, is more compelling because of the limitations imposed by both thermal fluctuations and the autonomy of the constituent “particles”. This has made the design of microscale “active engines” a highly relevant and timely research objective. To better understand the requirements of this objective, this thesis explored how active matter systems can be harnessed to perform useful work.

After reviewing methods in Part 1, I surveyed a range of minimal models of work extraction from active matter and other non-equilibrium systems in Part 2. In the first chapter of this part, Chapter 4, I explored the dynamics of confined self-propelling particles that switch their self-propulsion direction by interacting stochastically with boundaries. The (Doi-Peliti) field-theoretic framework developed in this chapter allowed the derivation of the fully time-dependent solution to the probability density of these “boundary tumbling” particles. Further analysis revealed a shape transition of the density depending on the interplay between boundary reaction rate, self-propulsion speed, and the effective length scale of the reaction region. Particularly relevant is that these boundary interactions, when the system is mapped to a ring, can enhance the rate of work extraction. This comes at the expense of a diverging energetic cost/entropy production rate associated with precisely measuring when a particle has undergone an irreversible boundary reaction. Thus, an avenue for further research would be to restore finite entropy production in this model by generalising it to include reversible reactions at the boundaries. This would then allow a study of the thermodynamic efficiency of the work extraction in this model.

In Chapter 5, I introduced an experimentally motivated resetting model where a ratchet potential is used to mediate the resetting of a purely diffusive particle by switching on with a constant rate and switching off only upon the particle’s first passage to the origin. This generalised existing resetting models while also offering a new perspective on how to sustain a steady-state net current through finite-time resetting. The exact solutions of the steady-state probability densities, and corresponding net current, yielded a comprehensive overview of the system’s behaviour. The major contribution of this chapter to the overall thesis was the defining of an efficiency parameter that quantified useful power output, in terms of current, relative to the energy that needs to be input from an external controller to sustain the system. It was found that under certain conditions, arbitrarily perfect efficiency can be achieved.

Chapter 6 demonstrated that the same ratchet potential from the previous chapter can be used to extract work autonomously from run-and-tumble particles without needing

to be modulated in time. As in previous chapters, I derived the steady-state probability densities, currents, and entropy production which revealed interesting non-monotonic dependencies on the system parameters. It was found that the thermodynamic efficiency of the work extraction is optimised when the ratchet acts as a diode allowing motion in only one of the self-propulsion states.

Part 2 concluded with Chapter 7, in which optimal feedback protocols for maximising power extraction from active particles with hidden states were studied. An analytic calculation provided an upper bound to power extraction for any protocol, thereby setting an important benchmark for evaluating the performance of active engines. Alongside the analytics, I also studied a novel protocol, coined the “boundary update protocol”, based on the exact calculation of *conditional* splitting probabilities. This protocol was found to saturate the derived optimal bound, suggesting it is optimal for extracting work from active particles.

Finally, in the singular Chapter 8 of Part 3, I established the groundwork for the analytic study of *dense* active matter, which will be integral to the operation of active engines. This chapter characterised the properties of one such class of dense active matter, known as “active crystals”, which form from the condensation of interacting active particles in two dimensions. By deriving exact expressions for the fluctuations and entropy production, I provided a detailed picture of the crystal’s behaviour, while crucially avoiding effective one-dimensional approximations recently made in the literature. The entropy production offered insight into how energy is dissipated in these systems. This will be essential to understanding the efficiency of active engines that harness the collective motion of ensembles of active particles.

Overall, this thesis provided an exposition of work extraction from active matter systems. It is intended to lay the foundations for the design of *efficient* active engines, while also advancing our broader understanding of active matter by providing new models, methods, and predictions that will inform future research.

~ Part 5 ~

Appendices

A

Stochastic cloaking: a case study of interpreting a Langevin equation

This appendix is based on the following preprint:

C. Roberts, Z. Zhang, H. Rojas, S. Bo, C. Escudero, S. Guenneau, and G. Pruessner. Stochastic cloaking: concealing a region from diffusive particles, arXiv 2410.04124 (2024) [55].

The necessary permissions to reproduce this preprint as part of my thesis are included in Appendices B.2.1, B.2.3, B.2.4, B.2.7, B.2.8, and B.2.10.

Author contributions to original manuscript: GP and SG supervised the project. I performed the bulk of the numerical simulations with input from ZZ. I wrote the bulk of the manuscript and produced all figures. GP, SG, ZZ, and I interpreted the results. HR and CE provided guidance on the different interpretations of the Langevin equation and how to simulate them. SB provided guidance on recovering the different conventions of an overdamped Langevin equation from simulations involving the underdamped Langevin equation. All authors edited the manuscript.

Appendix summary

This appendix demonstrates that the interpretation of multiplicative noise in a stochastic equation can lead to different physical properties of a system. I demonstrate this for a novel model of cloaking in which a circular core is concealed from an ensemble of diffusing particles whose individual trajectories are governed by a Langevin equation. In particular, the effect of the chosen convention when numerically integrating the Langevin equation is investigated for an annular single-layer invisibility cloak of smoothly varying diffusivity in two dimensions. I find the Itô convention reproduces near-perfect cloaking, while the Stratonovich and Hänggi-Klimontovich conventions do not. The effectiveness of the cloaking is measured by the ability of the cloak to prevent particles from accessing the inner core while simultaneously preserving the particle density outside the cloak compared to simulations involving no core (and no cloak). Enhanced cloaking performance can be achieved by regularising the singular behaviour of the cloak, which I demonstrate through two different approaches. Aside from providing additional background to the methods deployed in this thesis, this appendix lays the foundations for stochastic cloaking, which is a significant milestone following that of optical and thermal cloaking.

A.1 Introduction

The advent of inhomogeneous “metamaterials” has led to the proposal of various exotic phenomena that were once considered the realm of science fiction [256–259]. Notably, by capitalising on the form-invariance of Maxwell’s equations under a coordinate transformation [260], Pendry et al. suggested that tuning the magnetic permeability and electric permittivity of a metamaterial could be used to deviate electromagnetic radiation around an object in such a way that the radiation is undisturbed from its original trajectory [261]. The metamaterial acts as an invisibility cloak in this case, since any external observer would be unable to detect the presence of the concealed object and, crucially, the metamaterial itself. This application of “transformation optics” has inspired research into cloaking for other forms of radiation.

A major milestone is thermal cloaking, based on “transformation thermodynamics” [262–264], where a metamaterial of spatially varying thermal conductivity protects a region from heat flux. Thermal cloaking demonstrated that transformation-based cloaking applies not only to elliptic differential equations—describing optics and acoustics [265, 266]—but also to parabolic differential equations. Yet, both are examples of *deterministic* differential equations.

Before the release of the work on which this appendix is based [55], no equivalent demonstration had been made for systems governed by *stochastic* differential equations, where behaviour can be predicted only on a *statistical* (rather than *precise*) basis. Such a demonstration is thus another significant milestone for cloaking, not least because of the inherent difficulties introduced by stochasticity. The major difficulty arises from the governing stochastic equation—the Langevin equation—being only a “pre-equation”, since it is uniquely determined only after choosing a particular convention under which to integrate it [267]. This is often called the Itô vs. Stratonovich dilemma [56, 267–270], named after the first two conventions to be proposed [58, 59]. Though both are over 60 years old, the fact that these conventions affect the physical properties of a system is still of great interest today [271].

Despite the difficulties posed by stochasticity, in this appendix I demonstrate that an annular metamaterial of spatially varying diffusivity can cloak an inner core from stochastically diffusing particles when interpreted under the Itô convention. The properties of the metamaterial, or “cloak”, are determined from a coordinate transformation that maps the inner core to the surrounding cloak, as in Figure A.1.

In analogy to optical and thermal cloaking, “stochastic” cloaking prevents particles from accessing the core, while preserving the particle density outside the cloak. The latter is quantified by analysing the arrival distribution of particles downstream of the cloak.

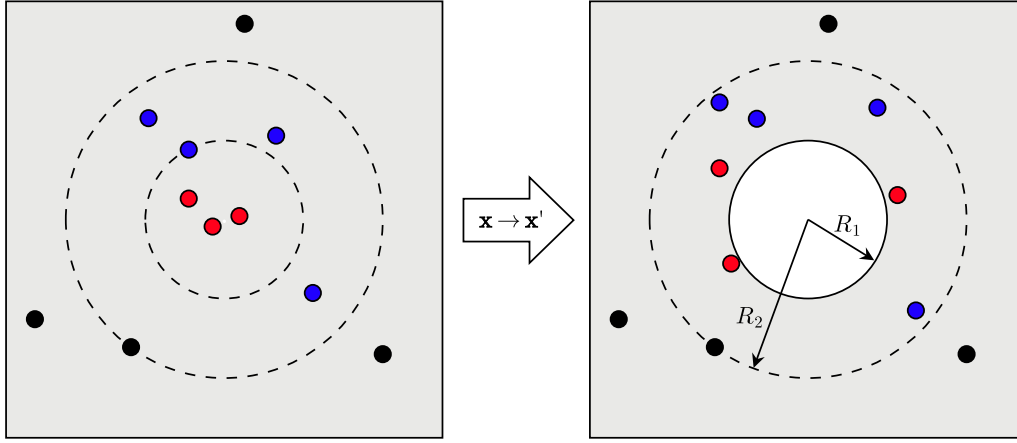


Figure A.1: Schematic representation of a coordinate transformation that tears a hole in the metric space of a two-dimensional plane (left) to produce a finite region, indicated in white, that particles are unable to enter (right). Particle positions at radii $r \geq R_2$ (black points) are invariant under the transformation, while the radii of particles at $r < R_2$ (red and blue points) increase under the transformation.

A.2 Langevin equation

The time evolution of a particle's position $x(t)$ in one dimension is described by the stochastic Langevin equation (see also Chapter 2),

$$\frac{m}{\gamma(x)} \ddot{x}(t) = -\dot{x}(t) + \sqrt{2D(x)}\xi(t), \quad (\text{A.1})$$

where m is the particle's mass, $\gamma(x)$ is the friction coefficient, $D(x)$ is the diffusivity, and $\xi(t)$ is Gaussian white noise with ensemble-averaged mean $\langle \xi(t) \rangle = 0$ and correlation $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$. In the overdamped regime, where the typical timescale τ_o of interest satisfies $\tau_o \gg m/\gamma$, the Langevin equation simplifies to

$$\dot{x}(t) = \sqrt{2D(x)}\xi(t), \quad (\text{A.2})$$

indicating the particle's dynamics are determined solely by $D(x)$.

A.3 Conventions

To simulate a particle trajectory, one can iteratively integrate Equation (A.2) in small timesteps Δt ,

$$x(t + \Delta t) = x(t) + \int_t^{t+\Delta t} ds \sqrt{2D(x(s))}\xi(s), \quad (\text{A.3})$$

which presents a choice when it comes to evaluating the integral on the right-hand side of Equation (A.3). Specifically, one must choose which value the random variable $x(t)$ takes in the interval $[x(t), x(t + \Delta t)]$ in order to evaluate the diffusivity. However, there is no uniquely determined point at which it *should* be evaluated. Instead, the choice is a matter

of the adopted convention, which is parameterised by the continuous variable $\alpha \in [0, 1]$ in the following [272],

$$x(t + \Delta t) = x(t) + \sqrt{2D [(1 - \alpha)x(t) + \alpha x(t + \Delta t)]} \int_t^{t+\Delta t} ds \xi(s), \quad (\text{A.4})$$

where the integral $\int_t^{t+\Delta t} ds \xi(s)$ is numerically evaluated by drawing from a Gaussian distribution of variance Δt .

Three common conventions are Itô ($\alpha = 0$) [58], Stratonovich ($\alpha = 1/2$) [59], and isothermal/Hänggi-Klimontovich ($\alpha = 1$) [60, 61], the latter of which I will refer to as “anti-Itô”. Each convention has its merits [268, 272, 273], however, any $\alpha > 0$ convention essentially requires evaluating the diffusivity at a future timestep. The simplest way to simulate $\alpha > 0$ is thus to reformulate the dynamics in terms of the non-anticipatory Itô convention, $\alpha = 0$, via a correction term [272] or an auxiliary step [274, 275]—see Appendix A.B. Importantly, the chosen convention affects the statistics of the particle’s dynamics, as elucidated by the Fokker-Planck equation describing the time evolution of the particle density,

$$\frac{\partial P(x, t)}{\partial t} = \frac{\partial}{\partial x} D^\alpha(x) \frac{\partial}{\partial x} D^{1-\alpha}(x) P(x, t). \quad (\text{A.5})$$

Though similar to a heat equation, the Fokker-Planck equation differs by having an associated Langevin equation that directly governs the motion of each individual particle. However, due to their similarity, I will leverage methods from transformation thermodynamics [262, 263] to inform the derivation of the spatially varying diffusivity that achieves stochastic particle cloaking in two dimensions. This diffusivity will then be used to simulate an ensemble of diffusive particles via the two-dimensional Langevin equation,

$$x_i(t + \Delta t) = x_i(t) + g_{ij}[(1 - \alpha)\mathbf{x}(t) + \alpha\mathbf{x}(t + \Delta t)] \int_t^{t+\Delta t} ds \xi_j(s), \quad (\text{A.6})$$

where $i, j \in \{1, 2\}$ index the components of vectors (such as the position $\mathbf{x} = (x_1, x_2)$ and noise $\boldsymbol{\xi} = (\xi_1, \xi_2)$), and matrices (such as the square root of the diffusivity/diffusion tensor $\mathbf{g} = \sqrt{2\mathbf{D}} = ((g_{11}, g_{21})^T, (g_{12}, g_{22})^T)$). Above and throughout, repeated indices imply summation.

A.4 Transformed Fokker-Planck equation

To derive the cloak’s spatially varying diffusivity, I consider a coordinate transformation that maps the protected circular core of radius R_1 to a surrounding annulus $R_1 \leq r' \leq R_2$, see Figure A.1, where r' is the radial distance from the centre of the core in the new coordinates. This annular region acts as the cloak, with its diffusivity determined through the specific mapping.

First, I consider the effect of a general coordinate transformation $\mathbf{x} \rightarrow \mathbf{x}'$ on the Fokker-Planck equation in two dimensions. Starting from the Fokker-Planck equation describing

homogeneous diffusion D_0 ,

$$\frac{\partial P(\mathbf{x}, t)}{\partial t} = \frac{\partial}{\partial x_i} D_0 \frac{\partial P(\mathbf{x}, t)}{\partial x_i}, \quad (\text{A.7})$$

I seek the transformed diffusion tensor $\mathbf{D}'$ in the new coordinates that renders the Fokker-Planck equation form-invariant. In other words, by manipulating the transformed Fokker-Planck equation into the same form as Equation (A.7), identification of $\mathbf{D}'$ in place of D_0 readily follows. Leaving the details to Appendix A.A, the Fokker-Planck equation after a general coordinate transformation becomes [262]

$$\frac{\partial P(\mathbf{x}', t)}{\partial t} = \frac{1}{\det(\mathbf{J})} \frac{\partial}{\partial x'_j} J_{kj}^{-1} D_0 J_{kl}^{-1} \det(\mathbf{J}) \frac{\partial P(\mathbf{x}', t)}{\partial x'_l}, \quad (\text{A.8})$$

where the Jacobian matrix $\mathbf{J}$ has components $J_{ij} = \partial_{x'_j} x_i$. Equation (A.8) poses the dynamics on an effective manifold [276], whereas the recipe for finding $\mathbf{D}'$ requires the coordinate transformation to leave the Fokker-Planck equation in an invariant “Euclidean” form analogous to Equation (A.7). What prevents this from happening is the space-dependent factor $1/\det(\mathbf{J})$ preceding the spatial derivatives. In transformation thermodynamics, this factor is merely absorbed into the specific heat capacity [262, 263]. However, there is no analogous trick for the case of stochastic particle diffusion, since it depends solely on the diffusivity $\mathbf{D}'(\mathbf{x})$. Hence, the Fokker-Planck equation is generally not form-invariant under a coordinate transformation, as Equation (A.8) is its most simplified form before considering specific transformations.

A.5 Non-linear transformation

Equation (A.8) suggests a transformation with constant $\det(\mathbf{J})$ would render the Fokker-Planck equation invariant. The most-studied transformation is the linear mapping $r' = R_1 + r(R_2 - R_1)/R_2$ for $r \leq R_2$ [261, 277, 278]. This has non-constant $\det(\mathbf{J}) = (R_2/(R_2 - R_1))^2 (r' - R_1)/r'$ for $r \leq R_2$, and so alternative transformations need to be considered. As it turns out, a transformation that simultaneously maps the protected region, $r' < R_1$, to the annulus, $R_1 \leq r' \leq R_2$, while maintaining constant $\det(\mathbf{J})$ is difficult to find. *Close* to satisfying both properties is the non-linear transformation [279, 280],

$$r' = \begin{cases} \sqrt{\beta r^2 + R_1^2}, & r \leq R_2, \\ r, & r > R_2, \end{cases} \quad (\text{A.9})$$

where $\beta = (R_2^2 - R_1^2)/R_2^2$ and the azimuthal coordinate $\theta = \theta'$ is invariant under the transformation. In Cartesian coordinates $\mathbf{x}' = (x', y')$, the Jacobian for this non-linear

transformation is

$$\begin{aligned} J &= \frac{\partial(x, y)}{\partial(r, \theta)} \frac{\partial(r, \theta)}{\partial(r', \theta')} \frac{\partial(r', \theta')}{\partial(x', y')} \\ &= \begin{cases} R(\theta') \text{diag} \left(\frac{r'}{r\beta}, \frac{r}{r'} \right) R(-\theta'), & R_1 < r' \leq R_2, \\ \mathbb{1}, & r' > R_2, \end{cases} \end{aligned} \quad (\text{A.10})$$

where $R(\theta)$ and $\mathbb{1}$ are the 2×2 rotation and identity matrices, respectively. The Jacobian (A.10) has a piecewise-constant determinant,

$$\det(J) = \begin{cases} \frac{1}{\beta}, & R_1 < r' \leq R_2, \\ 1, & r' > R_2, \end{cases} \quad (\text{A.11})$$

suggesting Equation (A.8) can be brought into the desired form (A.7) on a piecewise basis under the transformation (A.9) above. On this piecewise basis, the factors of $\det(J)$ in Equation (A.8) cancel, allowing one to approximate the Fokker-Planck equation under this transformation by

$$\frac{\partial P(\mathbf{x}', t)}{\partial t} \approx \frac{\partial}{\partial x'_j} D'_{jk} \frac{\partial P(\mathbf{x}', t)}{\partial x'_k}, \quad (\text{A.12})$$

where the piecewise diffusion tensor is identified as

$$D' = D_0 J^{-T} J^{-1} = \begin{cases} D_0 \beta R(\theta') \text{diag} \left(\frac{r'^2 - R_1^2}{r'^2}, \frac{r'^2}{r'^2 - R_1^2} \right) R(-\theta'), & R_1 < r' \leq R_2, \\ D_0 \mathbb{1}, & r' > R_2, \end{cases} \quad (\text{A.13})$$

from which homogeneous diffusion $D' = D_0 \mathbb{1}$, as in Equation (A.7), can be recovered by setting $R_1 = 0$. Strictly speaking, Equation (A.12) is an equality everywhere except at $r' = R_2$, where there is an additional divergent contribution arising from the sharp jump in $\det(J)$, Equation (A.11). By neglecting this term, the diffusion tensor in Equation (A.13) is naïvely expected to yield far-from-perfect cloaking. Furthermore, Equation (A.12) has the appearance of a two-dimensional analogue to the one-dimensional Fokker-Planck equation (A.5) with $\alpha = 1$, naïvely suggesting the anti-Itô convention [60, 61] of the Langevin equation (A.6) would yield the best cloaking performance. However, such a prediction is based on the misguided presumption that the identification of α from Equation (A.12) equally applies to Fokker-Planck equations other than just the one-dimensional case [272]. In fact, in higher dimensions, the correction term that arises when treating anti-Itô as a perturbation to Itô is generally not of the divergence form necessary to write the Fokker-Planck equation as a two-dimensional analogue of Equation (A.5) [268]. As a result, I also trialled the diffusion tensor D' , Equation (A.13), in the Langevin equation (A.6) for conventions other than just anti-Itô. This was further justified *a posteriori*, since I found the Itô convention [58] resulted in the best cloaking performance.

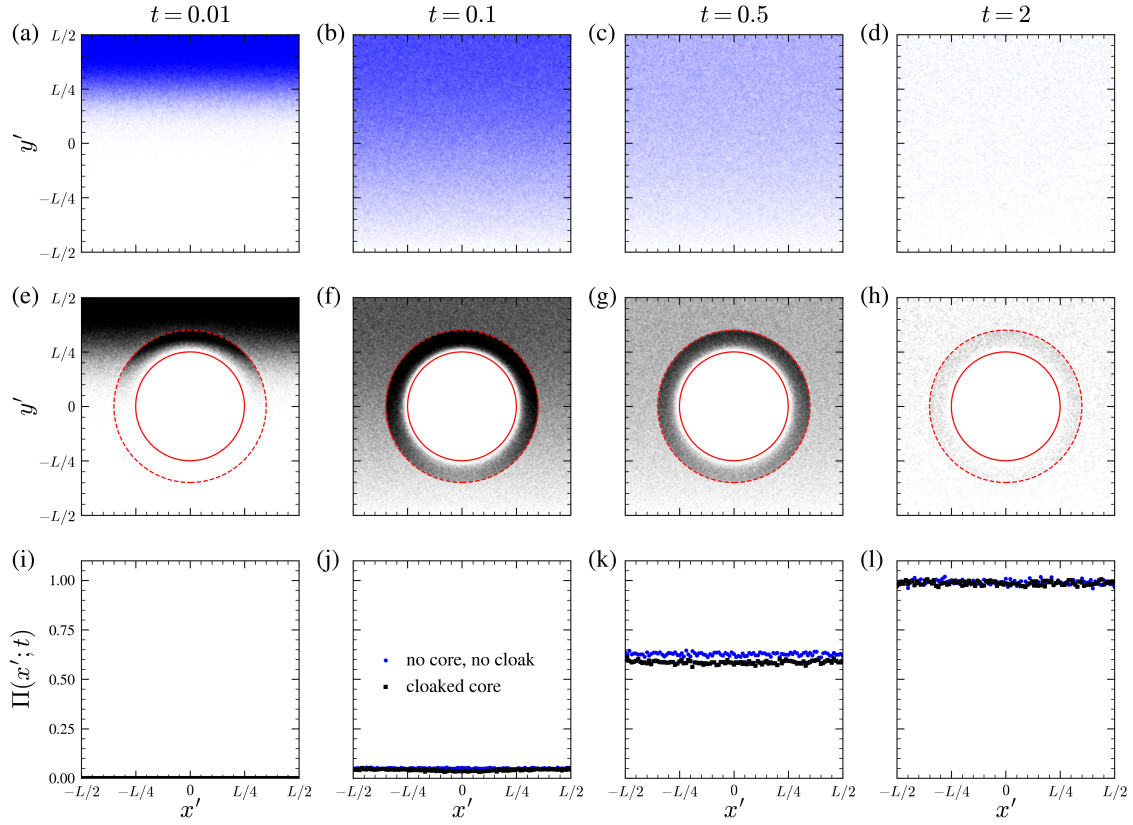


Figure A.2: Comparison between simulations of no core (a)–(d), and a cloaked core (e)–(h), with their corresponding arrival distributions $\Pi(x'; t)$, Equation (A.14), (i)–(l) at times $t = 0.01$ in (a), (e), and (i); $t = 0.1$ in (b), (f), and (j); $t = 0.5$ in (c), (g), and (k); and $t = 2$ in (d), (h), and (l). Each data point in (a)–(h) represents the position of one of $N = 10^6$ particles. The simulation parameters used in all subfigures were $\Delta t = 10^{-5}$, $L = 1$, $D_0 = 1$. In (e)–(h), the inner core has radius $R_1 = 0.25$ (solid red line) and is surrounded by an annular cloak of outer radius $R_2 = 0.35$ (dashed red line). Particles are prevented from penetrating the core by the cloak in (e)–(h), and the arrival distributions $\Pi(x'; t)$ in (i)–(l) show that of the cloaked core closely matches that of no core for all times t , suggesting the diffusion tensor, Equation (A.13), used in the cloaking simulations produces near-perfect cloaking.

A.6 Simulation setup

I performed simulations to determine how well the cloak, with diffusivity given by Equation (A.13), conceals the inner core. The core of radius R_1 is centred in a square box of linear size L . The box has periodic boundary conditions at the sides, $x' = -L/2$ and $x' = L/2$, a reflecting boundary at the top, $y' = L/2$, and an absorbing boundary at the bottom, $y' = -L/2$, through which all particles eventually leave the system. A uniform line of N particles is initialised at the top, $y' = L/2$, at time $t = 0$, i.e. $P(x', y'; t = 0) = \delta(y' - L/2) \sum_{i=1}^N \delta(x' + L/2 - iL/N)/N$. This setup is notably different to that of thermal cloaking, where the temperatures at the top and bottom of the box are kept fixed. Here, the setup is analogous to a single pulse of radiation emitted from the line

$y' = L/2$ at $t = 0$. Strictly speaking, each particle contributes a Dirac delta function to the overall particle density $P(x', y'; t)$. However, for finite N , the particle density is rather viewed in a coarse-grained sense, i.e. the simulation box is envisaged as being divided into small cells of linear length ℓ , such that the density in a particular cell is well approximated by $n/(N\ell^2)$, where n is the number of particles contained in that cell. In this sense, the true particle density $P(x', y'; t)$ is recovered in the thermodynamic limit $N \rightarrow \infty$, while also taking $\ell \rightarrow 0$.

After initialisation, particles diffuse according to Equation (A.6) with diffusivity given by Equation (A.13)—see Appendix A.B for full details. In case particles penetrated the core $r' \leq R_1$, I chose it to have the same homogeneous diffusivity D_0 as the medium surrounding the cloak. Perfect cloaking would prevent particles from penetrating the core, $r' \leq R_1$, while also ensuring the density outside the cloak, $r' > R_2$, matches that of a simulation containing no core at all times t . In other words, any observer measuring the density at a radius $r' > R_2$ would be unable to detect the presence of the core *and* the cloak because the density would be the same as in their absence. How closely these densities match gives a measure of the cloak’s performance. To formally quantify this, I measured the cumulative arrival distribution $\Pi(x, t_f)$ of particles at the absorbing boundary, which is analogous to a “splitting probability” in a first-passage time problem [56],

$$\Pi(x'; t_f) = \int_0^{t_f} dt D_0 \frac{\partial P(x', y'; t)}{\partial y'} \Big|_{y'=-L/2}, \quad (\text{A.14})$$

where $D_0 \partial_y P(x', y'; t)$ is the particle current at $\mathbf{x}' = (x', y')$ in the negative- y' direction. Equation (A.14) is the density of particles that have arrived at position x' on the absorbing boundary by time t_f . The spatial average of $\Pi(x'; t_f)$ asymptotically approaches unity as $t_f \rightarrow \infty$, i.e. $\lim_{t_f \rightarrow \infty} \int_{-L/2}^{L/2} dx' \Pi(x'; t_f)/L = 1$, signifying the absorption of all particles. For the cloaking to be considered effective, the arrival distribution in the simulation of the cloaked core must closely match that of a simulation of no core (and no cloak).

A.7 Simulation results

I performed the simulations described above for the Itô ($\alpha = 0$) [58], Stratonovich ($\alpha = 1/2$) [59], and anti-Itô ($\alpha = 1$) [60, 61] conventions of interpreting the Langevin equation (A.6). The Stratonovich and anti-Itô conventions resulted in poorer cloaking than that of Itô, signified by: particles penetrating the core; spurious large jumps near $r' = R_1$; and noticeable differences in the arrival distributions, Equation (A.14), compared to that of no core. This is not surprising given the application of these conventions to systems involving “problematic” boundaries—like the discontinuity at $r' = R_2$ and singularity at $r' = R_1$ in the diffusivity, Equation (A.13)—can lead to ill-posed results, as mentioned in Refs. [268, 281–283]. Given their relatively poor performance, I will omit further discussion of the Stratonovich and anti-Itô conventions.

The key result of this appendix is that, remarkably, the Itô convention exhibited near-perfect cloaking signified by no particle penetration of the core and an arrival distribution,

Equation (A.14), that closely matched that of no core for all times t , see Figure A.2. “Near perfect” is to caveat a small discrepancy in the number of particles that have been absorbed up to time t between the simulations of the cloaked core and no core. However, this is similar to time-lags typically seen in thermal cloaking [284]. Moreover, this discrepancy all but disappears through regularisation procedures that I introduce in Appendix A.C. Strikingly, the particle density inside the cloak $R_1 < r' \leq R_2$ is markedly different to that seen for thermal cloaking, where the density typically decays smoothly from the outer region $r' > R_2$ to the inner cloak boundary $r' = R_1$ [262]. Here, there is a distinct “halo” of high particle density in the cloak to accommodate those particles that would otherwise be inside the core $r' < R_1$. This also suggests why the smooth decay in density for thermal cloaking comes at the cost of penetration of the core [262].

A.8 Conclusion

Inspired by optical and thermal cloaking [261, 262], I demonstrated “stochastic” cloaking of a region from diffusive particles. This is in spite of the lack of form-invariance of the Fokker-Planck equation under a general coordinate transformation, as well as the inherent difficulties introduced by stochasticity. The setup involved a circular core that was concealed from the diffusive particles by surrounding it with an annular metamaterial of spatially varying diffusivity. To quantify the cloaking performance, I measured the arrival distribution, Equation (A.14), of particles along a tangential line downstream of the cloak. The hallmark of cloaking in this case is an arrival distribution that matches that of a simulation involving no core for all times. Based on this, the key result of this appendix is a demonstration of near-perfect cloaking for the diffusion tensor D' in Equation (A.13) if the Langevin equation is interpreted under the Itô convention [58], see Figure A.2. The same is not true for other interpretations, such as Stratonovich and Hänggi-Klimontovich, thus demonstrating that the interpretation of multiplicative noise in a Langevin equation can lead to different physical properties of the system under consideration. The cloaking performance under the Itô convention can be further improved through regularisation procedures introduced in Appendix A.C. While near-perfect cloaking was demonstrated under the Itô convention, the specific coordinate transformation I considered resulted in invariance of the Fokker-Planck equation only on a piecewise basis. Therefore, future work should focus on establishing a firmer theoretical basis for the cloaking that results from the Itô convention. Another interesting avenue for further research would be to test stochastic cloaking on other cloak geometries, such as diamonds [285]. Aside from demonstrating that the interpretation of a Langevin equation can lead to different physical properties, this appendix has laid the foundations for a novel class of cloaking and thereby provides a completely new way to explore this intriguing phenomenon.

APPENDIX A APPENDICES

A.A Coordinate transformation of the Fokker-Planck equation

In this supplementary section, I derive Equation (A.8) of the main text, i.e. the result of applying a coordinate transformation to the Fokker-Planck equation (A.7) describing homogeneous diffusion of strength D_0 . For convenience, I repeat the latter here,

$$\frac{\partial P(\mathbf{x}, t)}{\partial t} = \frac{\partial}{\partial x_i} D_0 \frac{\partial P(\mathbf{x}, t)}{\partial x_i}, \quad (\text{A.15})$$

where, as in the main text, a repeated index implies summation over that index.

The standard way [262] to proceed is to integrate Equation (A.15) against a scalar “test function” $\phi(\mathbf{x})$, where $\mathbf{x} = (x_1, x_2)$, whose properties are arbitrary aside from being infinitely differentiable and having compact support on the region $\Omega(\mathbf{x}) = [-L/2, L/2] \times [-L/2, L/2]$ in which the particles reside. From integrating Equation (A.15),

$$\int_{\Omega(\mathbf{x})} dx_1 dx_2 \frac{\partial P(\mathbf{x}, t)}{\partial t} \phi(\mathbf{x}) = - \int_{\Omega(\mathbf{x})} dx_1 dx_2 \frac{\partial \phi(\mathbf{x})}{\partial x_i} D_0 \frac{\partial P(\mathbf{x}, t)}{\partial x_i}, \quad (\text{A.16})$$

where the boundary term from the integration by parts on the right-hand side vanishes due to the compact support property of $\phi(\mathbf{x})$.

Now, I consider the effect of a general coordinate transformation $\mathbf{x} = (x_1, x_2) \rightarrow \mathbf{x}' = (x'_1, x'_2)$. Under the change of coordinates, all instances of ∂_{x_j} in Equation (A.16) are replaced with $J_{ij}^{-1} \partial_{x'_j}$, where $J_{ij} = \partial_{x'_j} x_i$ are elements of the Jacobian matrix $\mathbf{J}$, and $dx_1 dx_2 = \det(\mathbf{J}) dx'_1 dx'_2$, i.e.

$$\int_{\Omega(\mathbf{x}')} dx'_1 dx'_2 \det(\mathbf{J}) \frac{\partial P(\mathbf{x}', t)}{\partial t} \phi(\mathbf{x}') = - \int_{\Omega(\mathbf{x}')} dx'_1 dx'_2 J_{ji}^{-1} \frac{\partial \phi(\mathbf{x}')}{\partial x'_i} D_0 J_{jk}^{-1} \det(\mathbf{J}) \frac{\partial P(\mathbf{x}', t)}{\partial x'_k}. \quad (\text{A.17})$$

The integrand on the right-hand side of Equation (A.17) is merely the scalar product of the two vectors $\partial_{x'_i} \phi(\mathbf{x}')$ and $J_{ji}^{-1} D_0 J_{jk}^{-1} \det(\mathbf{J}) \partial_{x'_k} P(\mathbf{x}', t)$. Hence, upon another integration by parts to return the derivative $\partial_{x'_j}$ acting on the former to acting on the latter, followed by some rearrangement,

$$\int_{\Omega(\mathbf{x}')} dx'_1 dx'_2 \phi(\mathbf{x}') \left(\det(\mathbf{J}) \frac{\partial P(\mathbf{x}', t)}{\partial t} - \frac{\partial}{\partial x'_i} J_{ji}^{-1} D_0 J_{jk}^{-1} \det(\mathbf{J}) \frac{\partial P(\mathbf{x}', t)}{\partial x'_k} \right) = 0, \quad (\text{A.18})$$

where the boundary term resulting from the integration by parts once again vanishes. It follows that if $P(\mathbf{x}', t)$ satisfies Equation (A.18) for an arbitrary test function $\phi(\mathbf{x}')$, then it also satisfies Equation (A.8).

A.B Simulations of different conventions for interpreting the Langevin equation

Here, I detail how the simulations of the different discretisation conventions of the Langevin equation were performed. As discussed in the main text, the most direct route to simulating the $\alpha > 0$ cases is by reformulating the numerical integration of the Langevin equation (A.6) in terms of the non-anticipatory Itô convention [58], $\alpha = 0$, either through a correction term [272] or an auxiliary step [274, 275]. The correction term that arises when treating the other conventions as a perturbation to Itô typically involves spatial derivatives of the diffusion tensor D' . Since the diffusion tensor here, Equation (A.13), has a jump discontinuity at $r' = R_1$, this makes it difficult to simulate the dynamics through the correction-term approach. Thus, I instead opt for the auxiliary-step approach, which is able to handle discontinuities [274]. Qualitatively, this approach involves first generating an auxiliary position $\tilde{\mathbf{x}}(t + \Delta t)$ at the future timestep under the Itô convention. This auxiliary position is then interpreted as the “future” timestep at which to evaluate the diffusion tensor for an $\alpha > 0$ simulation, but still treating the Langevin equation (A.6) under the Itô convention. This correctly recovers the statistics of an $\alpha > 0$ simulation [274, 275]. More explicitly, the simulations are implemented by the pseudocode in Algorithm 1, where all positions are to be understood as those in the new coordinates *after* applying the coordinate transformation.

A.C Regularisation and realistic cloaks

To corroborate the findings in the main text of near-perfect cloaking under the Itô convention, Figure A.2, I also performed simulations for two cases of stochastic cloaking that could more feasibly be implemented in an experiment.

A.C.a Underdamped dynamics

The first of these is for the more general underdamped dynamics described by the two-dimensional analogue of Equation (A.1), i.e.

$$m\ddot{\mathbf{x}}(t) = -\gamma(\mathbf{x})\dot{\mathbf{x}} + \gamma(\mathbf{x})\mathbf{g}(\mathbf{x})\boldsymbol{\xi}(t), \quad (\text{A.19})$$

where the symbols retain their same definitions as in the main text. Here, the sharp jumps in the diffusivity D' , Equation (A.13), are regularised by the particles having inertia. The results of the overdamped case in the main text can be recovered for the underdamped dynamics by taking particle mass $m \rightarrow 0$ for a spatially varying diffusivity but constant friction coefficient. This is consistent with the recipe to recover the Itô convention of an overdamped Langevin equation from a discretisation-independent underdamped Langevin equation [286]. A snapshot of the particle density and arrival distribution from an underdamped simulation for constant $\gamma = 1$ (corresponding to $\alpha = 0$ in the overdamped regime) is illustrated in Figure A.3. As for the overdamped dynamics considered in the main text, Figure A.2, spatially varying γ (corresponding to $\alpha = 1$ in the overdamped regime) in

```

initialise:
    • Set particle index:  $n = 1$ ;
1 while  $n \leq N$  do
    initialise:
        • Set initial conditions:  $t = 0$ ,  $y(0) = L/2$ ,  $x(0) = nL/N - L/2$ ;
2 while  $t < t_f$  and  $y(t) > -L/2$  do
3     • Generate two independent random numbers,  $\mathcal{N}_1(0, \Delta t)$  and  $\mathcal{N}_2(0, \Delta t)$ ,
        drawn from a Gaussian distribution of mean 0 and variance  $\Delta t$ , i.e. a
        distribution  $G(x) = \exp(-x^2/(2\Delta t))/\sqrt{2\pi\Delta t}$ ;
4     • Calculate auxiliary “Itô” position:
5      $\tilde{x}_I(t + \Delta t) = x(t) + g_{11}[\mathbf{x}(t)]\mathcal{N}_1(0, \Delta t) + g_{12}[\mathbf{x}(t)]\mathcal{N}_2(0, \Delta t)$ ;
6      $\tilde{y}_I(t + \Delta t) = y(t) + g_{21}[\mathbf{x}(t)]\mathcal{N}_1(0, \Delta t) + g_{22}[\mathbf{x}(t)]\mathcal{N}_2(0, \Delta t)$ ;
7     • Calculate  $\alpha$ -dependent position:
8     if  $0 < \alpha \leq 1$  then
9          $x(t + \Delta t) = x(t) + g_{11}[(1 - \alpha)\mathbf{x}(t) + \alpha\tilde{\mathbf{x}}_I(t + \Delta t)]\mathcal{N}_1(0, \Delta t) + g_{12}[(1 -$ 
10          $\alpha)\mathbf{x}(t) + \alpha\tilde{\mathbf{x}}_I(t + \Delta t)]\mathcal{N}_2(0, \Delta t)$ ;
11          $y(t + \Delta t) = y(t) + g_{21}[(1 - \alpha)\mathbf{x}(t) + \alpha\tilde{\mathbf{x}}_I(t + \Delta t)]\mathcal{N}_1(0, \Delta t) + g_{22}[(1 -$ 
12          $\alpha)\mathbf{x}(t) + \alpha\tilde{\mathbf{x}}_I(t + \Delta t)]\mathcal{N}_2(0, \Delta t)$ ;
13     else
14         if  $\alpha = 0$  then
15              $x(t + \Delta t) = \tilde{x}_I(t + \Delta t)$ ;
16              $y(t + \Delta t) = \tilde{y}_I(t + \Delta t)$ ;
17     • Implement periodic boundary conditions:
18     if  $x(t + \Delta t) \geq L/2$  then
19         •  $x(t + \Delta t) = x(t + \Delta t) - L$ ;
20     if  $x(t + \Delta t) < -L/2$  then
21         •  $x(t + \Delta t) = x(t + \Delta t) + L$ ;
22     • Implement reflecting boundary condition:
23     if  $y(t + \Delta t) > L/2$  then
24         •  $y(t + \Delta t) = L - y(t + \Delta t)$ ;
25     • Increment time:  $t = t + \Delta t$ ;
26     • Increment particle number:  $n = n + 1$ ;
    
```

Algorithm 1: Pseudocode to implement the different discretisation conventions of the overdamped Langevin equation (A.6). In the pseudocode, t_f is the final time that the simulation is run to for each particle, Δt is the simulation timestep, N is the total number of particles, and g_{ij} are the elements of the matrix $\mathbf{g} = \sqrt{2\mathbf{D}}$, as in the main text, where $\mathbf{D}$ can represent either the singular diffusion tensor of Equation (A.13), or the non-singular diffusion tensor of Equation (A.23), see Appendix A.C, depending on which diffusion tensor is being simulated.

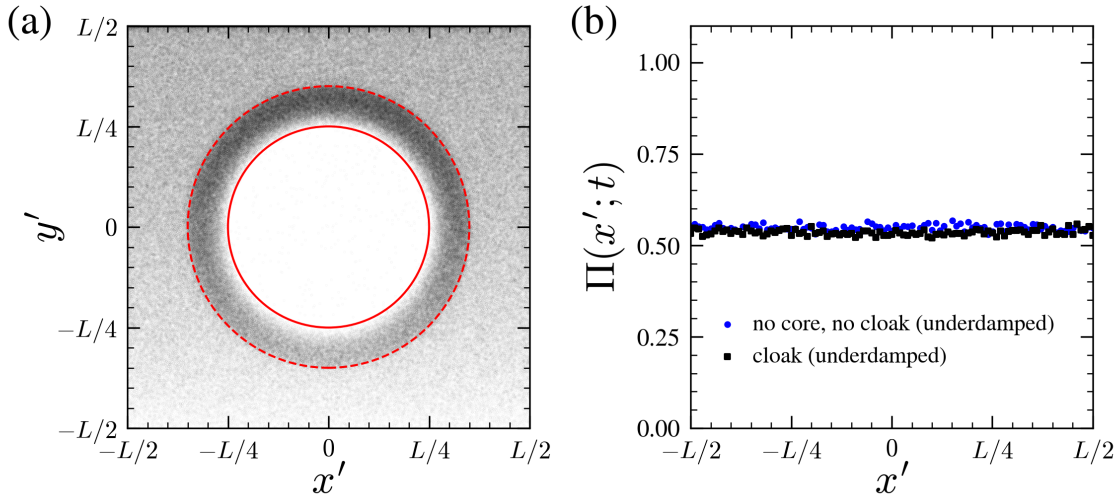


Figure A.3: (a) Snapshot at time $t = 0.5$ from a simulation of the underdamped dynamics described by Equation (A.19), for constant $\gamma = 1$ and using the diffusion tensor given in Equation (A.13). Details of how the underdamped dynamics were simulated are given in Appendix A.C.a. Each data point in (a) represents the position of one of $N = 10^6$ particles. (b) Corresponding cumulative arrival distribution $\Pi(x; t)$, Equation (A.14), for the underdamped simulations of a cloaked core compared against that of no core. The simulation parameters used in both subfigures were $\Delta t = 10^{-5}$, $L = 1$, $D_0 = 1$, $m = 10^{-3}$, $R_1 = 0.25$, and $R_2 = 0.35$. I considered a small mass m such that the inertial timescale $m/\gamma \ll L^2/D_0$, thus making the dynamics close to the overdamped regime, illustrated in Figure A.2. However, the fact that there is a finite mass m is enough to regularise the singular behaviour of the diffusion tensor, Equation (A.13), as evidenced by the cumulative arrival distribution $\Pi(x; t)$ for the cloaked core now more closely matching that of no core compared to the overdamped case. Furthermore, compared to the overdamped simulations illustrated in Figure A.2, less particles have been absorbed at $y' = -L/2$ up to time $t = 0.5$ because some particles “stick” to the reflecting boundary $y' = L/2$ for short periods of time due to their inertia. There is also some (albeit a very small amount of) particle penetration of the inner core in the underdamped case, which is the price paid for the regularisation provided by the finite mass m .

the underdamped dynamics yet again produced relatively poor cloaking. For the finite but small m used in Figure A.3, the most notable difference to that of the overdamped dynamics, Figure A.2, is that the arrival distributions between the cloaked core and no core in the underdamped case agree more closely at all times than for the overdamped dynamics—though this comes at the price of some particle penetration of the inner core.

The pseudocode for implementing the underdamped Langevin equation (A.19) is given in Algorithm 2. By Einstein’s relation, diffusion D satisfies $\gamma D = k_B T$, where γ is the friction coefficient, k_B is the Boltzmann constant, and T is the temperature of the heat bath from which the diffusion derives. Hence, spatial modulation of the particle diffusivity can be achieved through either that of the friction γ or the temperature T . In the limit of particle mass $m \rightarrow 0$, the former corresponds to an anti-Itô convention [60, 61], $\alpha = 1$, of

the overdamped Langevin equation (A.6), while the latter corresponds to that of an Itô convention [58], $\alpha = 0$ [286].

A.C.b A non-singular non-linear diffusion tensor

The second experimentally relevant case I consider is to directly regularise the diffusion tensor $\mathbf{D}'$ in Equation (A.13), which is singular at the cloak's inner boundary $r' = R_1$. This singularity resulted from the implicit blowing up of an infinitesimally small “puncture” in the original coordinates to a finite region (circular core of radius R_1) under the coordinate transformation, see Figure A.1 of the main text. This can be regularised from instead starting from a finite region of radius ϵ in the original coordinates [287], given by the following coordinate transformation,

$$r' = \begin{cases} \frac{R_1}{\epsilon} r, & r \leq \epsilon, \\ \sqrt{\beta_\epsilon r^2 + \lambda_\epsilon}, & \epsilon < r \leq R_2, \\ r, & r > R_2, \end{cases} \quad (\text{A.20})$$

where $\lambda_\epsilon = R_2^2(R_1^2 - \epsilon^2)/(R_2^2 - \epsilon^2)$, $\beta_\epsilon = (R_2^2 - R_1^2)/(R_2^2 - \epsilon^2)$, and the azimuthal coordinate is once again invariant under the coordinate transformation, i.e. $\theta' = \theta$. The transformation in Equation (A.20) maps a region of finite radius ϵ to the inner core of radius R_1 , i.e. $r' = R_1$ when $r = \epsilon$. In the limit $\epsilon \rightarrow 0$, one recovers the singular non-linear transformation of Equation (A.9), with the singular behaviour at $r = 0$ now more evident from Equation (A.20) when taking this limit.

As in the main text, I calculate the Jacobian for this transformation in Cartesian coordinates. This results in

$$\mathbf{J} = \frac{\partial(x, y)}{\partial(r, \theta)} \frac{\partial(r, \theta)}{\partial(r', \theta')} \frac{\partial(r', \theta')}{\partial(x', y')} = \begin{cases} \frac{\epsilon}{R_1} \mathbb{1}, & r' \leq R_1, \\ \mathbf{R}(\theta') \text{diag} \left(\frac{r'}{r\beta_\epsilon}, \frac{r}{r'} \right) \mathbf{R}(-\theta'), & R_1 < r' \leq R_2, \\ \mathbb{1}, & r' > R_2, \end{cases} \quad (\text{A.21})$$

which has a piecewise-constant determinant given by

$$\det(\mathbf{J}) = \begin{cases} \frac{\epsilon^2}{R_1^2}, & r' \leq R_1, \\ \frac{1}{\beta_\epsilon}, & R_1 < r' \leq R_2, \\ 1, & r' > R_2. \end{cases} \quad (\text{A.22})$$

By bringing the general expression for the coordinate transformation of the Fokker-Planck equation into a form analogous to Equation (A.7) on a piecewise basis, as done for the singular case in the main text, one can identify the piecewise diffusion tensor for the

```

initialise:
  • Set particle index:  $n = 1$ ;
  • Choose  $\alpha \in \{0, 1\}$ ;
1 while  $n \leq N$  do
  initialise:
    • Set initial conditions:  $t = 0$ ,  $y(0) = L/2$ ,  $x(0) = nL/N - L/2$ ,  $v_x(0) = 0$ ,  $v_y(0) = 0$ ;
2  while  $t < t_f$  and  $y(t) > -L/2$  do
3    • Generate two independent random numbers,  $\mathcal{N}_1(0, \Delta t)$  and  $\mathcal{N}_2(0, \Delta t)$ , drawn from a Gaussian distribution of mean 0 and variance  $\Delta t$ , i.e. a distribution  $G(x) = \exp(-x^2/(2\Delta t))/\sqrt{2\pi\Delta t}$ ;
4    • Update velocity according to the Langevin equation (A.19):
5    if  $\alpha = 1$  then
6      • Friction term is spatially varying, i.e.
7      
$$v_x(t + \Delta t) = v_x(t) + \frac{1}{m} \left[ -v_x(t)\Delta t (\mathbf{D}^{-1}[\mathbf{x}(t)])_{11} - v_y(t)\Delta t (\mathbf{D}^{-1}[\mathbf{x}(t)])_{12} + 2(\mathbf{g}^{-1}[\mathbf{x}(t)])_{11}\mathcal{N}_1(0, \Delta t) + 2(\mathbf{g}^{-1}[\mathbf{x}(t)])_{12}\mathcal{N}_2(0, \Delta t) \right];$$

8      
$$v_y(t + \Delta t) = v_y(t) + \frac{1}{m} \left[ -v_x(t)\Delta t (\mathbf{D}^{-1}[\mathbf{x}(t)])_{21} - v_y(t)\Delta t (\mathbf{D}^{-1}[\mathbf{x}(t)])_{22} + 2(\mathbf{g}^{-1}[\mathbf{x}(t)])_{21}\mathcal{N}_1(0, \Delta t) + 2(\mathbf{g}^{-1}[\mathbf{x}(t)])_{22}\mathcal{N}_2(0, \Delta t) \right];$$

9    else
10     if  $\alpha = 0$  then
11       • Friction term is constant, i.e.
12       
$$v_x(t + \Delta t) = v_x(t) + \frac{1}{m} \left[ -v_x(t)\Delta t + g_{11}[\mathbf{x}(t)]\mathcal{N}_1(0, \Delta t) + g_{12}[\mathbf{x}(t)]\mathcal{N}_2(0, \Delta t) \right];$$

13       
$$v_y(t + \Delta t) = v_y(t) + \frac{1}{m} \left[ -v_y(t)\Delta t + g_{21}[\mathbf{x}(t)]\mathcal{N}_1(0, \Delta t) + g_{22}[\mathbf{x}(t)]\mathcal{N}_2(0, \Delta t) \right];$$

14     • Increment position:
15     
$$x(t + \Delta t) = x(t) + v_x(t + \Delta t)\Delta t;$$

16     
$$y(t + \Delta t) = y(t) + v_y(t + \Delta t)\Delta t;$$

17     • Implement periodic boundary conditions:
18     if  $x(t + \Delta t) \geq L/2$  then
19       •  $x(t + \Delta t) = x(t + \Delta t) - L$ ;
20     if  $x(t + \Delta t) < L/2$  then
21       •  $x(t + \Delta t) = x(t + \Delta t) + L$ ;
22     • Implement reflecting boundary condition:
23     if  $y(t + \Delta t) > L/2$  then
24       •  $y(t + \Delta t) = L - y(t + \Delta t)$ ;
25     • Increment time:  $t = t + \Delta t$ ;
26   • Increment particle number:  $n = n + 1$ ;

```

Algorithm 2: Pseudocode to implement the underdamped Langevin equation (A.19). For simplicity, I set $k_B T = 1$ in the case of $\alpha = 1$, leading to $\gamma = \mathbf{D}^{-1}$, and set $\gamma = k_B = 1$ in the case of $\alpha = 0$, leading to $\mathbf{D} = T$. As in Algorithm 1, t_f is the final time that the simulation is run to for each particle, Δt is the simulation timestep, N is the total number of particles, and g_{ij} are the elements of the matrix $\mathbf{g} = \sqrt{2\mathbf{D}}$.

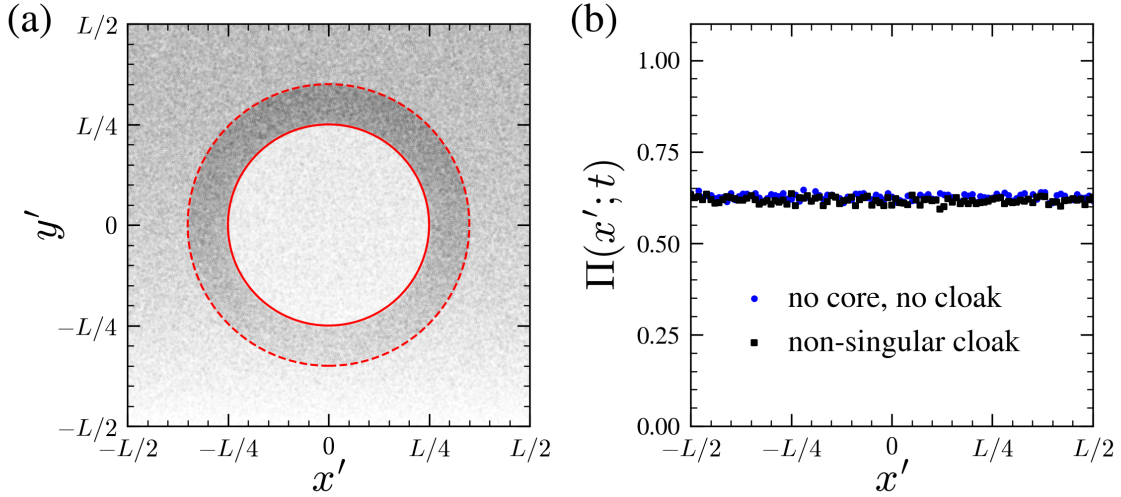


Figure A.4: (a) Snapshot at time $t = 0.5$ from a simulation using the non-singular diffusion tensor, Equation (A.23), derived in Appendix A.C.b. Each data point in (a) represents the position of one of $N = 10^6$ particles. (b) Corresponding cumulative arrival distribution $\Pi(x; t)$, Equation (A.14), for the simulations of the non-singular diffusion tensor compared against that of no core. The simulation parameters used in both subfigures were $\Delta t = 10^{-5}$, $L = 1$, $D_0 = 1$, $\epsilon = 0.2$, $R_1 = 0.25$, and $R_2 = 0.35$. Compared to the simulations of the singular diffusion tensor, Equation (A.13), illustrated in Figure A.2, there is significant particle penetration of the inner core. However, if the core has a homogeneous diffusivity of $D_0 R_1^2 / \epsilon^2$, which is the case here, then the cumulative arrival distribution $\Pi(x; t)$ of the cloak better matches that of no core at all times, signifying that cloaking (in the sense that the particle density *outside* the cloak remains invariant) is achieved to a greater degree.

non-singular transformation as

$$D'_\epsilon = D_0 J^{-T} J^{-1} = \begin{cases} D_0 \frac{R_1^2}{\epsilon^2} \mathbb{1}, & r' \leq R_1, \\ D_0 \beta_\epsilon R(\theta') \text{diag} \left(\frac{r'^2 - R_1^2}{r'^2}, \frac{r'^2}{r'^2 - R_1^2} \right) R(-\theta'), & R_1 < r' \leq R_2, \\ D_0 \mathbb{1}, & r' > R_2. \end{cases} \quad (\text{A.23})$$

This regularised diffusion tensor is more easily mimicked by a metamaterial in an experiment, but comes at the price of allowing particles to penetrate the protected region $r' \leq R_1$. However, if the core is of homogeneous diffusivity, then it is still possible to conceal it from an external observer. Specifically, *given* a core of homogeneous diffusivity that one wishes to conceal, cloaking is achieved by tuning the parameter ϵ in the cloak's spatially varying diffusivity such that the value $D_0 R_1^2 / \epsilon^2$ matches that of the core's given diffusivity.

Figure A.4 shows a snapshot of the particle density and arrival distribution in the case of the non-singular diffusion tensor, Equation (A.23), where particle positions evolve according to the overdamped Langevin equation (A.6) interpreted under the Itô convention [58], $\alpha = 0$. The density is indistinguishable outside the cloak from that of a simulation of

no core, as indicated by the arrival distribution more closely matching that of no core than for the singular diffusion tensor, Equation (A.13), presented in the main text, Figure A.2.

B

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Sent: Fri 15 November 2024, 08:26

Subject: Right to reproduce joint work

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To: Connor Roberts <connor.roberts16@imperial.ac.uk>

Sent: Fri 15 November 2024, 08:47

Subject: Re: Right to reproduce joint work

Dear Connor,

Of course, you have my permission to reproduce our joint work.

Best wishes,
Stefano

B.2.2 Luca Cocconi

From: Connor Roberts <connor.roberts16@imperial.ac.uk>
To: Luca Cocconi <luca.cocconi@ds.mpg.de>
Sent: Mon 29 July 2024, 14:17
Subject: Right to reproduce published work

Dear Luca,

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From: Luca Cocconi <luca.cocconi@ds.mpg.de>
To: Connor Roberts <connor.roberts16@imperial.ac.uk>
Sent: Mon 29 July 2024, 21:58
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Luca

B.2.3 Carlos Escudero

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To: Carlos Escudero Liebana <cescudero@mat.uned.es>
Sent: Fri 15 November 2024, 08:28
Subject: Right to reproduce joint work

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To: Connor Roberts <connor.roberts16@imperial.ac.uk>
Sent: Sun 17 November 2024, 18:04
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Best regards,
Carlos

B.2.4 Sébastien Guenneau

From: Connor Roberts <connor.roberts16@imperial.ac.uk>
To: Sébastien Guenneau <s.guenneau@imperial.ac.uk>
Sent: Fri 15 November 2024, 08:31
Subject: Right to reproduce joint work

Dear Sebastien,

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Kind regards,
Connor

From: Sébastien Guenneau <s.guenneau@imperial.ac.uk>
To: Connor Roberts <connor.roberts16@imperial.ac.uk>
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Dear Connor,

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Kind regards,

Sébastien

B.2.5 Jacob Knight

From: Connor Roberts <connor.roberts16@imperial.ac.uk>
To: Jacob Knight <j.knight21@imperial.ac.uk>
Sent: Fri 26 July 2024, 13:45
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To: Connor Roberts <connor.roberts16@imperial.ac.uk>
Sent: Fri 26 July 2024, 15:54
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Best wishes,

Jacob

B.2.6 Eloise Lardet

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To: Eloise Lardet <eloise.lardet21@imperial.ac.uk>

Sent: Fri 26 July 2024, 13:52

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Dear Eloise,

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Best wishes,

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B.2.7 Gunnar Pruessner

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To: Gunnar Pruessner <g.pruessner@imperial.ac.uk>

Sent: Thu 25 July 2024, 09:48

Subject: Right to reproduce published work

Dear Gunnar,

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From: Gunnar Pruessner <g.pruessner@imperial.ac.uk>
To: Connor Roberts <connor.roberts16@imperial.ac.uk>
Sent: Thu 25 July 2024, 10:16
Subject: Re: Right to reproduce published work

Of course, I am happy for you to reproduce anything you like of our joint work.

All the best,
Gunnar

B.2.8 Helder Rojas

From: Connor Roberts <connor.roberts16@imperial.ac.uk>
To: Helder A Rojas Molina <h.rojas-molina23@imperial.ac.uk>
Sent: Fri 15 November 2024, 08:22
Subject: Right to reproduce joint work

Dear Helder,

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Kind regards,
Connor

From: Helder A Rojas Molina <h.rojas-molina23@imperial.ac.uk>
To: Connor Roberts <connor.roberts16@imperial.ac.uk>
Sent: Sat 16 November 2024, 18:09
Subject: Re: Right to reproduce joint work

Dear Connor,

Of course, you can use our paper as part of your thesis. In fact, thank you very much for considering me and asking about it.

Sincerely,
Helder Rojas

B.2.9 Emir Sezik

From: Connor Roberts <connor.roberts16@imperial.ac.uk>

To: Emir Sezik <emir.sezik19@imperial.ac.uk>

Sent: Fri 26 July 2024, 13:53

Subject: Right to reproduce published work

Dear Emir,

I am in the process of writing my PhD thesis, entitled ‘Work extraction from active matter systems’.

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From: Emir Sezik <emir.sezik19@imperial.ac.uk>

To: Connor Roberts <connor.roberts16@imperial.ac.uk>

Sent: Fri 26 July 2024, 13:55

Subject: Re: Right to reproduce published work

Hello Connor,

You have my permission to include this article as part of your thesis however you wish.

Best,
Emir

B.2.10 Ziluo Zhang

From: Connor Roberts <connor.roberts16@imperial.ac.uk>

To: Ziluo Zhang <zhangzl@wiucas.ac.cn>

Sent: Fri 15 November 2024, 08:25

Subject: Right to reproduce joint work

Dear Ziluo,

I am in the process of writing my PhD thesis, entitled ‘Work extraction from active matter systems’.

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Kind regards,

Connor

From: Ziluo Zhang <zhangzl@wiucas.ac.cn>

To: Connor Roberts <connor.roberts16@imperial.ac.uk>

Sent: Fri 15 November 2024, 08:33

Subject: Re: Right to reproduce joint work

Dear Connor,

I give my approval of the use of this manuscript in your phd thesis.

Congratulations!

Ziluo

B.2.11 Zigan Zhen

From: Connor Roberts <connor.roberts16@imperial.ac.uk>

To: Zigan Zhen <z.zhen19@imperial.ac.uk>

Sent: Fri 26 July 2024, 13:42

Subject: Right to reproduce published work

Dear Zigan,

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Kind regards,
Connor

From: Zigan Zhen <z.zhen19@imperial.ac.uk>
To: Connor Roberts <connor.roberts16@imperial.ac.uk>
Sent: Tue 30 July 2024, 15:22
Subject: Re: Right to reproduce published work

Dear Connor,

You have my permission to include this article. I hope everything goes well with your thesis!

Best wishes,
Zigan

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