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A generalized Dean–Kawasaki equation for an interacting Brownian gas in a partially absorbing medium

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The Dean–Kawasaki (DK) equation is a stochastic partial differential equation (SPDE) for the global density $\rho = N^{-1}\sum_{j=1}^{N}\delta(x - X_j(t))$ of a gas of N overdamped Brownian particles, where $X_j(t)$ is the position of the jth particle. In the thermodynamic limit $N \to \infty$ with weak pairwise interactions, the expectation $\langle\rho\rangle$ with respect to the white noise processes converges in distribution to the solution of a McKean–Vlasov (MV) equation. In this article, we use an encounter-based approach to derive a generalized DK equation for an interacting Brownian gas on the half-line with a partially absorbing boundary at $x = 0$. Each particle is independently absorbed when its local time $L_j(t)$ at $x = 0$ exceeds a random threshold $\widehat{\ell}_j$. The global density is now summed over the set of particles that have not yet been absorbed, and expectations are taken with respect to the Gaussian noise and the random thresholds $\widehat{\ell}_j$. Assuming the DK equation has a well-defined mean-field limit, we derive the corresponding MV equation on the half-line. We illustrate the theory by (i) analysing stationary solutions for a Curie–Weiss (quadratic) interaction potential and a totally reflecting boundary; and (ii) calculating the effective rate of particle loss in the weak absorption limit. Extensions to finite intervals and partially absorbing traps are also considered.

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1. Introduction

There are many natural processes that can be modelled in terms of systems of interacting particle systems, ranging from galaxy clusters and ionic plasmas to active colloids and aggregating microorganisms such as bacteria [1–4]. Interacting particle systems are also used to model the collective decision making of agents in social networks [5]. Mean-field theory is often used to reduce the complexity of such systems by constructing nonlinear partial differential equations for macroscopic quantities such as the global density [6–8]. Much of the focus in recent years has been on interacting passive or active Brownian particles with long-range interactions. The Dean–Kawasaki (DK) equation is a stochastic partial differential equation (SPDE) that describes hydrodynamic fluctuations in the global density $\rho(\mathbf{x},t)=N^{-1}\sum_{j=1}^{N}\delta(\mathbf{x}-\boldsymbol{X}_j(t))$ of N over-damped Brownian particles (Brownian gas) with positions $\boldsymbol{X}_j(t)\in\mathbb{R}^d$ at time t [9,10]. More specifically, suppose that the positions evolve according to the stochastic differential equation (SDE)

$$d\boldsymbol{X}_j(t)=-\frac{1}{N\gamma}\sum_{k=1}^{N}\boldsymbol{\nabla}K(\boldsymbol{X}_j(t)-\boldsymbol{X}_k(t))dt+\sqrt{2D}d\mathbf{W}_j(t), \tag{1.1}$$

where D is the diffusivity, γ is a drag coefficient with $D\gamma=k_BT$, K is a smooth pairwise potential and $\mathbf{W}_j(t)$ is a vector of independent Brownian motions. The DK equation then takes the form [9]

$$\begin{aligned}\frac{\partial\rho(\mathbf{x},t)}{\partial t}&=\sqrt{\frac{2D}{N}}\boldsymbol{\nabla}\cdot\left[\sqrt{\rho(\mathbf{x},t)}\boldsymbol{\eta}(\mathbf{x},t)\right]+D\boldsymbol{\nabla}^2\rho(\mathbf{x},t)\\&\quad+\frac{1}{\gamma}\boldsymbol{\nabla}\cdot\left(\rho(\mathbf{x},t)\int_{\mathbb{R}^d}\rho(\mathbf{y},t)\boldsymbol{\nabla}K(\mathbf{x}-\mathbf{y})d\mathbf{y}\right),\end{aligned} \tag{1.2}$$

where $\boldsymbol{\eta}(\mathbf{x},t)$ is a vector of independent spatio-temporal white noise processes. Formally speaking, equation (1.2) is an exact equation for the global density in the distributional sense, and provides a basis for accurate and efficient numerical simulations of the density fluctuations in interacting diffusing particles [11]. The DK equation has also been used to construct a statistical field theory of a non-interacting Brownian gas [12]. If particle–particle interactions are included, then averaging the DK equation with respect to the Gaussian noise processes results in a moment closure problem for the one-particle density $\langle\rho\rangle$. One approximation scheme for achieving moment closure, which is used extensively in non-equilibrium statistical physics, is dynamical density functional theory (DDFT) [13–16]. A crucial assumption of DDFT is that the relaxation of the system is sufficiently slow such that the pair correlation can be equated with that of a corresponding equilibrium system at each point in time. An alternative approach is to use mean-field theory. There is an extensive mathematical literature on the rigorous stochastic analysis of the mean-field limit $N\to\infty$ for weak pairwise interactions, see for example [17–20]. In particular, if the initial positions of the N particles are independent and identically distributed, i.e. the joint probability density at $t=0$ takes the product form $p(\mathbf{x}_1,\ldots,\mathbf{x}_N,0)=\prod_{j=1}^{N}\phi_0(\mathbf{x}_j)$, then it can be proven that $\langle\rho\rangle$ converges in distribution to the solution of the McKean–Vlasov (MV) equation [6]

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t}=D\boldsymbol{\nabla}^2\phi(\mathbf{x},t)+\frac{1}{\gamma}\boldsymbol{\nabla}\cdot\left(\phi(\mathbf{x},t)\int_{\mathbb{R}^d}\phi(\mathbf{y},t)\boldsymbol{\nabla}K(\mathbf{x}-\mathbf{y})d\mathbf{y}\right), \tag{1.3}$$

with $\phi(\mathbf{x},0)=\phi_0(\mathbf{x})$. Equation (1.3) has an alternative interpretation as the nonlinear Fokker–Planck (FP) equation for the so-called nonlinear McKean SDE

$$d\boldsymbol{X} = -\frac{1}{\gamma}\left[\int_{\mathbb{R}^d} \nabla K(\boldsymbol{X}(t) - \mathbf{y})\rho(\mathbf{y}, t)d\mathbf{y}\right]dt + \sqrt{2D}d\mathbf{W}(t). \tag{1.4}$$

The interacting Brownian gas is said to satisfy the propagation of chaos property. The MV equation is known to have a rich mathematical structure, which includes the existence of multiple stationary solutions and associated phase transitions [21]. This has been explored in various configurations, including double-well confinement and Curie–Weiss interactions on $\mathbb{R}$ [7,22,23], and interacting particles on a torus [24,25].

Most studies of interacting Brownian gases ignore the effects of boundaries, with a few notable exceptions that consider the mean-field limit in the presence of totally reflecting boundaries [26,27]. There have also been a few studies of absorbing boundaries within the contexts of mathematical finance [28] and mean-field games [29,30]. In the case of the FP equation for single-particle diffusion in a bounded domain Ω, the most general classical boundary condition is the Robin condition $D\nabla p(\mathbf{x}, t) \cdot \boldsymbol{n} + \kappa_0 p(\mathbf{x}, t) = 0$ for all $x \in \partial\Omega$, where κ_0 is a positive reactivity constant, and $\boldsymbol{n}$ is the outward unit normal at a point on the boundary $\partial\Omega$. The Dirichlet and Neumann boundary conditions are recovered in the limits $\kappa_0 \to \infty$ and $\kappa_0 = 0$, respectively. However, implementing these boundary conditions at the level of the SDE is non-trivial. In the case of a totally reflecting boundary, the underlying SDE is modified by including an impulsive kick term that keeps the particle within Ω. This term can be written as the differential of the boundary local time, which is a Brownian functional that determines the amount of contact time between particle and boundary [31–36]. The modified SDE is known as the Skorokhod equation. Probabilistic versions of the Robin boundary condition can also be constructed using the local time [37]. One of the assumptions of the Robin boundary condition is that the surface reactivity is a constant. However, various surface-based reactions are better modelled in terms of a reactivity that is a function of the local time [38,39]. That is, the surface may need to be progressively activated by repeated encounters with a diffusing particle, or an initially highly reactive surface may become less active due to multiple interactions with the particle (passivation). Recently, a theoretical framework for analysing a more general class of partially absorbing boundary has been developed using a so-called encounter-based approach [40–43].

In this article, we use the encounter-based method to derive a generalized DK equation for a weakly interacting Brownian gas on the half-line with a partially absorbing boundary at $x = 0$. We begin by considering the simpler problem of diffusion on the half-line with a totally reflecting boundary at $x = 0$ (§2). This requires using a multi-particle version of the stochastic Skorokhod equation for reflected Brownian motion. Heuristically speaking, each particle is independently given an impulsive lick whenever it encounters the boundary, which can be represented as the differential of the local time $L_j(t)$ at $x = 0$, that is, $dL_j(t) = D\delta(X_j(t))$ for the jth particle. Averaging the DK equation with respect to the white noise processes and assuming that there exists a well-defined mean-field limit, we recover the MV equation for reflected diffusions, which was previously obtained using methods from stochastic analysis [26,27]. The straightforward extension to a Brownian gas on a finite interval is also described. In §3, we consider the stationary solutions of the MV equation in the case of a Curie–Weiss (quadratic) interaction potential for both the semi-infinite and finite intervals. In the latter case, we explore how the existence of phase transitions depends on the size of the domain.

The core of the paper is presented in §4, where we use local times to combine the generalized DK equation with the encounter-based model of a partially absorbing boundary at $x = 0$. Each particle is independently absorbed when its local time $L_j(t)$ exceeds a random threshold $\widehat{\ell}_j$ with probability distribution $\Psi(\ell) = \mathbb{P}[\widehat{\ell}_j > \ell]$, $j = 1, \ldots, N$ [40–43]. The corresponding global joint density μ only sums over the set of particles that have not yet been absorbed, that is,[1]

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$$\mu(x,\hat{\ell},t)=\frac{1}{N}\sum_{j=1}^{N}\delta(x-X_j(t))\mathbf{1}_{L_j(t)<\hat{\ell}_j}. \tag{1.5}$$

We derive the generalized DK equation for μ and then use a mean-field ansatz to obtain a MV equation for $p^{\Psi}(x,t)=\mathbb{E}[\langle\mu(x,\hat{\boldsymbol{\ell}},t)\rangle]$, where $\langle\cdot\rangle$ and $\mathbb{E}[\cdot]$ denote, respectively, averaging with respect to the Gaussian noise processes and the random local time thresholds. We show that in the particular case of the exponential distribution, $\Psi(\ell)=\exp(-\kappa_0\ell/D)$, the density $p^{\Psi}(x,t)$ satisfies the MV equation with a Robin boundary condition at $x=0$, where κ_0 is the corresponding reactivity. Hence, assuming a solution of the nonlinear Robin BVP exists, the corresponding solution for a non-exponential distribution $\Psi(\ell)$ can be constructed along identical lines to [41,43]. We illustrate the theory by considering the effective rate of particle loss in the weak absorption limit. Finally, in §5, we describe possible extensions of the theory, including an interacting Brownian gas in $\mathbb{R}$ with a finite interval acting as a partially absorbing trap. Absorption is now conditioned on the occupation time (time spent within the trapping region) crossing a random threshold [41,43].

2. Generalized DK equation for a totally reflecting boundary

In this section, we derive the generalized DK equation for a Brownian gas on $[0,\infty)$ with a totally reflecting boundary at $x=0$. Although the results can be obtained more simply using other methods, our particular formulation prepares the ground for dealing with partially absorbing boundaries, in particular, by introducing the notion of a local time. We begin with a non-interacting gas.

(a) Non-interacting Brownian gas

Consider N identical, non-interacting Brownian particles on the half-line. Each particle is subject to a totally reflecting boundary at $x=0$. Let $L_j(t)$ be the boundary local time of the jth particle, which is a Brownian functional of the form

$$L_j(t)=\lim_{\epsilon\to 0^+}\frac{D}{\epsilon}\int_0^t\mathbf{1}_{(0,\epsilon)}(X_j(s))ds, \tag{2.1}$$

where $\mathbf{1}$ is the indicator function. (The factor of D means that $L_j(t)$ has units of length.) It can be proven that $L_j(t)$ exists and is a non-decreasing, continuous function of t [32,33]. The SDE for $X_j(t)\in[0,\infty)$ is given by the so-called Skorokhod equation for reflecting Brownian motion,

$$dX_j(t)=\sqrt{2D}dW_j(t)+dL_j(t),\quad dL_j(t)=D\delta(X_j(t))dt, \tag{2.2}$$

with $W_j(t)$, $j=1,\ldots,N$, a set of independent Brownian motions. The differential $dL_j(t)$ represents an impulsive kick applied to the jth particle whenever it hits $x=0$. A compact description of the dynamics can be obtained by considering a 'hydrodynamic' formulation of equation (2.2), which involves the (normalized) global density

$$\rho(x,t)=\frac{1}{N}\sum_{j=1}^{N}\rho_j(x,t),\quad \rho_j(x,t)=\delta(X_j(t)-x). \tag{2.3}$$

We construct an SPDE for the global density ρ by adapting the derivation of the DK equation for a Brownian gas in $\mathbb{R}$ [9,10]. Consider an arbitrary smooth test function $f(x)$, and set

$$F(t)=\frac{1}{N}\sum_{j=1}^{N}f(X_j(t))=\int_0^{\infty}\rho(x,t)f(x)dx. \tag{2.4}$$

Using Ito's lemma to determine the differential $dF(t)$, we have

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$$\left[\int_0^\infty f(x)\frac{\partial\rho(x,t)}{\partial t}dx\right]dt = \frac{1}{N}\sum_{j=1}^{N}\left[f'(X_j(t))dL_j(t) + Df''(X_j(t)dt + \sqrt{2D}f'(X_j(t))dW_j(t)\right] \equiv dF(t)\,. \tag{2.5}$$

Since $dL_j(t) = D\delta(X_j(t))dt$, it follows that

$$\int_0^\infty f(x)\frac{\partial\rho(x,t)}{\partial t} = \frac{1}{N}\int_0^\infty \sum_{j=1}^{N}\rho_j(x,t)\left[D\delta(x)f'(0) + Df''(x) + \sqrt{2D}f'(x)\xi_i(t)\right]dx. \tag{2.6}$$

We have formally set $dW_i(t) = \xi_i(t)dt$, where ξ_i is a d-dimensional white noise term such that

$$\langle\xi_i(t)\rangle = 0, \quad \langle\xi_i(t)\xi_j(t')\rangle = \delta(t-t')\delta_{i,j}. \tag{2.7}$$

Integrating by parts the terms on the right-hand side of equation (2.6) and noting that the terms involving $f'(0)$ cancel, we have

$$\int_0^\infty f(x)\frac{\partial\rho(x,t)}{\partial t}dx = \int_0^\infty f(x)\left(-\frac{1}{N}\sum_{j=1}^{N}\sqrt{2D}\partial_x\rho_i(x,\ell,t)\xi_i(t) + D\partial_{xx}\rho(x,t)\right)dx - f(0)\left(\frac{\sqrt{2D}}{N}\sum_{j=1}^{N}\rho_j(0,t)\xi_j(t) - D\partial_x\rho(0,t)\right). \tag{2.8}$$

Since $f(x)$ is arbitrary, we obtain the following SPDE (in the weak sense):

$$\frac{\partial\rho(x,t)}{\partial t} = -\frac{\sqrt{2D}}{N}\sum_{j=1}^{N}\frac{\partial\rho_j(x,t)}{\partial x}\xi_j(t) + D\frac{\partial^2\rho(x,t)}{\partial x^2} - \delta(x)\mathcal{J}(0,t), \tag{2.9a}$$

with

$$\mathcal{J}(x,t) \equiv \frac{\sqrt{2D}}{N}\sum_{j=1}^{N}\rho_j(x,t)\xi_j(t) - D\frac{\partial\rho(x,t)}{\partial x}\,. \tag{2.9b}$$

Following along analogous lines to [9], we introduce the space-dependent Gaussian noise

$$\xi(x,t) = -\frac{1}{N}\sum_{j=1}^{N}\left[\partial_x\rho_j(x,t)\xi_j(t)\right], \tag{2.10}$$

with zero mean and the correlation function

$$\langle\xi(x,t)\xi(y,t')\rangle = \frac{1}{N^2}\delta(t-t')\sum_{j=1}^{N}\partial_x\partial_y\left(\rho_j(x,t)\rho_j(y,t)\right). \tag{2.11}$$

Since $\rho_j(x,t)\rho_j(y,t) = \delta(x-y)\rho_i(x,t)$, it follows that

$$\langle\xi(x,t)\xi(y,t')\rangle = \frac{1}{N}\delta(t-t')\partial_x\partial_y\left(\delta(x-y)\rho(x,t)\right). \tag{2.12}$$

Finally, we introduce the global density-dependent noise field

$$\hat{\xi}(x,t) = \frac{1}{\sqrt{N}}\frac{\partial}{\partial x}\left(\eta(x,t)\sqrt{\rho(x,t)}\right), \tag{2.13}$$

where $\eta(x,t)$ is a spatio-temporal white noise term:

$$\langle\eta(x,t)\eta(y,t')\rangle = \delta(t-t')\delta(x-y). \tag{2.14}$$

It can be checked that the Gaussian noises ξ and $\hat{\xi}$ have the same correlation functions and are thus statistically identical. Hence, we obtain a closed SPDE for the global density on the half-line

$$\frac{\partial\rho(x,t)}{\partial t} = \sqrt{\frac{2D}{N}}\frac{\partial\sqrt{\rho(x,t)}\eta(x,t)}{\partial x} + D\frac{\partial^2\rho(x,t)}{\partial x^2}, \quad x>0, \tag{2.15a}$$

$$D\frac{\partial \rho(0,t)}{\partial x} = -\sqrt{\frac{2D}{N}}\sqrt{\rho(0,t)}\eta(0,t). \tag{2.15b}$$

(Equation (2.15b) immediately follows from the Dirac delta function term on the right-hand side of equation (2.9a). This can be seen by integrating the latter with respect to a boundary layer around $x = 0$. Alternatively, one simply sets the sum of all terms multiplying $f(0)$ to zero.) Finally, averaging with respect to the white noise and setting $p(x,t) = \langle \rho(x,t) \rangle$ yields the diffusion equation on the half-line with a totally reflecting boundary at $x = 0$:

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}, \quad D\frac{\partial p(0,t)}{\partial x} = 0\,. \tag{6} \quad (2.16)$$

Note here $p(x,t)$ represents the density of a large system of non-interacting particles rather than the probability density of a single particle.

(b) Interacting Brownian gas

We now modify the SDE (2.2) by introducing an external potential $V(x)$ and a pairwise interaction potential $K(x)$ such that

$$dX_j(t) = -\frac{1}{\gamma}\left[V'(X_j(t)) + N^{-1}\sum_{k=1}^{N} K'(X_j(t) - X_k(t))\right]dt + \sqrt{2D}dW_j(t) + dL_j(t). \tag{2.17}$$

The potentials contribute extra terms on the right-hand side of equation (2.6) given by

$$\mathcal{A} = -\frac{1}{\gamma N}\int_0^\infty \sum_{j=1}^{N} \rho_i(x,t)\left[V'(x) + \frac{1}{N}\sum_{k=1}^{N}\int_0^\infty dy\, \delta(y - X_k(t))K'(x-y)\right]f'(x)dx\,. \tag{2.18}$$

Integrating by parts with respect to x yields

$$\mathcal{A} = \int_0^\infty f(x)\partial_x H_\rho(x,t)dx + H_\rho(0,t)f(0), \tag{2.19}$$

with

$$H_\rho(x,t) = \gamma^{-1}\rho(x,t)\left(V'(x) + \int_0^\infty \rho(y,t)K'(x-y)dy\right). \tag{2.20}$$

The non-interacting terms are calculated along identical lines to the derivation of equation (2.15), which leads to the following generalized DK equation for the interacting Brownian gas, which we write in the form of a conservation equation:

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial \mathcal{J}(x,t)}{\partial x}, \quad \mathcal{J}(0,t) = 0, \tag{2.21a}$$

with the probability flux

$$\mathcal{J}(x,t) = -\sqrt{\frac{2D}{N}}\sqrt{\rho(x,t)}\eta(x,t) - D\frac{\partial \rho(x,t)}{\partial x} - H_\rho(x,t)\,. \tag{2.21b}$$

As with the classical DK equation (1.2), averaging equation (2.21) with respect to the Gaussian noise processes leads to a PDE that couples the one-particle density $p(x,t) = \langle \rho(x,t) \rangle$ to the two-point correlation function $\langle \rho(x,t)\rho(x',t) \rangle$ etc., resulting in a moment closure problem. Assuming that the mean-field ansatz $\langle \rho(x,t)\rho(x',t) \rangle \to p(x,t)p(x',t)$ as $N \to \infty$ still holds in the presence of a reflecting boundary, we obtain the following MV equation for an interacting gas on the half-line with a totally reflecting boundary at $x = 0$:

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}, x > 0, \quad J(0,t) = 0, \tag{2.22a}$$

$$J(x,t) = -D\frac{\partial p(x,t)}{\partial x} - \frac{1}{\gamma}\left[p(x,t)\left(V'(x) + \int_0^\infty p(y,t)K'(x-y)dy\right)\right]. \tag{2.22b}$$

This is equivalent to the MV equation derived previously by proving the propagation of chaos property in the thermodynamic limit [26,27].

(c) Brownian gas on a finite interval

Our derivation of the generalized DK equation can easily be extended to diffusion on the finite interval $[-R, R]$ with reflecting boundaries at both ends. The main modification is in the definition of the local time of the jth particle:

$$L_j(t) = \lim_{\epsilon \to 0^+} \frac{D}{\epsilon}\left[\int_0^t I_{(R-\epsilon,R)}(X_j(s))ds + \int_0^t I_{(-R,-R+\epsilon)}(X_j(s))ds\right]. \tag{2.23}$$

The derivation of the corresponding DK equation for the global density $\rho(x,t)$ proceeds along similar lines to the half-line. In particular, equation (2.21) becomes

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial \mathcal{J}(x,t)}{\partial x}, \quad x \in (-R,R), \quad \mathcal{J}(\pm R,t) = 0, \tag{2.24}$$

with the probability flux given by equation (2.21b) and

$$H_\rho(x,t) = \gamma^{-1}\rho(x,t)\left(V'(x) + \int_{-R}^R \rho(y,t)K'(x-y)dy\right). \tag{2.25}$$

Averaging with respect to the Gaussian's noise processes, imposing the mean-field ansatz, results in the following MV equation on the interval $[-R, R]$:

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}, x \in (-R,R), \quad J(-R,t) = 0 = J(R,t), \tag{2.26a}$$

$$J(x,t) = -D\frac{\partial p(x,t)}{\partial x} - \frac{1}{\gamma}p(x,t)\left(V'(x) + \int_{-R}^R p(y,t)K'(x-y)dy\right). \tag{2.26b}$$

3. Stationary states for the Curie–Weiss interaction potential

For a finite system of interacting Brownian particles moving in a confining potential, one finds that the associated linear FP equation has a unique stationary state given by the Boltzmann distribution. On the other hand, the MV equation is a nonlinear non-local FP equation that describes an interacting Brownian gas in the thermodynamic limit. Consequently, it can support the existence of multiple stationary solutions and their associated phase transitions [7,21–25]. However, establishing the existence of a stationary solution of the MV equation is non-trivial, even in the absence of boundaries. Here, we explore this issue for the MV equation on the half-line and finite interval in the case of a Curie–Weiss (quadratic) interaction potential $K(x) = \lambda x^2/2$, $\lambda > 0$.

(a) Stationary states on the half-line

In the case of the half-line, the SDE (2.17) reduces to the form

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$$dX_j(t) = -\frac{1}{\gamma}\left[V'(X_j(t)) + \frac{\lambda}{N}\sum_{k=1}^{N}[X_j(t) - X_k(t)]\right]dt + \sqrt{2D}dW_j(t) + dL_j(t). \tag{3.1}$$

The interaction term can be rewritten as $-\lambda[X_j(t) - X(t)]$, where $X = N^{-1}\sum_{k=1}^{N} X_k(t)$. It is an example of a cooperative coupling that tends to make the system relax towards the 'centre of gravity' of the multi-particle ensemble. If $V(x)$ is taken to be a multi-well potential then there is competition between the cooperative interactions and the tendency of particles to be distributed across the different potential wells according to the classical Boltzmann distribution.

The time-independent version of equation (2.22) is

$$\frac{\partial J(x)}{\partial x} = 0, x > 0, \quad J(0) = 0, \tag{3.2}$$

with

$$J(x) := -D\left[\frac{\partial p(x)}{\partial x} + \beta p(x)\left(V'(x) + \lambda\int_0^\infty (x-y)p(y)dy\right)\right]. \tag{3.3}$$

We have used the Einstein relation $D\gamma = k_B T = \beta^{-1}$. Note that the integral term reduces to $\lambda(x - \langle y\rangle)$ with $\langle y\rangle = \int_0^\infty y p(y)dy$. Suppose, for the moment, that $\langle y\rangle = a$ for some fixed a, which parameterizes the density p. The totally reflecting boundary condition in (3.2) implies that $J(x) = 0$ for all $x \in [0, \infty)$ and, hence,

$$p(x) = p_a(x) = Z(a)^{-1}\exp\left(-\beta[V(x) + \lambda x^2/2 - a\lambda x]\right). \tag{3.4}$$

The factor $Z(a)$ ensures the normalization $\int_0^\infty p_a(x)dx = 1$. The unknown parameter a is then determined by imposing the self-consistency condition

$$a = m(a) \equiv \int_0^\infty x p_a(x)dx. \tag{3.5}$$

A necessary condition for the existence of a non-trivial solution $p_a(x)$ is that $V(x) + \lambda x^2/2 \to 0$ as $x \to \infty$. The number of equilibrium solutions is then equal to the number of solutions of equation (3.5). Note that one major difference when diffusion is restricted to the half-line is that $a > 0$ for any non-trivial solution $p_a(x)$.

A common choice for V in the case of a Brownian gas on $\mathbb{R}$ is the double-well potential $V(x) = x^4/4 - x^2/2$. Although is not possible to analytically solve the corresponding equation $a = \int_{-\infty}^{\infty} x p_a(x)dx$, one can prove that there exists a phase transition at a critical temperature T_c such that $a = 0$ for $T > T_c$ and $a = \pm a_0 \neq 0$ for $T < T_c$ [7,22,23]. On the other hand, since the double-well potential only has a single minimum in $[0, \infty)$, we expect there to exist at most one stationary solution for the reflected boundary problem. Therefore, we focus here on the existence of a unique stationary density for the simpler quadratic potential $V(x) = \nu x^2/2$, $\nu > 0$. We then have

$$\begin{aligned} Z(a) &= \int_0^\infty \mathrm{e}^{-\beta[(\nu+\lambda)x^2/2 - a\lambda x]}dx \\ &= \sqrt{\frac{\pi}{2\beta[\nu+\lambda]}}\mathrm{e}^{\beta a^2\lambda^2/2[\nu+\lambda]}\mathrm{erfc}(-a\lambda\sqrt{\beta/2[\nu+\lambda]}), \end{aligned} \tag{3.6}$$

and equation (3.5) becomes

$$a = Z(a)^{-1}\int_0^\infty x e^{-\beta[(\nu+\lambda)x^2/2 - a\lambda x]}dx = \frac{1}{\lambda\beta}\frac{\partial \log Z(a)}{\partial a}$$
$$= \frac{a\lambda}{\nu+\lambda} + \sqrt{\frac{2}{\pi\beta[\nu+\lambda]}}\frac{e^{-\beta a^2\lambda^2/2[\nu+\lambda]}}{\operatorname{erfc}(-a\lambda\sqrt{\beta/2[\nu+\lambda]})}. \tag{3.7}$$

Rearranging this equation implies that a is the implicit solution of

$$a = F(a) := \frac{\nu+\lambda}{\nu}\sqrt{\frac{2}{\pi\beta[\nu+\lambda]}}\frac{e^{-\beta a^2\lambda^2/2[\nu+\lambda]}}{\operatorname{erfc}(-a\lambda\sqrt{\beta/2[\nu+\lambda]})}. \tag{3.8}$$

In figure 1*a*, we plot the function $F(a)$ for different values of ν and $\lambda = \beta = 1$. This provides a graphical proof that there exists a unique stationary solution. The variation of the solution a with ν is plotted in figure 1*b*. We also compare with the mean position in the absence of interactions ($\lambda = 0$). It can be seen that as $\nu \to \nu_c = 0$, the effects of the cooperative interactions become more significant.

(b) Stationary states on $[-R, R]$

The stationary solution (3.4) still holds in the finite interval except that a is now a solution of the modified self-consistency condition

$$a = m(a) \equiv \int_{-R}^{R} x p_a(x)dx. \tag{3.9}$$

In the case of the quartic confining potential $V(x) = x^4/4 - x^2/2$, we recover the results of [7,22] in the limit $R \to \infty$. That is, for sufficiently large R, there is a phase transition at a critical inverse temperature $\beta_c(R)$ between a single stationary state $a = 0$ when $\beta < \beta_c$, and three stationary states $a = 0, \pm a_0(\beta, L)$, $a_0 > 0$, when $\beta > \beta_c$. This is illustrated in figure 2*a* for $R = 100$. We find numerically that $\beta_c \approx 2$ when $\lambda = 1$, which is consistent with the critical point obtained in the limit $R \to \infty$ [7,22]. Our generalized mathematical framework allows us to explore how the phase transition depends on the size R of the domain. As might be expected, for fixed $\beta > \beta_c^*$, where β_c^* is the critical point in the limit $R \to \infty$, there exists a critical length $R_c(\beta)$ at which $a_0(\beta, R_c(\beta)) = 0$, see figure 2*b*.

4. Generalized DK equation for a partially absorbing boundary: an encounter-based model

So far we have focused on totally reflecting boundary conditions, which can be handled using Skorokhod SDEs and differentials of the local time. However, the introduction of individual local times also allows us to incorporate a much more general class of boundary conditions via the encounter-based approach to diffusion-mediated surface absorption [40–43]. In this section, we derive a generalized DK equation on the half-line with a partially absorbing boundary at $x = 0$. In order to extend the DK construction to include partial absorption, it is necessary to significantly modify the definition of the empirical measure. We begin by considering the example of a single Brownian particle. We show how Ito's lemma can be used to develop an alternative formulation of the encounter-based approach that is particularly suitable for multiple particles.

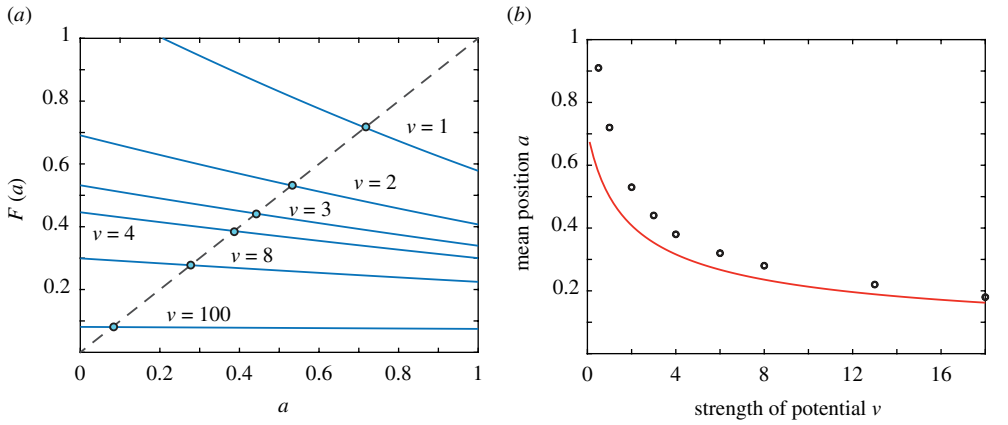

Figure 1. Brownian gas on the half-line. (*a*) Plot of function $F(a)$ defined in the the self-consistency condition (3.8) for the mean position a and various values of strength ν of the quadratic confining potential. The intercepts with the diagonal determine the unique solution a. Other parameters are $\lambda = \beta = 1$. (*b*) Plot of intercepts as a function of ν for $\lambda = 1$. The solid curve shows the mean position in the absence of coupling ($\lambda = 0$)).

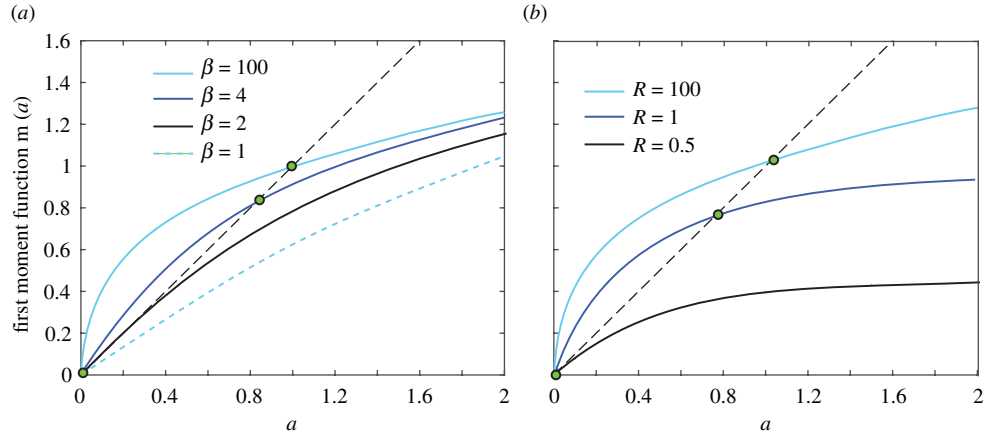

Figure 2. Brownian gas on $[-R, R]$. (*a*) Plot of first moment $m(a)$ as function of a and various inverse temperatures β. The intercepts with the diagonal determine the positive solutions a. Other parameters are $\lambda = 1$, $R = 100$. (*b*) Corresponding plots for $\beta = 10$ and various sizes of R.

(a) Single Brownian particle

At the single-particle level, the encounter-based approach assumes that a diffusion process is killed when its local time $L(t)$ at $x = 0$, as defined in equation (2.1), exceeds a randomly distributed threshold $\hat{\ell}$. In other words, the particle is absorbed at $x = 0$ at the stopping time

$$\mathcal{T} = \inf\{t > 0 : L(t) > \hat{\ell}\}, \qquad \mathbb{P}[\hat{\ell} > \ell] \equiv \Psi(\ell)\,. \tag{4.1}$$

Since $L(t)$ is a non-decreasing process, the condition $t < \mathcal{T}$ is equivalent to the condition $L(t) < \hat{\ell}$. Hence, the corresponding single-particle SDE is

$$dX(t) = [\sqrt{2D}dW(t) + dL(t)]\mathbf{1}_{L(t)<\hat{\ell}}, \tag{4.2}$$

where $\mathbf{1}_{L(t)<\hat{\ell}} \equiv \Theta(\hat{\ell} - L(t))$ with $\Theta(x)$ a Heaviside function. In anticipation of the multi-particle case, we introduce the single-particle empirical measure

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$$\mu(x, \hat{\ell}, t) = \delta(x - X(t))\mathbf{1}_{L(t) < \hat{\ell}}. \tag{4.3}$$

Let $f(x)$ be a bounded smooth test function and set

$$F(\hat{\ell}, t) = f(X(t))\mathbf{1}_{L(t) < \hat{\ell}}. \tag{4.4}$$

Using Ito's lemma and the definition of the local time, we have

$$\begin{aligned} dF(\hat{\ell}, t) = &\left[Df''(X(t))dt + \sqrt{2D}f'(X(t))dW(t) + Df'(X(t))\delta(X(t))dt\right]\mathbf{1}_{L(t) < \hat{\ell}} \\ &- Df(0)\delta(X(t))\delta(L(t) - \hat{\ell}). \end{aligned} \tag{4.5}$$

It follows that

$$\begin{aligned} \left[\int_0^\infty f(x)\frac{\partial \mu(x, \hat{\ell}, t)}{\partial t}dx\right]dt &= dF(\hat{\ell}, t) \\ &= \int_0^\infty \mu(x, \hat{\ell}, t)\left[Df''(x)dt + \sqrt{2D}f'(x)dW(t) + D\delta(x)f'(0)\right]dx \\ &\quad - Df(0)\delta(X(t))\delta(L(t) - \hat{\ell}). \end{aligned} \tag{4.6}$$

Integrating by parts and using the arbitrariness of f yields an SPDE for μ:

$$\frac{\partial \mu(x, \hat{\ell}, t)}{\partial t} = D\frac{\partial^2 \mu(x, \hat{\ell}, t)}{\partial x^2} + \sqrt{2D}\frac{\partial \mu(x, \hat{\ell}, t)}{\partial x}\xi(t), \qquad x > 0 \tag{4.7a}$$

and

$$D\frac{\partial \mu(0, \hat{\ell}, t)}{\partial x} = \sqrt{2D}\xi(t)\mu(0, \hat{\ell}, t) + D\delta(X(t))\delta(L(t) - \hat{\ell}). \tag{4.7b}$$

The latter equation follows from equating the sum of terms multiplying $f(0)$ to zero.

In order to derive a generalized FP equation, we need to take expectations with respect to both the white noise process and the random threshold. Recall that these are denoted by $\langle \cdot \rangle$ and $\mathbb{E}[\cdot]$, respectively. Note, in particular, that

$$\mathbb{E}\left[\mathbf{1}_{L(t) < \hat{\ell}}\right] = \Psi(L(t)), \qquad E\left[\delta(L(t) - \hat{\ell})\right] = \psi(L(t)) := -\Psi'(L(t)). \tag{4.8}$$

Introducing the pair of densities

$$p^\Psi(x, t) = \mathbb{E}[\langle \mu(x, \hat{\ell}, t)\rangle] = \langle \delta(x - X(t))\mathbb{E}[\mathbf{1}_{L(t) < \hat{\ell}}]\rangle = \left\langle \delta(x - X(t)\Psi(L(t))\right\rangle, \tag{4.9a}$$

$$\nu^\psi(x, t) = \left\langle \delta(x - X(t))\mathbb{E}[\delta(L(t) - \hat{\ell})]\right\rangle = \left\langle \delta(x - X(t)\psi(L(t))\right\rangle, \tag{4.9b}$$

and taking expectations of equation (4.7) gives

$$\frac{\partial p^\Psi(x, t)}{\partial t} = D\frac{\partial^2 p^\Psi(x, t)}{\partial x^2}, \ x > 0, \quad D\frac{\partial p^\Psi(x, t)}{\partial x}\bigg|_{x=0} = D\nu^\psi(0, t). \tag{4.10}$$

For a general local time threshold distribution Ψ, we do not have a closed equation for the marginal density $p^\Psi(x, t)$. However, in the particular case of the exponential distribution $\Psi(\ell) = \mathrm{e}^{-\kappa_0 \ell/D}$, we have $\psi(\ell) = \kappa_0 \Psi(\ell)/D$ and equation (4.10) reduce to the classical Robin BVP with reactivity κ_0:

$$\frac{\partial p(x, t)}{\partial t} = D\frac{\partial^2 p(x, t)}{\partial x^2}, \quad x > 0, \tag{4.11a}$$

$$D\frac{\partial p(0, t)}{\partial x}\bigg|_{x=0} = \kappa_0 p(0, t). \tag{4.11b}$$

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(We have set $p^{\Psi} = p$ for $\Psi(\ell) = \mathrm{e}^{-\kappa_0 \ell/D}$.) Within the context of the encounter-based formalism, we now make the crucial observation that the solution of the Robin BVP is equivalent to the Laplace transform of the so-called local time propagator with respect to ℓ:

$$p(x,t) = \int_0^\infty \mathrm{e}^{-z\ell} P(x,\ell,t)\,d\ell = \widetilde{P}(x,z,t), \quad z = \kappa_0/D, \tag{4.12}$$

where [40–43]

$$P(x,\ell,t) := \langle \delta(X(t)-x)\delta(L(t)-\ell)\rangle\,. \tag{4.13}$$

Assuming that the Laplace transform $\widetilde{P}(x,z,t)$, can be inverted with respect to z, the solution of equation (4.10) is obtained from equation (4.9a):

$$p^{\Psi}(x,t) = \int_0^\infty \Psi(\ell) P(x,\ell,t)\,d\ell = \int_0^\infty \Psi(\ell)\mathcal{L}_\ell^{-1}\widetilde{P}(x,z,t)\,d\ell\,. \tag{4.14}$$

One way to implement a non-exponential law is to consider an ℓ-dependent reactivity $\kappa(\ell)$ such that

$$\Psi(\ell) = \exp(-D^{-1}\int_0^\ell \kappa(\ell')d\ell')\,. \tag{4.15}$$

Since the probability of absorption now depends on how much time the particle spends in a neighbourhood of the boundary, as specified by the local time, it follows that the stochastic process has memory. That is, absorption process itself is non-Markovian.

(b) Interacting Brownian gas on the half-line

Writing down the SDE for an interacting Brownian gas with a partially absorbing boundary condition at $x = 0$ requires that we only include particles that have not yet been absorbed. Given a set of local time thresholds $\widehat{\boldsymbol{\ell}} = \{\widehat{\ell}_1, \ldots \widehat{\ell}_N\}$ and the set of stopping conditions

$$\mathcal{T}_j = \inf\{t>0\colon L_j(t) > \widehat{\ell}_j\}, \quad \mathbb{P}[\widehat{\ell}_j > \ell] \equiv \Psi(\ell), \tag{4.16}$$

equation (2.17) becomes

$$\begin{aligned} dX_j(t) = \Big\{ -\frac{1}{\gamma}\Big[V'(X_j(t)) + N^{-1}\sum_{k=1}^N K'(X_j(t)-X_k(t))\mathbf{1}_{L_k(t)<\widehat{\ell}_k}\Big]dt \\ + \sqrt{2D}dW_j(t) + dL_j(t)\Big\}\mathbf{1}_{L_j(t)<\widehat{\ell}_j}\,. \end{aligned} \tag{4.17}$$

For simplicity, we assume that the particle absorption processes are independent and that the distributions Ψ of the local time thresholds are the same for all particles. That is, each particle is assigned its own independent local time $L_j(t)$ and local time threshold $\widehat{\ell}_j$. (See the discussion in §5 for further elaboration.) Introduce the global density or empirical measure

$$\mu(x,\widehat{\boldsymbol{\ell}},t) = \frac{1}{N}\sum_{j=1}^N \mu_j(x,\widehat{\ell}_j,t) = \frac{1}{N}\sum_{j=1}^N \delta(X_j(t)-x)\mathbf{1}_{L_j(t)<\widehat{\ell}_j}, \tag{4.18}$$

which tracks the spatial evolution of the surviving particles given the thresholds $\widehat{\boldsymbol{\ell}}$. For a given set of local time thresholds, we derive a generalized DK equation for μ by combining the analysis of §§2 and 4a. Introduce a smooth test function f and set

$$F(\widehat{\boldsymbol{\ell}},t) = \frac{1}{N}\sum_{j=1}^N f(X_j(t))\mathbf{1}_{L_j(t)<\widehat{\ell}_j} = \int_0^\infty \mu(x,\widehat{\boldsymbol{\ell}},t)f(x)dx\,. \tag{4.19}$$

Using similar arguments to the previous cases, we use Ito's lemma to evaluate $dF(\hat{\ell}, t)$, which yields

$$\begin{aligned}&\int_0^\infty f(x)\frac{\partial \mu(x,\hat{\boldsymbol{\ell}},t)}{\partial t}dx\\&=\frac{1}{N}\int_0^\infty \sum_{j=1}^N \mu_j(x,\hat{\ell}_j,t)\left[\sqrt{2D}f'(x)\xi_j(t)+Df''(x)+D\delta(x)f'(0)+\mathcal{A}(x)f'(x)\right]dx\\&\quad-\frac{Df(0)}{N}\sum_{j=1}^N \delta(X_j(t))\delta(L_j(t)-\hat{\ell}_j).\end{aligned} \tag{4.20}$$

with

$$\begin{aligned}\mathcal{A}(x)&=-\frac{1}{\gamma}\left[V'(x)+\frac{1}{N}\sum_{k=1}^N \mathbf{1}_{L_k(t)<\hat{\ell}_k}\int_0^\infty \delta(y-X_k(t))K'(x-y)dy\right]\\&=-\frac{1}{\gamma}\left[V'(x)+\int_0^\infty \mu(y,\hat{\boldsymbol{\ell}},t)K'(x-y)dy\right].\end{aligned} \tag{4.21}$$

Integrating by parts the various terms on the right-hand side of equation (4.20), which picks up additional terms at $x = 0$, and exploiting the arbitrariness of f, yields the following SPDE for μ:

$$\frac{\partial \mu(x,\hat{\boldsymbol{\ell}},t)}{\partial t}=-\frac{\partial \mathcal{J}(x,\hat{\boldsymbol{\ell}},t)}{\partial x}, \tag{4.22a}$$

$$-\mathcal{J}(0,\hat{\boldsymbol{\ell}},t)=D\nu(0,\hat{\boldsymbol{\ell}},t),\quad \nu(0,\hat{\boldsymbol{\ell}},t):=\frac{1}{N}\sum_{j=1}^N \delta(X_j(t))\delta(L_j(t)-\hat{\ell}_j), \tag{4.22b}$$

with the probability flux

$$\mathcal{J}(x,\hat{\boldsymbol{\ell}},t)=-\sqrt{\frac{2D}{N}}\sqrt{\mu(x,\hat{\boldsymbol{\ell}},t)}\eta(x,t)-D\frac{\partial \mu(x,\hat{\boldsymbol{\ell}},t)}{\partial x}-H_\mu(x,\hat{\boldsymbol{\ell}},t), \tag{4.23}$$

and

$$H_\mu(x,\hat{\boldsymbol{\ell}},t)=\gamma^{-1}\mu(x,\hat{\boldsymbol{\ell}},t)\left(V'(x)+\int_0^\infty \mu(y,\hat{\boldsymbol{\ell}},t)K'(x-y)dy\right). \tag{4.24}$$

Note that we have simplified the noise terms using identical arguments to the derivation of equation (2.15). However, the DK equation is not closed with respect to μ, since it couples to a second empirical measure

$$\nu(x,\hat{\boldsymbol{\ell}},t)=\frac{1}{N}\sum_{j=1}^N \delta(X_j(t)-x)\delta(L_j(t)-\hat{\ell}_j), \tag{4.25}$$

at $x = 0$

In order to obtain the analogue of the single-particle density equation (4.10), we take expectations of equation (4.22) with respect to the Gaussian noise processes and the random local time thresholds. We again make use of the identities

$$\mathbb{E}[\mathbf{1}_{L_j(t)<\hat{\ell}_j}]=\Psi(L_j(t)),\quad \mathbb{E}[\delta(L_j(t)-\hat{\ell}_j)]=\psi(L_j(t)). \tag{4.26}$$

However, in the interacting case, we have to deal with the fact that H_μ is a nonlinear, non-local function of $\mu(x,\hat{\boldsymbol{\ell}},t)$. Analogous to §2, see the discussion above equation (2.22), we will assume the mean-field ansatz[2]

$$\mathbb{E}\left[\left\langle \mu(x,\hat{\boldsymbol{\ell}},t)\mu(y,\hat{\boldsymbol{\ell}},t)\right\rangle\right]=\mathbb{E}\left[\left\langle \mu(x,\hat{\boldsymbol{\ell}},t)\right\rangle\right]\mathbb{E}\left[\left\langle \mu(y,\hat{\boldsymbol{\ell}},t)\right\rangle\right], \tag{4.27}$$

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holds in the thermodynamic limit $N \to \infty$. This then yields an MV equation for the marginal density on the half-line with a partially absorbing boundary at $x = 0$,

$$p^{\Psi}(x,t) = \mathbb{E}\Big[\big\langle \mu(x,\hat{\boldsymbol{\ell}},t)\big\rangle\Big], \tag{4.28}$$

which takes the form

$$\frac{\partial p^{\Psi}(x,t)}{\partial t} = -\frac{\partial J^{\Psi}(x,t)}{\partial x}, \quad -J^{\Psi}(0,t) = Dv^{\psi}(0,t), \tag{4.29a}$$

with probability flux

$$J^{\Psi}(x,t) = -D\frac{\partial p^{\Psi}(x,t)}{\partial x} - \gamma^{-1}p^{\Psi}(x,t)\left(V'(x) + \int_0^{\infty} p^{\Psi}(y,t)K'(x-y)dy\right), \tag{4.29b}$$

and

$$v^{\psi}(x,t) = \frac{1}{N}\sum_{j=1}^{N}\left\langle \delta(x-X_j(t))\delta(L_j(t)-\hat{\ell}_j)\right\rangle = \frac{1}{N}\sum_{j=1}^{N}\left\langle \delta(x-X_j(t)\psi(L_j(t))\right\rangle. \tag{4.29c}$$

First note that if $\Psi(\ell) = 1$ for all ℓ then $\psi(\ell) = 0$ and we recover the MV equation (2.22) for a totally reflecting boundary. For almost all other choices for Ψ, equation (4.29) does not yield a closed PDE for $p^{\Psi}(x,t)$ due to the dependence of the boundary condition at $x = 0$ on $v^{\psi}(0,t)$. However, as in the case of a single particle, see §4a, we do obtain a closed MV equation in the special case of an exponential distribution $\Psi(\ell) = \mathrm{e}^{-\varkappa_0\ell/D}$. The boundary condition then takes the Robin form

$$J^{\Psi}(0,t) = -\varkappa_0 p^{\Psi}(0,t), \tag{4.30}$$

where $\varkappa_0$ is the effective reactivity. It immediately follows by analogy with the single-particle case, that if we can solve the nonlinear Robin BVP then we can interpret the solution as the Laplace transform of a local time propagator. That is, from the definition (4.18) of the empirical measure μ, we can rewrite equation (4.28) as

$$\begin{aligned} p^{\Psi}(x,t) &= \frac{1}{N}\sum_{j=1}^{N}\mathbb{E}\left[\left\langle \delta(x-X_j(t))\mathbf{1}_{L_j(t)<\hat{\ell}_{j'}}\right\rangle\right] = \frac{1}{N}\sum_{j=1}^{N}\left\langle \delta(x-X_j(t))\Psi(L_j(t))\right\rangle \\ &= \int_0^{\infty}\Psi(\ell)P(x,\ell,t), \end{aligned} \tag{4.31}$$

where

$$P(x,\ell,t) = \frac{1}{N}\left\langle \delta(x-X_j(t))\delta(\ell-L_j(t)\right\rangle. \tag{4.32}$$

It immediately follows that $p^{\Psi}(x,t)$ and $P(x,\ell,t)$ are also related according to equation (4.14) at the multi-particle level. The relationships between the various equations obtained by combining the hydrodynamics of an interacting Brownian gas and an encounter-based model of partially absorbing boundaries are summarized in figure 3.

(i) Remark

As in the case of reflecting boundaries, it is possible to extend our results to an interacting Brownian gas confined on the interval $[-R,R]$ with a partially absorbing boundary at each end. The details of the absorption process will depend on whether or not we have separate thresholding conditions at the two ends (see the discussion in §5). Here, we consider the simpler case in which absorption of the jth particle occurs as soon as the joint local time $L_j(t)$

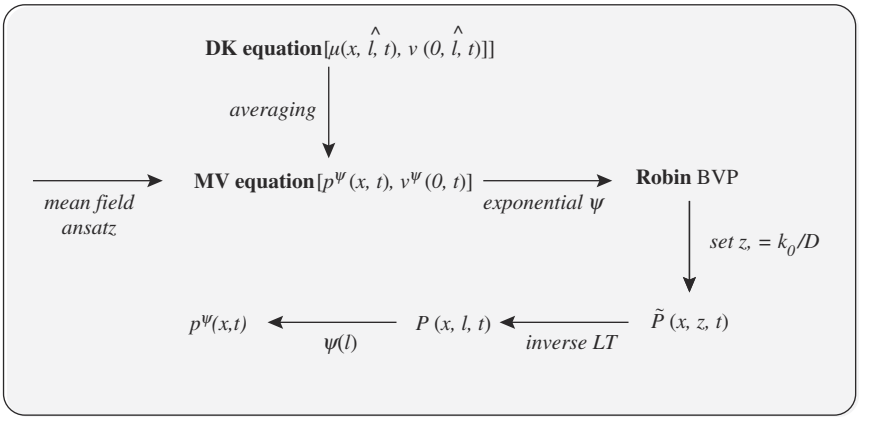

Figure 3. Hierarchy of equations obtained by combining the hydrodynamical theory of interacting Brownian gases with an encounter-based model of a partially absorbing boundary. The generalized DK equation (2.22) is an SPDE for $\mu(x, \hat{\ell}, t)$ that depends on a second measure $\nu(x, \hat{\ell}, t)$ at $x = 0$. Taking expectations with respect to the Gaussian noise processes and the local time thresholds and imposing a mean-field ansatz leads to the MV equation (4.29) for the marginal density $p^{\Psi}(x,t) = \int_0^{\infty} \Psi(\ell) P(x, \ell, t) d\ell$, which couples to the absorption flux $\nu^{\psi}(x,t) = \int_0^{\infty} \psi(\ell) P(0, \ell, t) d\ell$. In the exponential case $\Psi(\ell) = \mathrm{e}^{-\kappa_{\ell}/D}$, the MV equation reduces to a closed Robin BVP for the marginal density, which is equivalent to the Laplace transform of $P(x, \ell, t)$ with respect to ℓ. Inverting the Laplace transform then determines $P(x, \ell, t)$ and hence $p^{\Psi}(x,t)$.

given by equation (2.23) exceeds the random threshold $\hat{\ell}_j$, irrespective of which end this occurs. The corresponding MV equation is

$$\frac{\partial p^{\Psi}(x,t)}{\partial t} = -\frac{\partial J^{\Psi}(x,t)}{\partial x}, \quad J^{\Psi}(\pm R, t) = \pm D\nu(\pm R, t), \tag{4.33a}$$

with probability flux

$$J^{\Psi}(x,t) = -D\frac{\partial p^{\Psi}(x,t)}{\partial x} - \gamma^{-1} p^{\Psi}(x,t)\left(V'(x) + \int_{-R}^{R} p^{\Psi}(y,t) K'(x-y) dy\right). \tag{4.33b}$$

(c) Weak absorption limit

As a simple example, consider the half-line with the potential $V(x) = \nu x^2/2$ and take the interactions to be given by the Curie–Weiss potential $K(x) = \lambda x^2/2$, $\lambda > 0$. We also choose the exponential distribution $\Psi(x) = \mathrm{e}^{-\kappa_0 \ell/D}$ with $\kappa_0 \ll D/L$, so that absorption is much slower than diffusion. The probability flux becomes (after dropping the superscript Ψ)

$$\begin{aligned} J(x,t) &= -D\frac{\partial p(x,t)}{\partial x} - \frac{1}{\gamma} V'(x) p(x,t) - \frac{\lambda}{\gamma} p(x,t) \int_0^{\infty} p(y,t)(x-y) dy \\ &= -D\frac{\partial p(x,t)}{\partial x} - \frac{1}{\gamma} p(x,t)[V'(x) + \lambda\Lambda(t)x - \lambda m(t)], \end{aligned} \tag{4.34}$$

with the loss function and first moment defined, respectively, according to

$$\Lambda(t) = \int_0^{\infty} p(x,t) dx, \quad m(t) = \int_0^{\infty} x p(x,t) dx\,. \tag{4.35}$$

We thus obtain the non-autonomous FP equation

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x} = D\frac{\partial^2 p(x,t)}{\partial x^2} + \frac{1}{\gamma}\frac{\partial [A(x,t)p(x,t)]}{\partial x}, \quad x \in (0,\infty), \tag{4.36}$$

$$J(0,t) = -\epsilon\kappa_0 p(0,t), \tag{4.37}$$

with

$$A(x,t) = \lambda\, m(t) - V'(x) - \lambda x \Lambda(t)\,. \tag{4.38}$$

We have rescaled the reactivity by the small positive parameter in order to reflect the relative slow rate of absorption. We wish to calculate the loss function, which is the expected fraction of particles that have not been absorbed up to time t. (It is the analogue of the survival probability for a single particle.) It follows from integrating equation (4.36) with respect to x and using integration by parts that

$$\frac{d\Lambda(t)}{dt} = -\epsilon\kappa_0 p(0,t)\,. \tag{4.39}$$

In order to solve equation (4.36), we exploit the fact that when $\epsilon = 0$ there exists a unique stationary state $p = p_a(x)$, $m = m(a) = a$ and $\Lambda = 1$, see §3a. Using a quasi-steady-state approximation, we introduce the slow timescale $\tau = \epsilon t$ and assume that the solution can be decomposed as

$$p(x,t) = \Lambda(\tau)p_a(x) + \epsilon u(x,\tau), \tag{4.40}$$

with $\int_0^\infty u(x,\tau)dx = 0$, $\Lambda(0) = 1$ and $u(x,0) = 0$. In particular, we assume that the system starts in the stationary state of the reflecting BVP. Substituting the above decomposition into equation (4.39) implies that to leading order

$$\frac{d\Lambda(\tau)}{d\tau} = -\kappa_0 p_a(0)\Lambda(\tau), \tag{4.41}$$

so that

$$p(x,t) \sim \mathrm{e}^{-\epsilon\kappa_0 p_a(0)t} p_a(x). \tag{4.42}$$

Equations (3.4) and (3.6) imply that

$$p_a(0) = \frac{1}{Z(a)}, \quad Z(a) = \sqrt{\frac{\pi}{2\beta[\nu+\lambda]}}\mathrm{e}^{\beta a^2\lambda^2/2[\nu+\lambda]}\mathrm{erfc}(-a\lambda\sqrt{\beta/2[\nu+\lambda]}), \tag{4.43}$$

with a determined from equation (3.5). Example plots of the loss function $\Lambda(\tau) = \mathrm{e}^{-\tau/Z(a)}$ are shown in figure 4*a* for various first moments a. We absorb the constant κ_0 into the slow time τ. Finally, given the relationship between the solution to the Robin BVP and the Laplace transformed propagator, we can set

$$p(x,\ell,t) \sim \delta(\ell - \epsilon D p_a(0)t)p_a(x), \tag{4.44}$$

and for a general local time threshold distribution

$$p^{\Psi}(x,t) \sim \Psi(\epsilon D p_a(0)t)p_a(x)\,. \tag{4.45}$$

One example of a non-exponential threshold distribution is the gamma distribution

$$\psi_{\mathrm{gam}}(\ell) = \frac{r(r\ell)^{\sigma-1}\mathrm{e}^{-r\ell}}{\Gamma(\sigma)}, \quad \Psi_{\mathrm{gam}}(\ell) = \frac{\Gamma(\sigma, r\ell)}{\Gamma(\sigma)}, \sigma > 0, \quad r = \kappa_0/D, \tag{4.46}$$

where $\Gamma(\sigma)$ is the gamma function and $\Gamma(\sigma, z)$ is the upper incomplete gamma function:

$$\Gamma(\sigma) = \int_0^\infty \mathrm{e}^{-t}t^{\sigma-1}dt, \quad \Gamma(\sigma,z) = \int_z^\infty \mathrm{e}^{-t}t^{\sigma-1}dt, \ \sigma > 0. \tag{4.47}$$

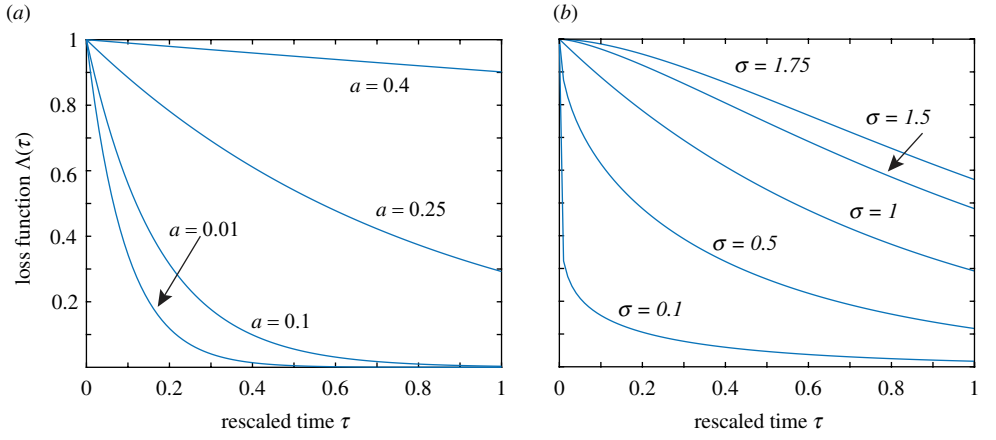

Figure 4. Loss function in the weak absorption limit for an interacting Brownian gas on the half-line. (*a*) Plot of the exponential loss function $\Lambda(\tau) = \mathrm{e}^{-\tau/Z(a)}$ for various values of the first moment a. (*b*) Plot of loss function $\Lambda(\tau) = \Psi_{\mathrm{gam}}(\tau/Z(a))$ for $\psi_{\mathrm{gam}}(\ell) = -\Psi'_{\mathrm{gam}}(\ell)$ given by the gamma distribution (4.46) and various values of the parameter σ. The first moment is $a = 0.25$. Other parameters are $D = \varkappa_0 = 1$.

The parameter r determines the effective absorption rate so that the boundary $x = 0$ is non-absorbing in the limit $r \to 0$ and totally absorbing in the limit $r \to \infty$. If $\sigma = 1$ then ψ_{gam} reduces to the exponential distribution $\psi_{\mathrm{gam}}(\ell)|_{\sigma=1} = r\mathrm{e}^{-r\ell}$. The parameter σ thus characterizes the deviation of $\psi_{\mathrm{gam}}(\ell)$ from the exponential case. If $\sigma < 1$ ($\sigma > 1$) then $\Psi(\ell)$ decreases more rapidly (slowly) as a function of the local time ℓ, that is, the boundary is more (less) absorbing. Example plots of the corresponding loss function $\Lambda(\tau) = \Psi_{\mathrm{gam}}(\tau/Z(a))$ are shown in figure 4*b*. We fix $D = 1$ and $a = 0.25$, and consider various values of the gamma distribution parameter σ. It can be seen that as the boundary becomes more absorbing (decreasing σ), the loss function decays more rapidly. Moreover, $\Lambda(\tau)$ is a convex down (up) function of τ for $\sigma > 1$ ($\sigma < 1$). Finally, note that a more detailed asymptotic analysis is needed in order to determine the validity of the quasi-steady-state approximation at large times.

5. Summary and extensions

In this article, we considered the problem of an interacting Brownian gas on the half-line. In order to handle a partially absorbing boundary condition at $x = 0$, we introduced a global density that depends on both the positions and local time thresholds of all of the surviving particles. We derived a generalized DK equation for the global density, see equation (4.22), which is an exact SPDE that prescribes how to incorporate the effects of spatio-temporal noise at the population level. We then used a mean-field ansatz to reduce the DK equation to a nonlinear MV equation in the thermodynamic limit, see equation (4.29). We also indicated how to extend the analysis to a finite interval. The rigorous mathematical proof that the mean-field limit exists via propagation of chaos has been carried out in the case of a reflecting boundary [26,27] but not, as far as we are aware, for a partially absorbing boundary. The latter also has the additional complication that there is a constant loss of particles due to absorption, so that for a large but finite number of particles and recurrent diffusion, any mean-field approximation will eventually break down. Independently of these particular issues, the boundary value problems for the generalized DK equation and the MV equations are of intrinsic interest. The former provides a starting point for developing various approximation schemes for large but

finite populations, whereas the latter is an example of a nonlinear, non-local PDE with rich mathematical structure.

One natural direction for future work is to consider higher dimensional versions of interacting Brownian gases in bounded domains. Here we briefly discuss two particular extensions of the encounter-based approach.

(a) Independently absorbing boundaries

In §4, we assumed that each particle is independently absorbed according to the stopping conditions (4.16), with all particles having the same local time threshold distribution Ψ. A simple generalization would be to take the distributions to be j-dependent. A related issue is that, in the case of the finite interval $[-R, R]$, we did not distinguish between absorption events at the two ends $x = \pm R$. That is $L_j(t)$ was taken to be the sum of the local times accrued at both ends, see equation (2.23). An alternative model would treat the absorption processes at $x = \pm R$ to be independent. At the single-particle level, this would mean introducing the pair of local times

$$L^+(t) = \lim_{\epsilon \to 0^+} \frac{D}{\epsilon} \int_0^t I_{(R-\epsilon, R)}(X(s))ds, \quad L^-(t) = \lim_{\epsilon \to 0^+} \frac{D}{\epsilon} \int_0^t I_{(-R, -R+\epsilon)}(X(s))ds \tag{5.1}$$

and the modified stopping condition

$$\mathcal{T} = \min\{\mathcal{T}^-, \mathcal{T}^+\}, \quad \mathcal{T}^\pm = \inf\{t > 0 \colon L^\pm(t) > \widehat{\ell}^\pm\}, \quad \mathbb{P}[\widehat{\ell}^\pm > \ell] \equiv \Psi \pm (\ell)\,. \tag{5.2}$$

The difference between the two scenarios also has a possible physical interpretation as illustrated in figure 5. In particular, recall that if Ψ is non-exponential, then the absorption process is non-Markovian, that is, some memory trace of previous particle-boundary encounters is maintained. Treating each particle as independently absorbed suggests that the memory traces are associated with internal states of the particles, see figure 5*a*. However, another possibility is that the individual boundaries maintain the memory traces, see figure 5*b*, so that the absorption process at the two ends can be separated. However, the latter significantly complicates the analysis of the multi-particle Brownian gas, since the probability that any one particle is absorbed will depend on previous interactions between the boundary and all other particles.

(b) Interacting Brownian gas in $\mathbb{R}$ with a partially absorbing trap

The encounter-based approach to single-particle absorption has also been developed within the context of heterogeneous media, where one or more subregions of a domain act as partially absorbing traps [41,43]. This is illustrated in figure 6 for an absorbing trap in the interval $[-R, R]$. A Brownian particle can freely enter and exit the trap but is only absorbed within the trap when its occupation time exceeds some random threshold. The occupation time is a Brownian functional defined according to [35]

$$A(t) = \int_0^t \mathbf{1}_{(-R,R)}(X(\tau))d\tau = \int_0^t \left(\int_{-R}^R \delta(x - X(\tau))dx \right) d\tau\,. \tag{5.3}$$

$A(t)$ specifies the amount of time the particle spends within $[-R, R]$ over the time interval $[0, t]$. The stopping time condition for absorption is

$$\mathcal{T} = \inf\{t > 0 \colon A(t) > \widehat{a}\}, \tag{5.4}$$

where $\widehat{a}$ is a random variable with probability distribution $\Psi(a) = \mathbb{P}[\widehat{a} > a]$. Hence, the corresponding single-particle SDE is

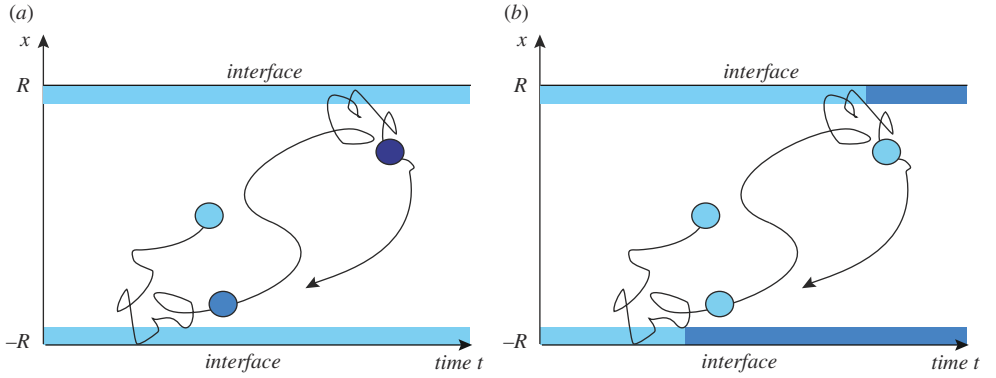

Figure 5. Schematic diagram indicating two different absorption scenarios for a Brownian particle diffusing in the interval $[-R, R]$. For the sake of illustration, the local times are taken to be the amount of time spent in a small boundary layer around $x = \pm R$. (*a*) The particle has an internal state $S(t)$ that increases strictly monotonically with the amount of time $L(t)$ spent in contact with either boundary. Absorption occurs when the internal state, and hence $L(t)$, crosses a threshold. (*b*) Each boundary has its own internal state denoted by $S^{\pm}(t)$, which is a strictly monotonic function of the amount of time the boundary is in contact with the particle, which is specified by the local time $L^{\pm}(t)$. Absorption occurs as soon as one of the internal states crosses its corresponding threshold. In both cases (*a*) and (*b*), the value of the internal state is represented by the colour of the shaded regions.

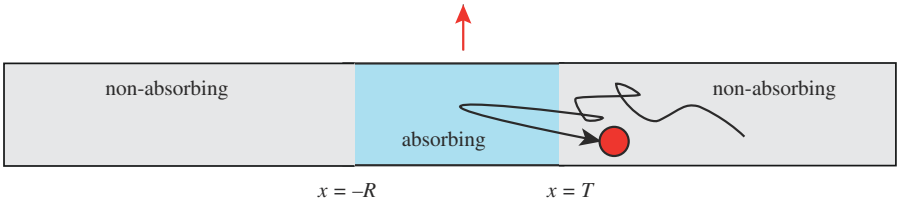

Figure 6. One-dimensional diffusion with a partially absorbing trap in the interval $[-R, R]$.

$$dX(t) = \sqrt{2D}dW(t)\mathbf{1}_{A(t)<\hat{a}}\,. \tag{5.5}$$

Here, we sketch how to adapt the previous analysis to an interacting Brownian gas in $\mathbb{R}$ with a partially absorbing trap. We begin by considering a single particle. Following along analogous time to an absorbing boundary, we introduce the single-particle empirical measure

$$\mu(x, \hat{a}, t) = \delta(x - X(t))\mathbf{1}_{A(t)<\hat{a}}, \tag{5.6}$$

and set $F(\hat{a}, t) = f(X(t))\mathbf{1}_{A(t)<\hat{a}}$ for a test function $f(x)$ in $\mathbb{R}$. Using Ito's lemma and the definition of the occupation time, we have

$$dF(\hat{a}, t) = \left[Df''(X(t))dt + \sqrt{2D}f'(X(t))dW(t)\right]\mathbf{1}_{A(t)<\hat{a}} - \delta(A(t) - \hat{a})\int_{-R}^{R}\delta(X(t) - y)f(y)dy\,. \tag{5.7}$$

It follows that

$$\begin{aligned}&\int_{-\infty}^{\infty} f(x)\frac{\partial\mu(x, \hat{a}, t)}{\partial t}dx\\ &= \int_{-\infty}^{\infty}\mu(x, \hat{a}, t)\left[Df''(x)dt + \sqrt{2D}f'(X(t))dW(t)\right]dx - \delta(A(t) - \hat{a})\int_{-R}^{R}\delta(X(t) - y)f(y)dy\,.\end{aligned} \tag{5.8}$$

Integrating by parts and using the arbitrariness of f yields an SPDE for μ:

$$\frac{\partial \mu(x,\hat{a},t)}{\partial t} = D\frac{\partial^2 \mu(x,\hat{a},t)}{\partial x^2} + \sqrt{2D}\frac{\partial \mu(x,\hat{a},t)}{\partial x}\xi(t) - \nu(x,\hat{a},t), \tag{5.9a}$$

with

$$\nu(x,\hat{a},t) = \delta(A(t)-\hat{a})\delta(X(t)-x)\mathbf{1}_{(-R,R)}(x). \tag{5.9b}$$

Note that ν vanishes outside the trap. Finally, averaging with respect to the white noise process and the random occupation time threshold yields

$$\frac{\partial p^{\Psi}(x,t)}{\partial t} = D\frac{\partial^2 p^{\Psi}(x,t)}{\partial x^2} - \nu^{\psi}(x,t)\mathbf{1}_{(-R,R)}(x), \tag{5.10}$$

with

$$p^{\Psi}(x,t) = \mathbb{E}[\langle \mu(x,\hat{a},t)\rangle] = \langle \delta(x-X(t)\Psi(A(t))\rangle, \tag{5.11a}$$

$$\nu^{\psi}(x,t) = \langle \delta(x-X(t))\delta(A(t)-\hat{a})\rangle = \langle \psi(A(t))\delta(x-X(t))\rangle. \tag{5.11b}$$

The subsequent solution strategy is analogous to the case of an absorbing boundary [41,43]. That is, for an exponential distribution $\Psi(a) = \mathrm{e}^{-\kappa_0 a}$, we recover the classical inhomogeneous diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}, \quad x \in (-\infty,-R)\cup(R,\infty), \tag{5.12a}$$

$$\frac{\partial q(x,t)}{\partial t} = D\frac{\partial^2 q(x,t)}{\partial x^2} - \kappa_0 q(x,t), \quad x \in (-R,R), \tag{5.12b}$$

together with the matching conditions

$$p(\pm R,t) = q(\pm R,t), \quad \partial_x p(\pm R,t) = \partial_x q(\pm R,t). \tag{5.12c}$$

We denote the solution within the trap by the function $q(x,t)$. The final step is to identify the solution p and q as the Laplace transforms of the corresponding propagators

$$P(x,a,t) = \langle \delta(x-X(t)\delta(a-A(t)\rangle, \quad x \in (-\infty,-R)\cup(R,\infty), \tag{5.13a}$$

$$Q(x,a,t) = \langle \delta(x-X(t)\delta(a-A(t)\rangle, \quad x \in (-R,R). \tag{5.13b}$$

Now suppose that there are N interacting Brownian particles with individual occupation times $A_j(t)$. The SDE (4.17) is replaced by

$$\begin{aligned} dX_j(t) = \Bigg\{ -\frac{1}{\gamma}\Bigg[V'(X_j(t)) + N^{-1}\sum_{k=1}^{N} K'(X_j(t)-X_k(t))\mathbf{1}_{A_k(t)<\hat{a}_k}\Bigg]dt \\ + \sqrt{2D}dW_j(t)\Bigg\}\mathbf{1}_{A_j(t)<\hat{a}_j}, \end{aligned} \tag{5.14}$$

and the global density is defined according to

$$\mu(x,\hat{\mathbf{a}},t) = \frac{1}{N}\sum_{j=1}^{N}\mu_j(x,\hat{a}_j,t) = \frac{1}{N}\sum_{j=1}^{N}\delta(X_j(t)-x)\mathbf{1}_{A_j(t)<\hat{a}_j}. \tag{5.15}$$

Introduce a smooth test function $f(x)$ for $x \in \mathbb{E}$ and set

$$F(\hat{\mathbf{a}},t) = \frac{1}{N}\sum_{j=1}^{N} f(X_j(t))\mathbf{1}_{A_j(t)<\hat{a}_j}. \tag{5.16}$$

Applying Ito's lemma, integrating by parts, and using the fact that f is arbitrary leads to the following generalized DK equation for μ:

$$\frac{\partial \mu(x,\hat{\boldsymbol{a}},t)}{\partial t} = -\frac{\partial \mathcal{J}(x,\hat{\boldsymbol{a}},t)}{\partial x} - \nu(x,\hat{\boldsymbol{a}},t)\mathbf{1}_{(-R,R)}(x), \tag{5.17a}$$

$$J(x,\hat{\boldsymbol{a}},t) = -\sqrt{\frac{2D}{N}}\sqrt{\mu(x,\hat{\boldsymbol{a}},t)}\eta(x,t) - D\frac{\partial \mu(x,\hat{\boldsymbol{a}},t)}{\partial x} - H_\mu(x,\hat{\boldsymbol{a}},t), \tag{5.17b}$$

with

$$H_\mu(x,\hat{\boldsymbol{a}},t) = \gamma^{-1}\mu(x,\hat{\boldsymbol{a}},t)\left(V'(x) + \int_{-\infty}^{\infty}\mu(y,\hat{\boldsymbol{a}},t)K'(x-y)dy\right), \tag{5.18}$$

and

$$\nu(x,\hat{\boldsymbol{a}},t) = \frac{1}{N}\sum_{j=1}^{N}\delta(A_j(t)-\hat{a}_j)\delta(X_j(t)-x)\,. \tag{5.19}$$

We have also transformed the noise terms. The final step is to take expectations with respect to the Gaussian noise and occupation time thresholds. Under a mean-field ansatz, we obtain an MV equation for the marginal density

$$p^\Psi(x,t) = \mathbb{E}\left[\left\langle \mu(x,\hat{\boldsymbol{a}},t)\right\rangle\right] = \frac{1}{N}\sum_{j=1}^{N}\left\langle \Psi(A_j(t))\delta(x-X_j(t))\right\rangle, \tag{5.20}$$

which takes the form

$$\frac{\partial p^\Psi(x,t)}{\partial t} = -\frac{\partial J^\Psi(x,t)}{\partial x} - \nu^\psi(x,t)\mathbf{1}_{(-R,R)}(x), \tag{5.21a}$$

with probability flux

$$J^\Psi(x,t) = -D\frac{\partial p^\Psi(x,t)}{\partial x} - \gamma^{-1}p^\Psi(x,t)\left(V'(x) + \int_{-\infty}^{\infty}p^\Psi(y,t)K'(x-y)dy\right), \tag{5.21b}$$

and absorption flux

$$\nu^\psi(x,t) = \frac{1}{N}\sum_{j=1}^{N}\left\langle \psi(A_j(t))\delta(x-X_j(t))\right\rangle. \tag{5.21c}$$

Data accessibility. This article has no additional data.

Declaration of AI use. I have not used AI-assisted technologies in creating this article.

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Endnotes

[1]Note that we normalize μ using the initial number of particles N, rather than the number of particles that have not yet been absorbed. This is consistent with the normalization of the interaction term, and avoids complications arising from the fact that the number of surviving particles is itself a stochastic variable. It follows that $\int_0^\infty \mu(x,\hat{e},t)dx$ is a decreasing function of t.

[2]In the case of a partially absorbing boundary, the fraction of surviving particles is a monotonically decreasing function of time. Clearly, for a large but finite number of particles and a recurrent diffusion process, the number of remaining particles will eventually approach zero so that any mean field approximation will break down. There have been a few rigorous mathematical studies of the mean field limit and propagation of chaos for mean field games with totally absorbing boundaries [28–30].

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