Imperial College
London

Imperial College London
The Blackett Laboratory
Quantum Optics & Laser Science Group

Orthogonal Polynomials and Open Quantum Systems

Mischa Prebin Woods

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Abstract

This thesis is concerned with the study of quantum systems coupled linearly to a continuous bath of oscillators examples of which are the spin-boson model and the Nelson model. The main theme throughout is to develop a better understanding of the properties of the bath of oscillators such that more efficient representations of it can be made to facilitate the understanding of the system dynamics. The main difficulty in simulating the system dynamics is that the bath of oscillators composes an infinite number of degrees of freedom. In this thesis, we investigate the mathematical properties of an approach in which the bath modes are written as a semi-infinite chain of nearest neighbour interacting harmonic oscillators such that the efficient time dependent density-matrix renormalisation group (t-DMRG) methods can be applied for simulation.

In the first section, we show how there are many different ways to represent the bath as semi-infinite chains and prove that seemingly unrelated methods can all be achieved using the same mathematical formalism. We show that in an iterative process the bath can be transformed into a chain of oscillators with nearest neighbour interactions. This is achieved using the formalism of orthogonal polynomials. This allows one to define a sequence of residual spectral densities at each site along the chain. We show that this sequence of residual spectral densities is provided by the so-called "sequence of secondary measures". We derive a systematic procedure to obtain the spectral density of the residual bath in each step. We find that these residual spectral densities are related to an old abstract problem in mathematics known as the "secondary measures". We solve this problem from the field of orthogonal polynomials to give an explicit expression for the residual spectral densities and go on to prove that these functions converge under very general conditions. That is, the asymptotic part of the chain is universal, translation invariant with universal spectral density. These results suggest efficient methods for handling the numerical treatment of the residual bath.

In the second section, we take a different approach. Rather than studying the properties of residual baths, we look at how system observables are affected by truncating the semi-infinite chain of harmonic oscillators to a finite length chain. By developing locality bounds for the dynamics, we derive an upper bound to the error introduced by such a truncation and show that for all finite times it can be made arbitrarily small by including a sufficient number of harmonic oscillators

before truncating. Furthermore, it is shown that the speed at which the system communicates with different harmonic oscillators in the chain is proportional to the maximum frequency of the environment but that this speed also depends on the particular version of the chain. These bounds are given for when the dynamics are calculated in the Interaction picture and in the Schrödinger picture.

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0.1 Background

Real quantum mechanical systems are never found in complete isolation, but invariably coupled to a macroscopically large number of "environmental" degrees of freedom, such as those provided by electromagnetic field modes, density fluctuations of the surrounding media (phonons) or ensembles of other quantum systems, like electronic or nuclear spins [1, 2, 3]. The fact that the environment is totally or partially inaccessible to experimental probing in these so called "open quantum systems" leads to the appearance of an effectively irreversible dynamics for the quantum system's observables, and mediate the fundamental processes of energy relaxation, phase decoherence and, possibly, the thermalization of the subsystem.

Accurate numerical or analytical description of general open quantum systems dynamics appears, prima facie, to be extremely difficult due to the large (often infinite) number of bath and system variables which need to be accounted for. When the environmental degrees of freedom are modeled as a *bath* of harmonic oscillators exact path integral solutions can be available but are rarely of practical use [10, 1, 2]. Hence assumptions such as weak system-environment coupling and vanishing correlation times of the environment, i.e. the Born-Markov approximation, are often invoked to obtain compact and efficiently solvable equations. These approaches suffer the drawback that their accuracy is hard to certify and that they become simply incorrect in many important situations. Indeed, our increasing ability to observe and control quantum systems on ever shorter time and length scales is constantly revealing new roles of noise and quantum coherence in important biological and chemical processes [4, 5, 6, 7, 8] and requires an accurate but efficient description of the system-environment interaction that go well beyond the Born-Markov approximation [8, 9] in order to understand the interaction of intrinsic quantum dynamics and environmental noise. In many biological, chemical and solid-state systems, deviations from strict Markovianity, which can be explicitly quantified [12, 13, 14], are significant and methods beyond standard perturbative expansions are required for their efficient description. A number of techniques have been developed to operate in this regime. Those include polaron approaches [15], the quasi-adiabatic path-integral (QUAPI) method [16], the hierarchical equation of motion approach [17] and extensions of the quantum state diffusion description to non-Markovian regimes [18].

Here we will focus on the exploration of the mathematics of an exact, analytical mapping of the standard model of a quantum system interacting with a continuum of harmonic oscillators to

an equivalent model in which the system couples to one end of a chain nearest-neighbour coupled harmonic oscillators, as illustrated in figure (1.1). This mapping has permitted the formulation of an efficient algorithm for the description of the system-environment coupling for spectral densities of the environment fluctuations [19, 20, 23]. This mapping was originally intended just as a practical means of implementing t-DMRG which would avoid approximate determination of the chain representation using purely numerical, and often unstable, transforms [21]. It was quickly realised that the scope of the mapping is much broader. Indeed, the mapping itself provides an extremely intuitive and powerful way of analysing universal properties of open quantum systems, that is, independent of the numerical method used to simulate the dynamics [19]. This conclusion was implied also in [23], where the authors also developed a, in principle, rather different chain representation of a harmonic environment using an iterative propagator technique [23].

Both of these theories establish chain representations as a novel and direct way of looking at how energy and correlations propagate into the environment in real time. In the chain picture the interactions cause excitations to propagate away from the system, allowing a natural, causal understanding of Markovian and non-Markovian dissipation in terms of the properties of the chain's couplings and frequencies.

Now we will briefly outline the novel results present in this thesis. A more comprehensive and detailed list is also given at the end of each chapter. In chapter 1, we generalise and extend the work of [19]. The basic idea of mapping a bath of bosons onto a chain representation has been around for a long time in many different formats and forms, all with different and novel features. Essentially, the chain mapping of [19], is the same as that of [21] but with the underlying method reformulated in terms of the language of orthogonal polynomials. This re-formulation has many benefits because many numerical algorithms have been developed in the field of orthogonal polynomials which can now be adopted to calculate the chain coefficients. This is advantageous because it provides stable and efficient algorithms for the calculation of the chain coefficients as well as the ability to find analytical solutions in some instances. It is also noteworthy that the method of applying orthogonal polynomials to develop chain mappings was around before the work of [19], but in the context of non-hermition Hamiltonians [22]. From the point of view of the maths, the proofs follow very similarly, the only main difference being that in [19] one uses real orthogonal polynomials, where as in [22], they use complex orthogonal polynomials. The generalisation found

in this chapter were motivated by [23], where they also find a chain mapping of a bosonic bath. Here though the form of the chain was different. The main novel results is the generalisation of [19] using orthogonal polynomials to find may different chain mappings. Chapter 2 begins with solving an old open problem in the field of orthogonal polynomials by providing an explicit formula for the so-called sequence of secondary measures. We then prove how this abstract construction has a physical interpretation by proving that they give rise to the residual spectral densities of the chain. We also give convergence conditions of the sequence of residual spectral densities. We also achieve a non trivial proof that the chain mapping of [23] is a special case of the general results obtained here. What's more, the algorithm derived here using orthogonal polynomials is much more efficient and straightforward to implement. We also derive rigorous convergence theorems for the residual spectral densities. In the chain mapping of [23], numerical studies were performed and one of the convergence theorems derived in this thesis was postulated. The derived results in this chapter also help relate it to the work of [26], where they derived a way to extract one mode from the bosonic bath. Since the equations derived in this section allow one to extract $n = 1, 2, 3, \ldots$ from the bath, it can also be viewed as a generalisation of this result. In chapter 3, the new result is a locality bound of the dynamics for class of Hamiltonians for which locality bounds were previously unknown. Namely, for locally coupled Hamitonians quadratic in canonically conjugate position and momenta operators and bilinearly coupled via these operators to bounded operators. This new result extends the work of [59], where locality bounds were derived for Hamitonians quadratic in the local canonically conjugate position and momenta only.

0.2 Mathematical and Physical Prerequisites

In order to comprehend this thesis, one should have a degree in physics or mathematics. A general understanding of quantum mechanics is also assumed. Although very deep results with advanced mathematics is used in this thesis, the material is introduced starting from a basic level and working the way up slowly to obtain the final results; with detailed proofs throughout. In some cases, there will be more advanced knowledge assumed, such as with the definition of the Hamiltonian in section 1, where a knowledge of second quantisation and fock space would be useful. However, in such instances the reader should be able to skip these parts without compromising to great extent his

or her understanding of the rest of the thesis.

0.3 Publications

During the doctoral years of the author, he has produced with co-authors several manuscripts which or either being reviewed or which are in preparation:

- Mappings of open quantum systems onto chain representations and Markovian embeddings. See [63], the material of the first two chapters of this thesis is based on this material. It is currently in review process.

- Simulating bosonic baths with error bounds. The material in the third chapter is based on this material. It is currently in preparation.

Chapter 1

Chain Mappings and Orthogonal Polynomials

The main goal of this chapter is to develope a general framework for mapping the bosonic environment of an open quantum system generally known as *Pauli-Fierz Hamiltonians* onto semi infinite 1D chain representations with nearest neighbour interactions where the system only couples to the first element in the chain. This general formalism allows the comparison between different chain mappings. It will be shown how this generalised chain mapping reduces to two known results mentioned in section 0.1 under special conditions. In addition, the method developed here is also valid when the spectral density of the system-enviroment interaction has a gap in its support. This is of practical interest as there are open quantum systems (such as photonic crystals [28]) that naturally exhibit such a spectral density and hence can only be mapped onto a chain using the method presented in this thesis.

The content of each section is as follows: In sections 1.1 and 1.2 the Hamiltonian is defined and the ideas behind the method of mapping the environment onto the chain representations is outlined. This is followed by section 1.3 which is concerned with introducing the necessary mathematical tools needed to fully develop the chain mapping. These consist in some elementary results in the field of orthogonal polynomials. This section also helps to introduce notation which will be used throughout this thesis. In section 1.4, with the aid of the results of section 1.3, the chain mapping idea introduced in section 1.2 is fully developed by providing a general framework for mapping

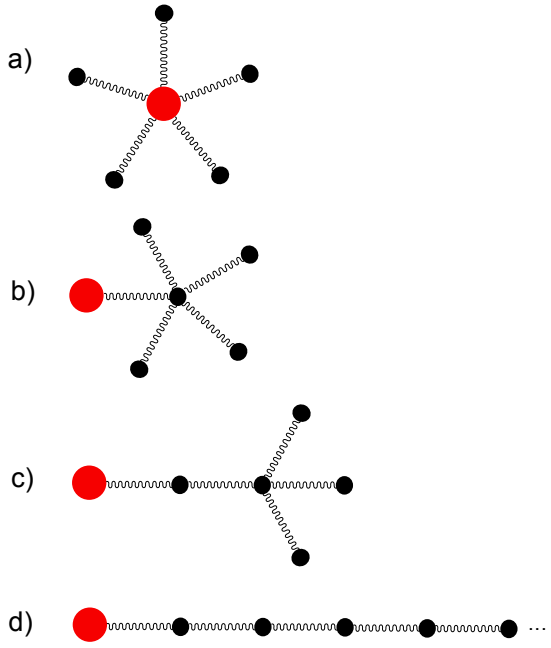


Figure 1.1: **a)** to **c)**: Conversion of a general bath of oscillators into a chain of oscillators with nearest neighbour interactions. All these baths are dynamically equivalent as far as the system is concerned. For a bath with infinitely many modes, the process yields an infinite chain whose asymptotic end is universal. This asymptotic end can be written as a universal bath of harmonic oscillators. We call the processes a) to c) *embeddings*. At each step we embed one more mode of the environment into the system and obtain the *new bath*. **d)** The limiting case where all bath oscillators have been converted to a semi-infinte chain

open quantum systems which are linearly coupled to an environment onto a representation where the environment is a semi-infinite chain with nearest neighbour couplings and define two special cases of particular interest, - the particle and phonon mappings.

The main results of this chapter is theorem 9 and corollaries 10 and 12.

1.1 The Hamiltonian

We consider a quantum system coupled to a bosonic bath. The separable Hilbert space $\mathcal{S}$ of the system carries a lower bounded "free" Hamiltonian $\hat{H}_{\mathcal{S}}$, where as the bosonic bath is described in

the Fock space $\Gamma(\mathfrak{h})$ over the mode Hilbert space $\mathfrak{h}$, with a free Hamiltonian $d\hat{\Gamma}(\hat{G})$ arising from the second quantization of a positive self-adjoint operator $\hat{G}$ on $\mathfrak{h}$. The coupling will be via one mode $h \in \mathfrak{h}$ and a suitable self-adjoint system operator $\hat{A}_s$, so that altogether we have on $\mathcal{S} \otimes \Gamma(\mathfrak{h})$ the Hamiltonian

$$\hat{H} = \hat{H}_{\mathcal{S}} \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \mathbb{I}_{\mathcal{S}} \otimes d\hat{\Gamma}(\hat{G}) + \hat{A}_s \otimes \hat{\Phi}(h). \tag{1.1}$$

Here $\hat{\Phi}$ denotes the usual field operator. If, for example, $\hat{G}$ is a function g of certain momentum variables $\vec{k}$, this is usually written in terms of creation and annihilation operators as $d\hat{\Gamma}(\hat{G}) = \int d\vec{k}\; g(\vec{k}) a^*_{\vec{k}} a_{\vec{k}}$ and $\hat{\Phi}(h) = \int d\vec{k}\; h(\vec{k})\big(a^*_{\vec{k}} + a_{\vec{k}}\big)$, where * denotes the adjoint operator. The form Eq. (1.1) is often referred to as a Pauli-Fierz Hamiltonian [30], specialized in our case by allowing one interaction term. It includes the spin-boson model obtained by choosing $\mathcal{S} = \mathbb{C}^2$, $\hat{H}_{\mathcal{S}} = \alpha\hat{\sigma}_z$, and $\hat{A}_s = \hat{\sigma}_x$, where α is a positive constant and $\hat{\sigma}_x$, $\hat{\sigma}_z$ are the Pauli matrices. This model has many applications. For example, it is used as a simple model to study dissipation of a particle trapped in a double well potential. In the context of quantum computation, the model can be used to study a qubit coupled to an environment with can decohere. It constitutes a basic model for the thermodynamic properties of amorphous solids. The certain coupling strength to the environment, there is also a phase transition from one in which the two level system goes from being delocalised between the two eigenstates two one in which it is localised to one of them. For a review, see [10]. More recently, it has also found application in the field of quantum biology [11]. In this case the model is used to understand decoherence effects in light harvesting complexsis. Pigment-protein complexes are modelled where the system plays the role of chromophores and the bath constitutes the fluctuations due to vibrations in the surrounding proteins.

The sufficient conditions for the operator Eq. (1.1) to be well-defined in the case that $\hat{A}_s$ is unbounded are quite involved and can be found in the literature [32]. However if $||\hat{A}_s|| < \infty$, then a sufficient requirement is that $h \in \mathfrak{h}$, $||\hat{G}^{-1/2}h|| < \infty$ which can be written in terms of g and h as

$$\int \frac{h^2(k)}{g(k)} dk < \infty. \tag{1.2}$$

Indeed, this implies that $\hat{G} \geq \lambda |h\rangle\langle h|$, for some $\lambda > 0$ and hence that the interaction term is infinitesimally bounded (see Vol 2, Section X.2: Perturbations of self-adjoint operators p. 162 of [33]) with respect to the free part. For a more detailed definition of the Hamiltonian Eq. (1.1) and its Hilbert space, see (A) in the appendix.

Note that the Hamiltonian depends only on the operator $\hat{G}$ and the vector h. Therefore, we can try to simplify the problem by applying unitaries in $\mathfrak{h}$ to bring these operators into a form treated more easily. Finding such a standard form is well known from problems not involving a given vector h: in that case we would immediately diagonalize $\hat{G}$, and expect to simplify computations considerably. Similarly we will use a standard form for the pairs $(\hat{G}, h)$. To begin with, there will be vectors in $\mathfrak{h}$, which are completely irrelevant to our problem, namely those orthogonal to h and all vectors $\hat{G}^n h$. More precisely (in the sense of not assuming $h \in \mathrm{dom}(\hat{G})$) we define the "cyclic subspace" $\mathfrak{h}_1$ as the closed subspace generated by all vectors $e^{it\hat{G}}h$ for $t \in \mathbb{R}$.

The direct sum $\mathfrak{h}_1 \oplus \mathfrak{h}_1^\perp$ leads to the tensor product of the respective Fock spaces, so that $\Gamma(\mathfrak{h}) \cong \Gamma(\mathfrak{h}_1) \otimes \Gamma(\mathfrak{h}_1^\perp)$ and the factor $\Gamma(\mathfrak{h}_1^\perp)$ is dynamically decoupled from the cyclic part and the system. Therefore, we can just trace out this factor, likewise replacing the initial state by its partial trace without any detectable change for the system and its interaction with the environment. Therefore we can and will assume in the sequel that $\mathfrak{h} = \mathfrak{h}_1$ is already cyclic.

Suppose now we have a second environment system $(\tilde{\mathfrak{h}}, \hat{\tilde{G}}, \tilde{h})$ and a unitary operator $\hat{U} : \mathfrak{h} \to \tilde{\mathfrak{h}}$ such that $\hat{U}h = \tilde{h}$ and $\hat{U}\hat{G}\hat{U}^* = \hat{\tilde{G}}$. Under such an isomorphism all details of system-environment will be mapped into each other. This is formally done by the unitary operator $\Gamma(\hat{U}) : \Gamma(\mathfrak{h}) \to \Gamma(\tilde{\mathfrak{h}})$, which multiplies any n-particle wave function with $\hat{U}^{\otimes n}$. Let $\hat{E}(dx)$ be the projection valued spectral measure of $\hat{G}$. Then we form the scalar measure

$$\mu(d\omega) = \langle h, \hat{E}(d\omega)h \rangle \ . \tag{1.3}$$

Obviously, this will not change under a unitary isomorphism $\hat{U}$. In fact, it completely determines the triple $(\mathfrak{h}, \hat{G}, h)$ up to isomorphism. Indeed we can set

$$\tilde{\mathfrak{h}} = \mathcal{L}^2(\mathbb{R}^+, \mu) \tag{1.4}$$

$$(\hat{\tilde{G}}\psi)(x) = x\psi(x) \ \forall \ \psi \in \tilde{\mathfrak{h}} \tag{1.5}$$

$$\tilde{h}(x) = 1 \tag{1.6}$$

The unitary operator defining the isomorphism, is given $\big(\hat{U}e^{it\hat{G}}h\big)(x) = e^{itx}$. One readily checks that this preserves scalar products, and since we have assumed $\mathfrak{h}$ to be cyclic it is defined on a dense set of vectors.

Definition 1. *We say that the triple $(\mathfrak{h}', \hat{G}', h')$ defined in Eqs (1.4) to (1.6), is the standard form of $(\mathfrak{h}, \hat{G}, h)$.*

Often the measure is absolutely continuous with respect to Lebesgue measure, in which case we write $\mu(dx) = \pi^{-1}J(x)dx$ with the *spectral density* J. (The factor $1/\pi$ is only introduced for conformity with [1]). For example, when $h \in \mathfrak{h} = \mathcal{L}^2([\vec{k_{min}}, \vec{k_{max}}], d\vec{k})$, with $-\infty \leq \vec{k_{min}} < \vec{k_{max}} \leq \infty$, and $(\hat{G}\psi)(\vec{k}) = g(\vec{k})\psi(\vec{k})$ for some monotone function g, we get

$$J(\omega) = \pi h\left(g^{-1}(\omega)\right)^2 \left|\frac{dg^{-1}(\omega)}{d\omega}\right|, \tag{1.7}$$

where g^{-1} is the inverse function of g. When g is not monotone, we would additionally get a sum over the inverse images $g^{-1}(\{\omega\})$, and if the momentum variable has more dimensions, we would also have an integral over the inverse image.

1.2 Extracting Chains

We can further unravel the standard form if we build up a basis of the Hilbert space starting from h and using the repeated action of $\hat{G}$ on h. This procedure, which will lead to the desired chain representation, is reminiscent also of the construction of nearest neighbor quantum walks from a unitary and an initial vector [34]. We consider the simplest case, based only on $\hat{G}$ and h in the spirit of the normal form described above.

We assume that h is in the domain of some power of $\hat{G}$, say $h \in \mathrm{dom}\hat{G}^N$, possibly with $N = \infty$, by which we mean that $\hat{G}^n h$ is defined for all integer $n \geq 0$. Then we can apply Gram-Schmidt orthogonalization to the sequence $h, \hat{G}h, \hat{G}^2h, \ldots$ to obtain an orthonormal set of vectors. If we do this in the standard form it amounts precisely to building the orthogonal polynomials P_n associated with the measure μ. Since $\hat{G}$ is hermitian, we find a three-term recursion relation connecting the P_n. In other words, $\langle P_n, \hat{G}P_m\rangle = 0$ unless $|n - m| \leq 1$.

The process may terminate before reaching the vector $\hat{G}^N h$, if the cyclic subspace $\mathfrak{h}$ is of dimension $< N$. Then, and only then, one of the off-diagonal matrix elements of $\hat{G}$ might vanish. Excluding this trivial case (as we will from now on) we can successively choose the phases of the polynomials so that the off-diagonal elements are positive. With this convention the P_n are uniquely determined by $\hat{G}$ and h, and hence we find a unique orthonormal system P_n for $n \leq N$ such that $P_0 = h$, and

1. For $n < N$: $P_n \in \mathrm{dom}\hat{G}$ for and $\hat{G}P_n \in span\{P_m | m \leq N\}$.

2. $\langle P_n, \hat{G} P_m \rangle = 0$ for $|n-m| > 1$ and $n, m \leq N$.

3. $\langle P_n, \hat{G} P_{n+1} \rangle = \langle P_{n+1}, \hat{G} P_n \rangle = \sqrt{\beta_n} > 0$ for $n < N$.

If we write $\hat{G}$ in this basis we see that it represents one oscillator for each n, with frequency $\omega_n^2 = \langle P_n, \hat{G} P_m \rangle$, and harmonic coupling to its neighbor with strength $\sqrt{\beta_n}$. In second quantization we get exactly the bath representation of figure (1.1) (compare theorem 9).

Note that the idea works also when N is finite, in which case we write the system as a finite chain, which is coupled at the end to a terminal bath. When at this juncture we still have $h \in \mathrm{dom}\hat{G}$ the process may be continued. Nevertheless such a finite chain extraction may be useful to obtain a good numerical truncation and thus simplification of the bath. We note that one can also apply these ideas to the symplectic structure of the bath: in that case we do not just allow unitary transformations of $\mathfrak{h}$, but also real linear transformations, which preserve the imaginary part of the scalar product. In terms of oscillators this still gives canonical transformations, and in second quantization a more general kind of Bogolyubov transformations (no longer gauge invariant ones). Clearly, this requires a more in depth study of some properties of the orthogonal polynomials P_n, and this will be done in the following section (we will later come back to the study of orthogonal polynomias in section 2.1).

1.3 Introduction to Notation and Basic Tools

Let us consider a *measure* $d\mu$ on the real line. Its support is contained in a smallest interval $I = [a, b]$, where $a = -\infty$ and $b = +\infty$ are admitted. For measures with unbounded support we need to assume that all moments

$$C_n(d\mu) := \int_a^b x^n d\mu(x) \quad n = 0, 1, 2, \ldots, \tag{1.8}$$

are finite. Moreover, unless stated otherwise, we will assume throughout that $d\mu(x) = \bar{\mu}(x)dx$ is absolutely continuous with respect to Lebesgue measure, and denote its density by $\bar{\mu}(x)$.

An important distinction concerns the presence or absence of gaps in the support of $d\mu$. We call the measure *gapless* if the support is equal to the interval $[a, b]$, and *gapped* otherwise. In this case there is at least one open interval $[b_1, a_1]$ with $a < b_1 < a_1 < b$ on which $d\mu$ vanishes. If not stated otherwise, the measure can be gapped or gapless and a, b finite or infinite.

Remark 2. *A few of the results in this thesis (most noticeably, theorems 49 and 50), are restricted to the finite interval case. Gaplessness quite often will be assumed but some results are valid in the gapped case (see remark 43 for more details on gapped examples).*

Let $\mathbb{P}$ denote the space of real polynomials. Then, for any $u(x)$ and $v(x) \in \mathbb{P}$ we will define an *inner product* as

$$\langle u, v \rangle_{\bar{\mu}} = \int_a^b u(x)v(x)d\mu(x). \tag{1.9}$$

We can now define the orthogonal polynomials. We call $\{P_n(d\mu; x)\}_{n=0}^{\infty}$ the set of *real orthonormal polynomials with respect to measure* $d\mu$ where each polynomial P_n is of degree n, if they satisfy

$$\langle P_n(d\mu), P_m(d\mu) \rangle_{\bar{\mu}} = \delta_{nm} \quad n, m = 0, 1, 2, \dots \ . \tag{1.10}$$

Similarly, we call $\{\pi_n(d\mu; x)\}_{n=0}^{\infty}$ the set of *real monic polynomials with respect to measure* $d\mu$ where each polynomial π_n is of degree n if they satisfy

$$\pi_n(d\mu; x) = P_n(d\mu; x)/a_n \quad n = 0, 1, 2, \dots \ , \tag{1.11}$$

where $a_n = a_n(d\mu)$ is the leading coefficient of $P_n(d\mu; x)$. Note that for any measure $d\mu(x)$, there always exists a set of real orthonormal polynomials and real monic polynomials (see [29] for a proof).

Theorem 3. *The monic polynomials $\pi_n(d\mu; x)$ satisfy the three term recurrence relation*

$$\pi_{n+1}(d\mu; x) = (x - \alpha_n)\pi_n(d\mu; x) - \beta_n \pi_{n-1}(d\mu; x) \qquad n = 0, 1, 2, \dots \ , \tag{1.12}$$

$$\pi_{-1}(d\mu; x) := 0, \tag{1.13}$$

where

$$\alpha_n = \alpha_n(d\mu) = \frac{\langle x\pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}}{\langle \pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}} \quad n = 0, 1, 2, \dots , \tag{1.14}$$

$$\beta_n = \beta_n(d\mu) = \frac{\langle \pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}}{\langle \pi_{n-1}(d\mu), \pi_{n-1}(d\mu) \rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots \ . \tag{1.15}$$

Proof. See [29]. □

We will define $\beta_0(d\mu)$ by

$$\beta_0(d\mu) = \langle \pi_0(d\mu), \pi_0(d\mu) \rangle_{\bar{\mu}}, \tag{1.16}$$

such that $\beta_0(d\mu) = C_0(d\mu)$. From Eqs. (1.14) and (1.15) one can easily show that if the measure $d\mu$ has bounded support, then $a < \alpha_n(d\mu) < b, \quad n = 0, 1, 2, \dots$, and $0 < \beta_n(d\mu) \leq \max(a^2, b^2), \quad n = 1, 2, 3, \dots$. A proof can be found in [29].

Theorem 4. *The orthonormal polynomials $P_n(d\mu; x)$ satisfy the three term recurrence relation*

$$t_n P_{n+1}(d\mu; x) = (x - s_n)P_n(d\mu; x) - t_{n-1}P_{n-1}(d\mu; x), \quad n = 0, 1, 2, \dots , \tag{1.17}$$

$$P_{-1}(d\mu; x) := 0, \qquad P_0(d\mu; x) = 1/\sqrt{\beta_0(d\mu)}, \tag{1.18}$$

where

$$s_n = s_n(d\mu) \;=\; \alpha_n(d\mu) \quad n = 0, 1, 2, \dots , \tag{1.19}$$

$$t_n = t_n(d\mu) \;=\; \sqrt{\beta_{n+1}(d\mu)} \quad n = 0, 1, 2, \dots . \tag{1.20}$$

Proof. See [29]. □

Definition 5. *We will call $Q_n(d\mu; x)$ the* secondary polynomial[1] *associated with polynomial $P_n(d\mu; x)$ defined by*

$$Q_n(d\mu; x) = \int_a^b \frac{P_n(d\mu; t) - P_n(d\mu; x)}{t - x} d\mu(t), \quad n = 0, 1, 2, \dots . \tag{1.21}$$

We note that since $t^q - x^q = (t-x)\sum_{p=0}^{p=q-1} t^p x^{q-1-p} \quad q = 1, 2, 3, \dots$ for real x, t and $C_0(d\mu) > 0$, we have that $Q_n(d\mu; x)$, $n = 1, 2, 3, \dots$ are real polynomials of degree $n - 1$ and $Q_0 = 0$.

Definition 6. *The* Stieltjes Transformation *of the gapless measure $d\mu(x) = \bar{\mu}(x)dx$ is defined by*[36]

$$S_{\bar{\mu}}(z) = \int_a^b \frac{d\mu(x)}{z - x}, \tag{1.22}$$

where $z \in \mathbb{C} - [a, b]$.

This is a function vanishing at infinity and analytic in the whole complex plane with the interval $[a, b]$ removed. (If $-a = b = +\infty$, then $S_{\bar{\mu}}$ is analytic separately in Im $z > 0$ and Im $z < 0$, the two branches being different in general.) If the measure is gapped, then the stieltjes transformation would have a zero in the interval $[a, b]$ (see appendix (E) for a proof), and then the L.H.S. of Eq. (1.23) below becomes incorrectly defined.

[1] also known as *polynomial of the second kind.*

Theorem 7. *If a gapless measure $d\rho(x) = \bar{\rho}(x)dx$ has Stieltjes transformation given by*

$$S_{\bar{\rho}}(z) = z - C_1(d\mu) - \frac{1}{S_{\bar{\mu}}(z)}, \tag{1.23}$$

with $C_0(d\mu) = 1$, then the secondary polynomials $\{Q_n(d\mu; x)\}_{n=1}^{\infty}$ form an orthogonal family for the induced inner product of $d\rho(x)$ and $d\mu(x)$ is also gapless.

Proof. See [37], or [38] for a direct proof. □

For two gapless measures $d\rho(x)$ and $d\mu(x)$ satisfying Eq. (1.23), $d\rho(x)$ is known as the secondary measure associated with $d\mu(x)$. In section 2.1.1, we will iterate this process to define a sequence of measures. With this we conclude our review of the basic properties of orthogonal polynomials. These results suffice to derive the chain mapping theorems which we will do next.

1.4 Chain Mappings

Now that we have developed the necessary mathematical tools in section 2.1, we will develop the physical theories of this chapter. These are the following theorems and corollaries. Theorem 9 is the formal theorem which shows how open quantum systems can be mapped onto chain representations and corollaries 10 and 12 give two particular examples of increased interest.

For later purposes, we will make the definitions $\omega_{min} := \inf g$, $\omega_{max} := \sup g$. In what follows, we will assume that $\mathbb{R} \ni x \to g(x)$ monotone and differentiable. Since the standard form (see definition 1) satisfies these requirements, we can assume this w.l.o.g.

We start this section with the following preliminary lemma.

Lemma 8. *Given a measure $d\mu(x)$ with $I = [G_q(\omega_{min}), G_q(\omega_{max})]$ and its corresponding monic orthogonal polynomials $\{\pi_n(d\mu; x)\}_{n=0}^{n=\infty}$, the following holds. One can construct the set of functions $\{\underline{\pi}_n(\underline{d\mu}; x)\}_{n=0}^{n=\infty}$,*

$$\underline{\pi}_n(\underline{d\mu}; x) := \pi_n\big(d\mu; G_q(g(x))\big), \quad n = 0, 1, 2, \dots, \tag{1.24}$$

where

$$G_q(x) := \frac{-q(1+q^2) + 2\sqrt{q^4 + 4(1-q^2)x^2}}{4(1-q^2)} \quad x \geq 0,\ q \in [0, 1] \tag{1.25}$$

which satisfy the 3-term recurrence relation

$$\underline{\pi}_{n+1}(\underline{d\mu};x) \;= (G_q(g(x)) - \alpha_n(d\mu))\,\underline{\pi}_n(\underline{d\mu};x) - \beta_n(d\mu)\underline{\pi}_{n-1}(\underline{d\mu};x), \tag{1.26}$$

$$\underline{\pi}_{-1}(\underline{d\mu};x) := 0 \quad n = 0,1,2,\ldots \tag{1.27}$$

and are orthogonal with respect to the measure $d\underline{\mu}(x)$

$$\int_{k_{min}}^{k_{max}} \underline{\pi}_n(\underline{d\mu};x)\underline{\pi}_m(\underline{d\mu};x)\underline{\bar{\mu}}(x)dx = \langle \pi_n(d\mu), \pi_n(d\mu)\rangle_{\bar{\mu}}\delta_{nm} \quad n,m = 0,1,2,\ldots, \tag{1.28}$$

where $\underline{d\mu}(x) =: \underline{\bar{\mu}}(x)dx$*, with*

$$\underline{\bar{\mu}}(x) = \bar{\mu}\left(G_q(g(x))\right)\left|\frac{dG_q(g(x))}{dx}\right|, \tag{1.29}$$

with $I = [k_{min}, k_{max}]$*. Furthermore, the converse is true: given the set of functions* $\{\underline{\pi}_n(\underline{d\mu};x)\}_{n=0}^{\infty}$ *defined in terms of a set of monic polynomials* $\{\pi_n(x)\}_{n=0}^{\infty}$ *which satisfy Eqs. (1.26) and (1.28) for a weight function* $\underline{\bar{\mu}}$ *defined in terms of a weight function* $\bar{\mu}$ *with* $I = [G_q(\omega_{min}), G_q(\omega_{max})]$*, then the set* $\{\pi_n(x)\}_{n=0}^{\infty}$ *are the corresponding monic orthogonal polynomials for the weight function* $\bar{\mu}$*.*

Proof. Eqs. (1.28) and (1.29) follow from perfoming a change of variable in $\langle \pi_n(d\mu), \pi_m(d\mu)\rangle_{\bar{\mu}} = \langle \pi_n(d\mu), \pi_n(d\mu)\rangle_{\bar{\mu}}\delta_{nm}$ and noting that $dG_q(g(x))/dx \geq 0$ if g is non-decreasing and $dG_q(g(x))/dx \leq 0$ if g is non-increasing. Eq. (1.26) follows from a change of variable in Eq. (1.12). The fact that the converse is true follows from the fact that G_q and g have well-defined inverse functions. □

Before we state our first main theorem, we briefly introduce the boson number operator $\mathfrak{n}$ as the second quantization of the identity operator on the one particle space $\mathfrak{n} := d\hat{\Gamma}(\mathbb{I}_{\mathfrak{h}})$. We will use this to define the domain of some new operators in the following.

Theorem 9. *Hamiltonians Eq. (1.1), with a spectral density* J *with finite moments, are equivalent to semi-infinite chains with only nearest-neighbors interactions, where the system only couples to the first site in the chain. More specifically, there exists, for every* $q \in [0,1]$*, a countably infinite set of new creation* $b_n^*(q)$ *and annihilation* $b_n(q)$ *operators*

$$b_n^*(q) = \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^q;x)\left[\cosh r_q\big(g(x)\big)a_x^* - \sinh r_q\big(g(x)\big)a_x\right], \tag{1.30}$$

$$b_n(q) = \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^q;x)\left[\cosh r_q\big(g(x)\big)a_x - \sinh r_q\big(g(x)\big)a_x^*\right], \tag{1.31}$$

$n = 0, 1, 2, \dots$, *well-defined on* $\mathcal{D}(\mathfrak{n}^{1/2})$ *which satisfy the commutation relations*

$$[b_n(q), b_m^*(q)] = \delta_{nm} \quad n, m = 0, 1, 2, \dots , \tag{1.32}$$

with transformed Hamiltonian

$$:\hat{H}: = \hat{H}_S \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \mathbb{I}_{\mathcal{S}} \otimes \hat{H}_{E,q} + \hat{H}_{int,q} \,, \tag{1.33}$$

$$\hat{H}_{E,q} = \sum_{n=0}^{\infty} \Big\{ E_{1n}(q)(b_n^*(q)b_n^*(q) + b_n(q)b_n(q)) + E_{2n}(q)b_n^*(q)b_n(q) \tag{1.34}$$

$$+ E_{3n}(q)(b_n^*(q)b_{n+1}^*(q) + b_n(q)b_{n+1}(q)) \tag{1.35}$$

$$+ E_{4n}(q)(b_n^*(q)b_{n+1}(q) + b_n(q)b_{n+1}^*(q)) \Big\}, \tag{1.36}$$

$$\hat{H}_{int,q} = E_5(q)\hat{A}_s \otimes (b_0^*(q) + b_0(q)). \tag{1.37}$$

where $E_{1n}(q)$, $E_{2n}(q)$, $E_{3n}(q)$, $E_{4n}(q)$, $E_5(q) \in \mathbb{R}$ *and* $q \in [0, 1]$ *is a free parameter of the mapping which determines the particular version.* $:\hat{H}:$ *is to indicate that the Hamiltonian* $\hat{H}$ *has been renormalized*[2]*. The constants* $E_{1n}(q)$, $E_{2n}(q)$, $E_{3n}(q)$, $E_{4n}(q)$, $E_5(q)$ *are determined when a particular spectral density* $J(x)$ *and value of* q *are specified. Expressions for the functions* $U(d\lambda^q; x)$ *and* $r_q(x)$ *are derived in the proof.* For a pictorial representation of this theorem, see figure (1.1).

Proof. The proof is by construction. Let us start by defining a local transformation of the creation and annihilation operators a_x^* and a_x into another set, c_x and c_x^*, which preserves the commutation relations. We can do this via a so called *Bogoliubov transformation*[43]

$$a_x = \cosh\big[r_q\big(g(x)\big)\big]c_x + \sinh\big[r_q\big(g(x)\big)\big]c_x^*, \tag{1.38}$$

$$a_x^* = \cosh\big[r_q\big(g(x)\big)\big]c_x^* + \sinh\big[r_q\big(g(x)\big)\big]c_x, \tag{1.39}$$

where $r_q(x) \in \mathbb{R}$ and $[a_x, a_y^*] = [c_x, c_y^*] = \delta(x - y)$. Notice how we have parametrised the argument of the cosh and sinh functions in terms of $r_q(g(x))$. As we will see later, there are a familiy of functions $r_q(x)$ for which it is usefull to perform this tranformation. The q is to denote which particular function is being used and will become clear soon. [3] If we now parameterise $r_q(x)$ by

[2]Specifically, a constant factor $C\mathbb{I}_{\mathcal{S}} \otimes \mathbb{I}_{\Gamma}(\mathfrak{h})$, $C \in \mathbb{R}$ has been neglected.

[3]We can replace the *cosh* and *sinh* functions with *cos* and *sin* functions for fermions. By doing so, we could work out a different version of this theorem which would be valid for the case where the initial bosonic creation-anhilation operators $\{a_x, a_x^*\}$ $x \in [k_{min}, k_{max}]$ where fermionic instead

introducing a new function $\xi_q(x)$ through $r_q(x) = \ln \xi_q(x)$ where $\xi_q(x) \in [0, +\infty)$ using Eq. (1.38) and (1.39) we find after renormalising

$$:\int_{k_{min}}^{k_{max}} dx\, g(x) a_x^* a_x: \;=\; \int_{k_{min}}^{k_{max}} dx \frac{g(x)}{4\xi_q^2(g(x))}\Big((\xi_q^4(g(x))-1)(c_x^* c_x^* + c_x c_x) + 2(\xi_q^4(g(x))+1)c_x^* c_x\Big). \tag{1.40}$$

System-environment term simplifies to

$$\hat{A}_s \otimes \int_{k_{min}}^{k_{max}} dx h(x)(a_x + a_x^*) = \hat{A}_s \otimes \int_{k_{min}}^{k_{max}} dx\, h(x)\xi_q(g(x))(c_x^* + c_x). \tag{1.41}$$

For appropriate choice of the function $\xi_q(x)$, we can define a measure

$$d\underline{\lambda}^q(x) \;=\; \underline{M}^q(x)dx, \tag{1.42}$$

$$\underline{M}^q(x) \;=\; h^2(x)\xi_q^2(g(x)). \tag{1.43}$$

With the set of monic polynomials $\{\pi_n(d\lambda^q; x)\}_{n=0}^{\infty}$ with measure $d\lambda^q(x)$, we are able to construct the set $\{\underline{\pi}_n(d\underline{\lambda}^q; x)\}_{n=0}^{\infty}$ of orthogonal functions with respect to measure $d\underline{\lambda}^q(x)$ defined in Lemma 8. We can use these to define the set of functions $\{U_n(d\lambda^q; x)\}_{n=0}^{\infty}$ through the relation

$$U_n(d\lambda^q; x) = \frac{\underline{\pi}_n(d\underline{\lambda}^q; x)\sqrt{\underline{M}^q(x)}}{\sqrt{\langle \underline{\pi}_n(d\underline{\lambda}^q), \underline{\pi}_n(d\underline{\lambda}^q)\rangle_{\underline{M}^q}}} = \frac{\underline{\pi}_n(d\underline{\lambda}^q; x)h(x)\xi_q(g(x))}{\sqrt{\langle \underline{\pi}_n(d\underline{\lambda}^q), \underline{\pi}_n(d\underline{\lambda}^q)\rangle_{\underline{M}^q}}}. \tag{1.44}$$

We can now define the set of creation and annihilation operators of the chain (we will specify their domain and show that they are well-defined later in the proof)

$$b_n^*(q) \;=\; \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^q; x) c_x^*(q), \tag{1.45}$$

$$b_n(q) \;=\; \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^q; x) c_x(q). \tag{1.46}$$

Substituting the inverse relations

$$c_x^*(q) \;=\; \sum_{n=0}^{\infty} U_n(d\lambda^q; x) b_n^*(q), \tag{1.47}$$

$$c_x(q) \;=\; \sum_{n=0}^{\infty} U_n(d\lambda^q; x) b_n(q), \tag{1.48}$$

into Eq. (1.41) we obtain

$$\hat{A}_s \otimes \int_{k_{min}}^{k_{max}} dx h(x)(a_x + a_x^*) = \sqrt{\beta_0(d\lambda^q)}\, \hat{A}_s \otimes (b_0^*(q) + b_0(q)). \tag{1.49}$$

So we note that for all functions $\xi_q(x)$ that result in a valid measure Eq. (1.42), one can achieve a coupling between system and reservoir which only interacts with the first element in the chain.

Now we will examine carefully what type of chain can be generated via this transformation.

Using the orthogonality conditions of the orthogonal polynomials and Eq. (1.47) and (1.48), we can transform terms of the form $\int_{k_{min}}^{k_{max}} c_{ax}c_{bx}dx$ into terms of the form $\sum_{n=0}^{\infty} W_n b_{an}b_{bn}$ where the W_n's are constants and the sub indices $a, b = 0$ denote that the operator is an annihilation operator and $a, b = 1$ denote that they are creation operators. Also, we can transform terms of the form $\int_{k_{min}}^{k_{max}} G_q(g(x))c_{ax}c_{bx}dx$ into $\sum_{n=0}^{\infty} W_n b_{an}b_{bn} + W_1 b_{a(n+1)}b_{bn} + W_{2n}b_{an}b_{b(n+1)}$ by using the three term recurrence relations Eq. (1.26) to eliminate the $G_q(g(x))$. We can also map terms of the form $\int_{k_{min}}^{k_{max}} (G_q(g(x)))^k c_{ax}c_{bx}dx \quad k = 2, 3, 4...$ using the three term recurrence relations in Eq. (1.26) k times, but this would result in every chain site coupling to its kth nearest neighbours. Given this resoning, we propose a trial solution to Eq. (1.40) which will reduce it to a chain of nearest neighbour interactions. This is:

$$\frac{g(x)}{4\xi_q^2(g(x))}(\xi_q^4(g(x)) - 1) = c_1 + g_1 G_q(g(x)), \tag{1.50}$$

$$\frac{g(x)}{2\xi_q^2(g(x))}(\xi_q^4(g(x)) + 1) = c_2 + g_2 G_q(g(x)). \tag{1.51}$$

Not all values of the real constants c_1, c_2, g_1, g_2 will result in a valid trial solution. We will parametrise a valid set of these constants in terms of q and hence there will be a different valid solution for the functions ξ_q and G_q for different values of q. This is where the q dependency enters in the proof. A valid and usefull parametrisation is $2g_1 = q, g_2 = 1, 8c_1 = -q^2, 4c_2 = q$, $q \in [0, 1]$. Solving Eqs. (1.50) and (1.51) for G_q and ξ_q for this parametrisation of the constants gives us

$$G_q(x) = \frac{-q(1+q^2) + 2\sqrt{q^4 + 4(1-q^2)x^2}}{4(1-q^2)} \quad x \geq 0, \tag{1.52}$$

$$\xi_q(x) = \left[\frac{q(1-q) + (1+q)4G_q(x)}{q(1+q) + (1-q)4G_q(x)}\right]^{1/4} \quad x \geq 0. \tag{1.53}$$

Now that we have explicit expresions for G_q and ξ_q, we will derive an expression for the measure $d\lambda^q(x) = M^q(x)dx$ from $d\underline{\lambda}^q = \underline{M}^q(x)dx$. From Eqs (1.43), (1.42) and (1.29), we have

$$h^2(x)\xi^2(g(x)) = \underline{M}^q(x) = M^q\big(G_q(g(x))\big)\left|\frac{dG_q(g(x))}{dx}\right|. \tag{1.54}$$

Solving this for M^q using Eqs (1.52) ,(1.53), (1.7), we find

$$M^q(x) = \frac{J\big(G_q^{-1}(x)\big)}{\pi} \frac{(1+q^2)q + 4(1-q^2)x}{(1+q)q + 4(1-q)x}, \tag{1.55}$$

where $G_q(G_q^{-1}(x)) = G_q^{-1}(G_q(x)) = x$ and is given by

$$G_q^{-1}(x) = \frac{1}{4}\sqrt{[q(1-q)+4(1+q)x][q(1+q)+4(1-q)x]} \quad x \geq \frac{-q(1-q)}{4(1+q)}, \tag{1.56}$$

and we recall from Lemma 8, that the interval I for $d\lambda^q = M^q(x)$ is $I = [G_q(\omega_{min}), G_q(\omega_{max})]$. Noting that M^q has finite moments on I since J does on $[\omega_{min}, \omega_{max}]$ and Eqs. (1.45), (1.46), (1.52), (1.53), we find that $U_n(d\lambda^q; x)\cosh r_q\big(g(x)\big)$, $U_n(d\lambda^q; x)\sinh r_q\big(g(x)\big) \in L^2([k_{min}, k_{max}])$, and hence $b_n^*(q)$ and $b_n(q)$ are well-defined operators on $\mathcal{D}(\mathfrak{n}^{1/2})$. Furthermore we can verify that they satisfy

$$(\Psi_1, b_n(q)\Psi_2) = (b_n^*(q)\Psi_1, \Psi_2)\,, \tag{1.57}$$

for all $\Psi_1, \Psi_2 \in \mathcal{D}(\mathfrak{n}^{1/2})$ hence confirming that $b_n^*(q)$ is the adjoint of $b_n(q)$. The commutation relation $[b_n(q), b_m^*(q)] = \delta_{n,m}$ follows from the orthogonality conditions for the monic polynomials and the commutator relation $[a_k, a_{k'}^*] = \delta(k-k')$. Now let us perform the trasnformation. After substituting Eqs. (1.47) and (1.48) into Eq. (1.40) and using the orthogonality conditions and 3-term recurrence relations of Lemma 8, we find

$$:\int_{k_{min}}^{k_{max}} dx\, g(x) a_x^* a_x : \tag{1.58}$$

$$= \sum_{n=0}^{\infty} \Big\{ \left(\frac{q}{2}\alpha_n(q) - \frac{q^2}{8}\right)\left(b_n^*(q)b_n^*(q) + b_n(q)b_n(q)\right) + \left(\alpha_n(q) + \frac{q}{4}\right) b_n^*(q)b_n(q) \tag{1.59}$$

$$+ \sqrt{\beta_{n+1}(q)}\left(q(b_n^*(q)b_{n+1}^*(q) + b_n(q)b_{n+1}(q)) + (b_n^*(q)b_{n+1}(q) + b_n(q)b_{n+1}^*(q))\right)\Big\},$$

where $\alpha(q) := \alpha(d\lambda^q)$, $\beta(q) := \beta(d\lambda^q)$. □

This theorem should be considered in many regards as the most crucial result of the whole thesis since all other results can be understood, in one form or another, as giving more in-depth insight into the consequences and properties of this chain mapping theorem. We should therefore pause for a moment to examine what we have achieved. Initially the system operator $\hat{A}_S$ coupled the system to every single mode of the environment. This is to say, there was no locality in

the coupling structure between the system and the bath, -the system was coupled to everything-. However, we have a very different story to tell after unravelling the chain through the chain mapping: now there is a lot of locality in the coupling structure. The system, via operator $\hat{A}_S$ is now only coupled with one mode of the environment, which in turn, is only coupled to one other mode of the environment, and so on and so on. This introduction of locality allows us to form the notion of interactions within the environment and with the system happening at a specific location and time. This is a useful picture to keep in mind when considering the rest of the physical results of this thesis. We should also note the relevance of the constraint that all moments of the spectral density be finite. This is a sufficient but not necessary condition for the Hamiltonian to be well defined (i.e. that $||\hat{G}^{-1/2}h|| < \infty$. See section 1.1). This constraint can be interpreted as telling us that we cannot map baths with frequencies which are too high. Alternatively, we can view it as saying we need to imply an ultra violet cut-off; something which arises very often in field theories. We will see later how this cut off will arise naturally as a very important parameter when developing locality bounds in chapter 3 and that even the way the cut off is implemented will play a role in chapter 2.

It might at this stage seem confusing to the reader why this result is referred to as *chain mapping* rather than, say, *chain representation*. This we be explained after the following corollary in the next section.

1.4.1 Special Cases

Corollary 10. *The generalised mapping* Eq. (1.33) *reduces to*

$$\hat{H} = \hat{H}_S \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \sqrt{\beta_0(0)}\hat{A}_s \otimes (b_0(0) + b_0^*(0)) \tag{1.60}$$

$$+ \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=0}^{\infty} \alpha_n(0) b_n^*(0) b_n(0) + \sqrt{\beta_{n+1}(0)}(b_{n+1}^*(0) b_n(0) + h.c.) \tag{1.61}$$

when $q = 0$. *We also find*

$$M^0(x) = \frac{J(x)}{\pi}, \quad \textit{with } I = [\omega_{min}, \omega_{max}] \tag{1.62}$$

and

$$G_0(x) = x, \tag{1.63}$$

$$b_n^*(0) = \int_{k_{min}}^{k_{max}} \frac{dx\, \pi_n(d\lambda^0; g(x))}{\sqrt{\langle \pi_n(d\lambda^0), \pi_n(d\lambda^0)\rangle_{M^0}}} \sqrt{\frac{J(g(x))}{\pi} \left|\frac{dg(x)}{dx}\right|} a_x^*, \quad n = 0, 1, 2, \ldots . \tag{1.64}$$

Proof. Follows from setting $q = 0$ in theorem 9 and simplifying the resultant expressions. □

Given that the coupling of the chain elements is excitation number preserving, the elementary excitations of the chain can be viwed as particles hopping on a 1d lattice. We therefore make the following definition.

Definition 11. *We shall refer to the transformation described in corollary* 10 *as the* particle mapping.

In the chain mapping of [20, 19], one had to first map $g(x) \mapsto x$ while maintaining J invariant through an appropriate mapping of h. The consequence of this was that the final Hamiltonian (the chain Hamiltonian) was not equal to the original Hamiltonian. Since from the definition of the α_n and β_n coefficients, we see that they only depend on J, this subtlety is only important in the relationship between the creation and annihilation operators $\{a_x, a_x^*\}$ and $\{b_n(0), b_n^*(0)\}_{n=0}^{\infty}$. This will, however, have consequences for writing the initial state of the Hamiltonian in the Fock basis of $b_n(0), b_n^*(0)$ operators. See (B) in the appendix. It is for this historical fact that we refer to the process described in theorem 9 as chain mapping.

Corollary 12. *When $q = 1$, the generalised mapping* Eq. (1.33) *reduces to*

$$:\hat{H}: = \hat{H}_S \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \sqrt{\beta_0(1)}\hat{A}_s \otimes X_0 + \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=0}^{\infty} \left(\sqrt{\beta_{n+1}(1)} X_n X_{n+1} + \frac{\alpha_n(1)}{2} X_n^2 + \frac{1}{2} P_n^2 \right). \tag{1.65}$$

where X_n and P_n are position and momentum operators, $X_n := (b_n^*(1) + b_n(1))$, $P_n := i(b_n^*(1) - b_n(1))/2$, on $\mathcal{D}(\mathfrak{n}^{1/2})$, $n = 0, 1, 2, \ldots$. We also find

$$M^1(x) = \frac{J(\sqrt{x})}{\pi}, \quad \textit{with } I = [\omega_{min}^2, \omega_{max}^2] \tag{1.66}$$

and

$$G_1(x) = x^2, \tag{1.67}$$

$$b_n^*(1) = \int_{k_{min}}^{k_{max}} \frac{dx\, \pi_n(d\lambda^1; g(x)^2)}{\sqrt{\langle \pi_n(d\lambda^1), \pi_n(d\lambda^1)\rangle_{M^1}}} \sqrt{\frac{J(x)}{\pi} \left|\frac{dg(x)}{dx}\right|} \Big(\frac{2g(x)+1}{2} a_x^* - \frac{2g(x)-1}{2} a_x \Big).$$

Proof. Follows from setting $q = 1$ in theorem 9 and simplifying the resultant expressions. □

Given that the coupling of the chain elements in Eq. (1.65) resemble that of springs obeying hooks law, the elementary excitations are phonons such as in solid state physics. We therefore make the following definition.

Definition 13. *We shall refer to the transformation described in corollary* 12 *as the* phonon mapping.

In light of definitions 11 and 13, we note that Eq. (1.33) interpolates between the two solutions.

1.5 Chapter Summary and Conclusion

In chapter 1 we have establish a general formalism for mapping an open quantum system of a specialized Pauli-Fierz Hamiltonian Eq. (1.1) onto chain representations using the theory of orthogonal polynomials. By chain representation we mean semi-infinite harmonic lattices with nearest neighbour coupling. The different versions of chain mappings were generated by choosing particular values of 4 real constants which we parameterised by one real variable q. The different versions differed in the form of the coupling between the oscillators. We defined two special cases and called them particle and phonon mapping due the physically simple form the coupling between the harmonic oscillators has. Thought the rest of this thesis, we will repeatedly mention these two special forms and gain a deeper understanding into their similarities and differences.

Chapter 2

Secondary Measures and Markovian Embeddings

In the chain mappings presented in the previous chapter, there is a natural and systematic way to "embed" degrees of freedom of the environment into the system (by "embed", we mean to redefine what we call system and environment by including some of the environmental degrees of freedom in the system. This is defined rigorously later in definition 38) See figure (1.1). One can make a non-Markovian system-environment interaction more Markovian by embedding some degrees of freedom of the environment into the system, a technique already employed in certain situations in quantum optics [26] and that recently has been demonstrated in [23]. What remains unclear however, is to quantify how efficient such procedures can be as well as determining the best way of performing the embedding. We will show that those issues can be understood and addressed much better with the formalism presented in this section.

Thus the second aim is to develop a method for understanding how Markovian such embeddings are by finding explicit analytical formulas for the spectral densities of the embeddings corresponding to the different chain mappings. Furthermore, we also derive universal convergence theorems for the spectral densities corresponding to the embedded systems and give rigourous conditions for when these limiting cases are achieved. This paves the way for a system interacting with a complex environment to be recast by moving the boundary of the system and environment, so that the non-trivial parts of the environment are embedded in the new effective "system" and the homogeneous chain represents the new, and much simpler, "environment". The advantage of this is that the

residual part of the environment might be simple enough for some of the approximations mentioned in section 0.1 to be applied, enabling us to integrate out these modes and dramatically reduce the number of sites of the chain that have to be accounted for explicitly. In order to achieve this, we have to first develop new mathematical tools and theorems regarding secondary measures and Jacobi operators, greatly extending and developing the application of orthogonal polynomials that was used for theorem 9. These results could be useful also in other areas of mathematics and mathematical physics which are related to the theory of Jacobi operators such as the Toda lattice [27].

For the first known result [20, 19] (c.f. corollary 10), the general method developed in this thesis gives analytical and non-iterative expressions for the spectral densities corresponding to the embeddings. For the other special case [23] (c.f. corollary 12), we derive calculable conditions for when the spectral densities corresponding to the embedding converge, -an aspect not addressed in [23]. As seen in the examples, we apply this technique to derive exact solutions for the family of spin-boson models which will allow us to illustrate how the different embedding methods are related.

The contents of each section is as follows: In section 2.1.1 we focus on deriving a formula which makes explicit a sequence of secondary measures solely in terms of the initial measure and its orthogonal polynomials. One should point out that although authors such as Gautschi introduce the concept and definition of secondary measures, here an analytical closed expression for them in terms of the initial measure and its orthogonal polynomials is provided. This result will turn out to be a vital ingredient in the development of the subsequent sections. Moreover, Gautschi states that the general solution derived here is unknown [29] p16-17. In section 2.1.2 the properties of the 3-term recursion coefficients of the orthogonal polynomials generated from their measures are studied. Then beta normalised measures which have more general and useful properties are defined. The main result of this section is the new theorem regarding the Jacobi matrix. This new theorem will be used extensively in section 2.2. Section 2.2 is concerned with embeddings of environmental degrees of freedom into the system. Here we also discuss how this interpretation allows one to view the chain mapping as a generalisation of the work of [35]. In section 2.2.1, the relation between this work and work by [23] is investigated. In order to do this we make

extensive use of the relations developed in section 2.1. It is shown how their mapping is a special case of the work presented here and find analytical non iterative solutions to quantities such as the sequence of residual spectral densities. In section 2.2.2 we develop convergence theorems for the sequence of residual spectral densities. We show rigorously that the sequence converges under certain conditions and give the universal functions the spectral densities converge to for the particle and phonon cases. The conditions for which the sequences converge are stated in terms of the initial spectral density. In section 2.3 we give explicit analytic examples for the family of spectral densities of the spin-boson model for the particle and phonon mapping cases.

The main results of this chapter are theorems 28, 36, 42, 41, 50 and corollaries 44, 45, 48.

2.1 Secondary Measures

Before we proceed further with the development of our understanding of the chain mapping, in section 2, we require a more indepth study of some properties of the orthogonal polynomials P_n, and this will be done in the following section greatly extending upon section 1.3 with the main new result being an explicit formula for the sequence of so-called *secondary meausres* in theorem 28.

2.1.1 Derivation of the Sequence of Secondary Normalised Measures

Definition 14. *We call the sequence of gapless measures* $d\mu_0$, $d\mu_1$, $d\mu_2, \ldots$ *generated from a gapless measure* $d\mu_0$ *by*

$$S_{\bar{\rho}_{n+1}}(z) = z - C_1(d\mu_n) - \frac{1}{S_{\bar{\mu}_n}(z)} \quad n = 0, 1, 2, \ldots , \tag{2.1}$$

$$d\mu_n(x) = \bar{\mu}_n(x)dx \quad n = 0, 1, 2, \ldots , \tag{2.2}$$

$$\bar{\mu}_n(x) = \frac{\bar{\rho}_n(x)}{C_0(d\rho_n)} \quad n = 1, 2, 3, \ldots , \tag{2.3}$$

the sequence of normalised secondary measures*, where* $C_0(d\mu_0) = 1$.

This sequence of measures is a slight adaptation from a basic result in the theory of orthogonal polynomials. In the standard version, the sequence of measures are not normalised. The fact that these objects are actually positive and gapless measures, is a well known result of the basic theory. See [37] or [38].

Lemma 15.

$$C_n(d\rho_{m+1}) = C_{n+2}(d\mu_m) - C_1(d\mu_m)C_{n+1}(d\mu_m) - \sum_{s=0}^{n-1} C_s(d\rho_{m+1})C_{n-s}(d\mu_m) \tag{2.4}$$

$n, m = 0, 1, 2, \ldots$.

Proof. For simplifity we will prove Eq. (2.4) for $m = 0$ as the generalisation is trivial. By Taylor expanding $S_{\bar{\mu}_0}(z)$ and $S_{\bar{\rho}_1}(z)$ in $x = 1/z$ we find

$$S_{\bar{\mu}_0}(z) = \sum_{n=0}^{\infty} \frac{C_n(d\mu_0)}{z^{n+1}} \quad \text{as } z \to \infty, \tag{2.5}$$

$$S_{\bar{\rho}_1}(z) = \sum_{n=0}^{\infty} \frac{C_n(d\rho_1)}{z^{n+1}} \quad \text{as } z \to \infty. \tag{2.6}$$

From Eq. (1.23) we have

$$S_{\bar{\rho}_1}(z)S_{\bar{\mu}_0}(z) = (z - C_1(d\mu_0))\, S_{\bar{\rho}_1}(z) - 1. \tag{2.7}$$

Hence substituting Eq. (2.5) and (2.6) into Eq. (2.7) we find

$$\sum_{n,m=0}^{\infty} C_n(d\mu_0)C_m(d\rho_1)x^{n+m+2} = \left(\frac{1}{x} - C_1(d\mu_0)\right) \sum_{s=0}^{\infty} C_s(d\mu_0)x^{s+1} - 1. \tag{2.8}$$

By comparing terms of the same power in x and taking into account $C_0(d\mu_0) = 1$ we deduce

$$\sum_{n=0}^{m} C_n(d\mu_0)C_{m-n}(d\rho_1) = C_{m+2}(d\mu_0) - C_1(d\mu_0)C_{m+1}(d\mu_0) \quad m = 0, 1, 2, \ldots . \tag{2.9}$$

By a change of variable in Eq. (2.9) we finally arrive at Eq. (2.4). □

Lemma 16. *A sequence of normalised secondary measures $d\mu_0$, $d\mu_1$, $d\mu_2$,..., $d\mu_n$, can be written as a continued fraction of the form*

$$S_0(z) = \cfrac{1}{z - C_{1,0} - \cfrac{d_0}{z - C_{1,1} - \cfrac{d_1}{z - C_{1,2} - \cfrac{d_2}{z - \cdots \cfrac{\cdots}{z - C_{1,n-1} - \cfrac{d_{n-1}}{z - C_{1,n} - d_n S_{n+1}(z)}}}}}} \tag{2.10}$$

where we have introduced the shorthand notation $S_n(z) := S_{\bar{\mu}_n}(z)$, $C_{n,s} := C_n(d\mu_s)$, $n, s = 0, 1, 2, \ldots$; $d_n := C_{2,n} - C_{1,n}^2$, $n = 1, 2, 3, \ldots$, *and* $d_0 := 1$.

Proof. By evaluating Eq. (2.4) for $n = 0$, and taking into account the above definition of d_n we see that $d_n = C(d\rho_n)$, $n = 1, 2, 3, \ldots$. Using our new notation, Eq. (2.1) for the sequence of gapless measures reads

$$S_{n+1}(z) = \frac{1}{d_n}[z - C_{1,n} - \frac{1}{S_n(z)}], \quad n = 0, 1, 2, \ldots \ . \tag{2.11}$$

Solving this for $S_n(z)$ followed by repeated substitution gives us Eq. (2.10). □

Theorem 17. *The following relations hold for the continued fraction Eq.* (2.10)

$$S_0(z) = \frac{u_n(-d_n S_{n+1}(z)) + u_{n+1}}{v_n(-d_n S_{n+1}(z)) + v_{n+1}}, \quad n = 0, 1, 2, \ldots \ , \tag{2.12}$$

with relations

$$u_{n+1} = (z - C_{1,n})u_n - d_{n-1}u_{n-1}, \quad v_{n+1} = (z - C_{1,n})v_n - d_{n-1}v_{n-1}, \tag{2.13}$$

and starting values

$$u_0 = 0, \quad u_1 = 1, \quad v_0 = 1, \quad v_1 = z - C_{0,1}. \tag{2.14}$$

Proof. These are elementary results from the theory of continued fractions (e.g. see section 4, connection with continued fractions [39]). □

Lemma 18.

$$\Delta_{n+1} := u_{n+1}v_n - v_{n+1}u_n = d_0 d_1 d_2 \ldots d_{n-1}, \quad n = 1, 2, 3, \ldots \ , \tag{2.15}$$

$$\Delta_1 = 1. \tag{2.16}$$

Proof. Using Eq. (2.13) to substitute for u_{n+1} and v_{n+1} into Eq. (2.15), we find the relation $\Delta_{n+1} = d_{n-1}\Delta_n$. Using Eq. (2.14) to verify Eq. (2.15) for the starting values, Eq. (2.15) follows by induction. □

Definition 19. *A* Padé Approximant *for a function g of type q/p in the neighbourhood of* 0 *is a rational fraction*

$$F(z) = \frac{Q(z)}{P(z)}, \tag{2.17}$$

with degree of $Q \leq q$, degree of $P \leq p$ and $g(z) - \frac{Q(z)}{P(z)}$ of order $\mathcal{O}(z^{p+q+1})$ in the neighbourhood of 0.

For more details, see [39].

Theorem 20. *$F_n(z) = \frac{u_{n+1}(z)}{v_{n+1}(z)}$ is a Padé Approximant for $S_0(z)$ of type $n/(n+1)$, $\quad n = 0, 1, 2, \ldots$.*

Proof. Using theorem 17, we can write $S_0(z) - \frac{u_{n+1}(z)}{v_{n+1}(z)}$ as

$$S_0(z) - \frac{u_{n+1}(z)}{v_{n+1}(z)} = \frac{\Delta_{n+1} d_n S_{n+1}(z)}{v_{n+1}(z)(v_{n+1}(z) - d_n v_n(z) S_{n+1}(z))}, \quad n = 0, 1, 2, \ldots . \tag{2.18}$$

Through lemma 18 we see that Δ_{n+1} is independent of z. By Taylor expanding $S_{n+1}(z)$ defined in definition 6 about $x = 1/z$, and remembering that $C_0(d\mu_n) = 1 \quad n = 1, 2, 3 \ldots$, we find using Eq. (2.18) that

$$S_{n+1}(z) = \frac{1}{z} + \mathcal{O}(\frac{1}{z^2}) \quad \text{as } z \to \infty \quad n = 0, 1, 2, \ldots . \tag{2.19}$$

By induction, we see that v_{n+1} and u_{n+1}, $\quad n = 0, 1, 2, \ldots$ given by Eq. (2.13) and (2.14), are degree $n + 1$ and n polynomials in z respectively, both with leading coefficients equal to unity. Hence we conclude that

$$S_0(z) - \frac{u_{n+1}(z)}{v_{n+1}(z)} = \frac{\Delta_{n+1} d_n}{z^{2n+3}} = \frac{d_0 d_1 \ldots d_n}{z^{2n+3}} \quad \text{as } z \to \infty \quad n = 0, 1, 2, \ldots . \tag{2.20}$$

Thus by definition 19 we conclude the proof. □

Lemma 21. *$u_n(z) = \lambda_n Q_n(d\mu_0; z)$ and $v_n(z) = \lambda_n P_n(d\mu_0; z) \quad n = 0, 1, 2, \ldots$, with $\lambda_n = 1/a_n$ where a_n is defined in Eq.* (1.11)*.*

Proof. From section 5.3.: moment problems and orthogonal polynomials (p213-220) of [39], and theorem 20 it follows that

$$\frac{u_{n+1}(z)}{v_{n+1}(z)} = \frac{Q_{n+1}(d\mu_0; z)}{P_{n+1}(d\mu_0; z)} \quad n = 0, 1, 2, \ldots . \tag{2.21}$$

By observing the starting values, we also have that

$$\frac{u_0(z)}{v_0(z)} = \frac{Q_0(d\mu_0; z)}{P_0(d\mu_0; z)}. \tag{2.22}$$

Hence

$$u_n(z) = \lambda_n Q_n(d\mu_0; z) \quad \text{and} \quad v_n(z) = \lambda_n P_n(d\mu_0; z) \quad n = 0, 1, 2, \ldots . \tag{2.23}$$

Given that u_n and v_n have leading coefficients equal to 1, we must have $\lambda_n = 1/a_n \quad$ n=0,1,2,. . . .

□

Theorem 22. $d_n = a_n^2/a_{n+1}^2 = \beta_{n+1}(d\mu_0) \quad n = 0, 1, 2, \dots$.

Proof. Proceeding in the same way as in page (18) of [29], we have

$$S_0(z) - \frac{Q_n(d\mu_0; z)}{P_n(d\mu_0; z)} = \frac{\gamma_n}{z^{2n+1}} \qquad \text{as } z \to \infty \quad n = 0, 1, 2, \dots . \tag{2.24}$$

where

$$\gamma_n = \frac{1}{a_n} \int_a^b x^n P_n(d\mu_0; x) d\mu_0(x) = \frac{\gamma_0 a_0^2}{a_n^2} \frac{\langle P_n(d\mu_0), P_n(d\mu_0)\rangle_{\bar{\mu}}}{\langle P_0(d\mu_0), P_0(d\mu_0)\rangle_{\bar{\mu}}} \quad n = 0, 1, 2, \dots . \tag{2.25}$$

Noting that $P_0(d\mu_0; x)/a_0 = \pi_0(d\mu_0; x) = 1$ and that $C_0(d\mu_0) = 1$, Eq. (2.25) tells us $\gamma_0 = 1$. Comparing Eq. (2.24) with Eq. (2.20) and (2.21), we deduce that

$$d_0 d_1 \dots d_{n-1} = \frac{a_0^2}{a_n^2} \frac{\langle P_n(d\mu_0), P_n(d\mu_0)\rangle_{\bar{\mu}}}{\langle P_0(d\mu_0), P_0(d\mu_0)\rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots . \tag{2.26}$$

By induction it follows

$$d_n = \frac{a_n^2}{a_{n+1}^2} \frac{\langle P_{n+1}(d\mu_0), P_{n+1}(d\mu_0)\rangle_{\bar{\mu}}}{\langle P_n(d\mu_0), P_n(d\mu_0)\rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots . \tag{2.27}$$

Due to definition 1.10, we see that $\langle P_n(d\mu_0), P_n(d\mu_0)\rangle_{\bar{\mu}} = 1 \quad n = 0, 1, 2, \dots$, hence

$$d_n = \frac{a_n^2}{a_{n+1}^2} \quad n = 1, 2, 3, \dots . \tag{2.28}$$

From Eq. (1.11), we see that Eq. (2.27) can be written in the form

$$d_n = \frac{\langle \pi_{n+1}(d\mu_0), \pi_{n+1}(d\mu_0)\rangle_{\bar{\mu}}}{\langle \pi_n(d\mu_0), \pi_n(d\mu_0)\rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots . \tag{2.29}$$

Hence, from definition 1.15 we conclude,

$$d_n = \beta_{n+1}(d\mu_0) \quad n = 1, 2, 3, \dots . \tag{2.30}$$

For $n = 1$, Eq. (2.26) gives us

$$d_0 = \frac{\langle \pi_1(d\mu_0), \pi_1(d\mu_0)\rangle_{\bar{\mu}}}{\langle \pi_0(d\mu_0), \pi_0(d\mu_0)\rangle_{\bar{\mu}}} = \frac{a_0^2}{a_1^2} = \beta_1(d\mu_0). \tag{2.31}$$

□

Theorem 23. *Gapless measures $d\mu(x) = \bar{\mu}(x)dx$ can be calculated from their Stieltjes transform by*

$$\bar{\mu}(x) = \frac{1}{2\pi i} \lim_{\epsilon \to 0^+} \left[S_{\bar{\mu}}(x - i\epsilon) - S_{\bar{\mu}}(x + i\epsilon) \right]. \tag{2.32}$$

Proof. This result is known as the *Stieltjes-Perron inversion formula*. See [40] for more details or Example 2.50: Stieltjes-Perron inversion formula [29] for an application and more references. □

Definition 24. *We call $\varphi(d\mu; x)$ the* reducer *of gapless measure $d\mu(x)$. It is given by*

$$\varphi(d\mu; x) = \lim_{\epsilon \to 0^+} \left[S_{\bar{\mu}}(x - i\epsilon) + S_{\bar{\mu}}(x + i\epsilon) \right]. \tag{2.33}$$

See appendix C for methods for calculating the reducer. The reducer allows us to write an explicit expression for the secondary measure associated with $\bar{\mu}(x)$ as follows.

Theorem 25. *For a gapless measure $d\mu(x)$ with secondary measure $d\rho(x)$, we have*

$$\bar{\rho}(x) = \frac{\bar{\mu}(x)}{\frac{\varphi^2(d\mu;x)}{4} + \pi^2 \bar{\mu}^2(x)} \tag{2.34}$$

Proof. See [38]. □

We will define the functions $Z_n(x) \in \mathbb{C} \quad n = 0, 1, 2, \dots$ as

$$Z_n(x) = \frac{\varphi_n(x)}{2} + i\pi \bar{\mu}_n(x) \quad n = 0, 1, 2, \dots , \tag{2.35}$$

where $\varphi_n(x) := \varphi(d\mu_n; x)$. These will turn out to be useful quantities which we will investigate in the following lemma and theorem in preparation for the proof of theorem 28.

Lemma 26. *The following recursion relations hold for $Z_{n+1}(x)$*

$$Z_{n+1}(x) = \frac{1}{d_n}[x - C_{1,n} - \frac{1}{Z_n(x)}], \quad n = 0, 1, 2, \dots . \tag{2.36}$$

Proof. We start by finding a relation between the Stieltjes transformation of a gapless measure $d\mu(x)$, and the reducer of its associated secondary measure $d\rho(x)$: By definition, we have

$$\varphi(d\rho; x) = \lim_{\epsilon \to 0^+} \left[S_{\bar{\rho}}(x - i\epsilon) + S_{\bar{\rho}}(x + i\epsilon) \right]. \tag{2.37}$$

Using Eq. (1.23), we find

$$\varphi(d\rho; x) = 2\big[x - C_1(d\mu)\big] - \lim_{\epsilon \to 0^+} \frac{S_{\bar{\mu}}(x - i\epsilon) + S_{\bar{\mu}}(x + i\epsilon)}{S_{\bar{\mu}}(x - i\epsilon) S_{\bar{\mu}}(x + i\epsilon)}. \tag{2.38}$$

Now using theorem 23 and definition 24, we find that

$$\lim_{\epsilon \to 0^+} \frac{S_{\bar{\mu}}(x - i\epsilon) + S_{\bar{\mu}}(x + i\epsilon)}{S_{\bar{\mu}}(x - i\epsilon) S_{\bar{\mu}}(x + i\epsilon)} = \frac{\varphi(d\mu; x)}{\frac{\varphi^2(d\mu;x)}{4} + \pi^2 \bar{\mu}^2(x)}. \tag{2.39}$$

Hence from Eq. (2.38) we arrive at

$$\varphi(d\rho;x) = 2\big[x - C_1(d\mu)\big] - \frac{\varphi(d\mu;x)}{\frac{\varphi^2(d\mu;x)}{4} + \pi^2\bar{\mu}^2(x)}. \tag{2.40}$$

Using the definition of a sequence of normalised secondary measures, definition 14 and the definition of d_n in Lemma 16, from Eq. (2.40) we find

$$\varphi_{n+1}(x) = \frac{1}{d_n}\left[2\big[x - C_{1,n}\big] - \frac{\varphi_n(x)}{\frac{\varphi_n^2(x)}{4} + \pi^2\bar{\mu}_n^2(x)}\right], \quad n = 0,1,2,\dots\ . \tag{2.41}$$

Similarly, we can also write theorem 25 for our sequence of normalised secondary measures using definition 14 and d_n. We find

$$\bar{\mu}_{n+1}(x) = \frac{1}{d_n}\left[\frac{\bar{\mu}_n(x)}{\frac{\varphi_n^2(x)}{4} + \pi^2\bar{\mu}_n^2(x)}\right], \quad n = 0,1,2,\dots\ . \tag{2.42}$$

If we write Eq. (2.35) for $Z_{n+1}(x)$ and then substitute Eq. (2.41) and Eq. (2.42) into the RHS we arrive at Eq. (2.36). □

Theorem 27. *The following relations hold between $Z_0(x)$ and $Z_{n+1}(x)$*

$$Z_0(z) = \frac{u_n(-d_nZ_{n+1}(z)) + u_{n+1}}{v_n(-d_nZ_{n+1}(z)) + v_{n+1}}, \quad n = 0,1,2,\dots\ , \tag{2.43}$$

were $u_n(z) = \lambda_n Q_n(d\mu_0;z)$ and $v_n(z) = \lambda_n P_n(d\mu_0;z)$ $\quad n = 0,1,2,\dots$, with $\lambda_n = 1/a_n$, a_n defined in Eq. (1.11).

Proof. By comparing Eq. (2.36) with eq. (2.11), we note that $Z_n(x)$ satisfies the same recursion relation as $S_n(x)$. Hence theorem 2.12 readily applies to Eq. (2.36) if we exchange $S_{n+1}(x)$ with $Z_{n+1}(x)$ and $S_0(x)$ with $Z_0(x)$. The relations between u_n, v_n and Q_n, P_n are proven in lemma 21. □

We are now ready a main result (this was developed by Roland Groux):

Theorem 28. *A sequence of normalised secondary measures starting from $d\mu_0$: $d\mu_0$, $d\mu_1$, $d\mu_2$,..., $d\mu_m$,... can be generated from the first measure in the sequence $d\mu_0$ by the formula*

$$\bar{\mu}_n(x) = \frac{1}{t_{n-1}^2(d\mu_0)} \frac{\bar{\mu}_0(x)}{\left(P_{n-1}(d\mu_0;x)\frac{\varphi(d\mu_0;x)}{2} - Q_{n-1}(d\mu_0;x)\right)^2 + \pi^2\bar{\mu}_0^2(x)P_{n-1}^2(d\mu_0;x)} \tag{2.44}$$

$n = 1,2,3,\dots$,

where the t_n coefficients are defined in theorem 4.

Proof. After solving Eq. (2.43) for $Z_n(x)$, we find

$$Z_n(x) = \frac{a_{n-1}}{a_n d_{n-1}} \frac{Z_0(x)P_n(d\mu_0;x) - Q_n(d\mu_0;x)}{Z_0(x)P_{n-1}(d\mu_0;x) - Q_{n-1}(d\mu_0;x)} \quad n = 1, 2, 3, \ldots . \tag{2.45}$$

From theorem 22 we see that

$$a_{n-1}/a_n = \kappa_n \sqrt{d_{n-1}} \quad n = 1, 2, 3, \ldots , \tag{2.46}$$

where κ_n is the sign of a_{n-1}/a_n. After using this relation to simplify the $a_{n-1}/a_n d_{n-1}$ coefficient in Eq. (2.45) and substituting for $Z_0(x)$ using Eq. (2.35), we take real and imaginary parts to achieve

$$\bar{\mu}_n(x) = \frac{\kappa_n}{\sqrt{d_{n-1}}} \frac{\bar{\mu}_0(x)\left[P_{n-1}(d\mu_0;x)Q_n(d\mu_0;x) - P_n(d\mu_0;x)Q_{n-1}(d\mu_0;x)\right]}{\left(P_{n-1}(d\mu_0;x)\frac{\varphi(d\mu_0;x)}{2} - Q_{n-1}(d\mu_0;x)\right)^2 + \pi^2\bar{\mu}_0^2(x)P_{n-1}^2(d\mu_0;x)} \tag{2.47}$$

$n = 1, 2, 3, \ldots$. Using the identities from lemmas 18 and 21, we note that

$$P_n(d\mu_0;x)Q_{n+1}(d\mu_0;x) - P_{n+1}(d\mu_0;x)Q_n(d\mu_0;x) = d_0 d_1 \ldots d_{n-1}/\lambda_n\lambda_{n+1} \tag{2.48}$$

$n = 1, 2, 3, \ldots$. Using theorem 22 and lemma 21 to write the RHS in terms of the a_n's, we find

$$d_0 d_1 \ldots d_{n-1}/\lambda_n\lambda_{n+1} = a_0^2 a_{n+1}/a_n = a_0^2/\kappa_{n+1}\sqrt{d_n} \quad n = 0, 1, 2, \ldots , \tag{2.49}$$

where in the last line we have used Eq. (2.46). We now note that by Eq. (1.11), $P_0(d\mu_0;x) = a_0$. We also have by definition 1.10, that $\langle P_0(d\mu_0;x)\ , P_0(d\mu_0;x)\rangle_{\bar{\mu}_0} = 1$. Hence

$$1 = \langle P_0(d\mu_0;x), P_0(d\mu_0;x)\rangle_{\bar{\mu}_0} = a_0^2 C_0(d\mu_0) = a_0^2. \tag{2.50}$$

Hence from Eq. (2.48), (2.49), (2.50), we find that we can write Eq. (2.47) as

$$\bar{\mu}_n(x) = \frac{1}{d_{n-1}} \frac{\bar{\mu}_0(x)}{\left(P_{n-1}(d\mu_0;x)\frac{\varphi(d\mu_0;x)}{2} - Q_{n-1}(d\mu_0;x)\right)^2 + \pi^2\bar{\mu}_0^2(x)P_{n-1}^2(d\mu_0;x)} \tag{2.51}$$

$n = 1, 2, 3, \ldots$. Finally, with the relations from theorems 22 and 4 we find $d_{n-1} = t_{n-1}^2(d\mu_0)$ $n = 1, 2, 3, \ldots$. □

2.1.2 Derivation of the Jacobi Matrix Theorem

Lemma 29. *The $\alpha_n(d\mu)$ and $\beta_n(d\mu)$ coefficients defined in theorem 3 are invariant under a change of scale of the measure $d\mu(x)$, while the change in $\beta_0(d\mu)$ scales linearly:*

$$\alpha_n(Cd\mu) = \alpha_n(d\mu) \quad n = 0, 1, 2, \ldots \tag{2.52}$$

$$\beta_n(Cd\mu) = \beta_n(d\mu) \quad n = 1, 2, 3, \ldots \tag{2.53}$$

$$\beta_0(Cd\mu) = C\beta_0(d\mu) \tag{2.54}$$

where $C > 0$.

Proof. First we will show that $\pi_n(Cd\mu; x) = \pi_n(d\mu; x) \quad n = 0, 1, 2, \ldots$.
From Eq. (1.11), we have that

$$1 = \langle P_n(d\mu), P_n(d\mu)\rangle_{\bar{\mu}} \quad n = 0, 1, 2, \ldots . \tag{2.55}$$

By multiplying and dividing by C we find

$$1 = \langle \frac{P_n(d\mu)}{\sqrt{C}}, \frac{P_n(d\mu)}{\sqrt{C}}\rangle_{c\bar{\mu}} \quad n = 0, 1, 2, \ldots . \tag{2.56}$$

From Eq. (1.11), we conclude

$$P_n(Cd\mu; x) = \frac{P_n(d\mu; x)}{\sqrt{C}} \quad n = 0, 1, 2, \ldots . \tag{2.57}$$

By observing Eqs. (1.11), (2.57), we conclude

$$a_n(Cd\mu) = a_n(d\mu)/\sqrt{C} \quad n = 0, 1, 2, \ldots . \tag{2.58}$$

Hence, from Eqs. (2.57), (2.58), (1.11) it follows

$$\pi_n(Cd\mu; x) = P_n(Cd\mu; x)/a_n(Cd\mu) = P_n(d\mu; x)/a_n(d\mu) = \pi_n(d\mu; x) \tag{2.59}$$

$n = 0, 1, 2, \ldots$. Now we can see how the α_n and β_n coefficients change:
Using definition 3 and Eq. (2.59) we have

$$\alpha_n(Cd\mu) = \frac{\langle x\pi_n(Cd\mu), \pi_n(Cd\mu)\rangle_{c\bar{\mu}}}{\langle \pi_n(Cd\mu), \pi_n(Cd\mu)\rangle_{c\bar{\mu}}} \tag{2.60}$$

$$= \frac{\langle x\pi_n(d\mu), \pi_n(d\mu)\rangle_{\bar{\mu}}}{\langle \pi_n(d\mu), \pi_n(d\mu)\rangle_{\bar{\mu}}} \tag{2.61}$$

$$= \alpha_n(d\mu), \quad n = 0, 1, 2, \ldots . \tag{2.62}$$

Similarly, we find

$$\beta_n(Cd\mu) = \beta_n(d\mu), \quad n = 1, 2, 3, \dots . \tag{2.63}$$

In the case of β_0 we have

$$\beta_0(Cd\mu) = \langle \pi_0(Cd\mu), \pi_0(Cd\mu) \rangle_{c\bar{\mu}} = C\beta_0(d\mu). \tag{2.64}$$

□

Theorem 30. *If $d\rho(x)$ is the secondary measure associated with $d\mu(x)$, then*

$$\alpha_{n+1}(d\mu) = \alpha_n(d\rho) \quad n = 0, 1, 2, \dots \tag{2.65}$$

$$\beta_{n+1}(d\mu) = \beta_n(d\rho) \quad n = 1, 2, 3, \dots \tag{2.66}$$

Proof. See [29], theorem 1.36 (page 16). □

Lemma 31. *A sequence of normalised secondary measures $d\mu_0(x)$, $d\mu_1(x)$, $d\mu_2(x)$, ..., satisfy*

$$\alpha_{m+n}(d\mu_0) = \alpha_n(d\mu_m) \quad n, m = 0, 1, 2, \dots , \tag{2.67}$$

$$\beta_{m+n}(d\mu_0) = \beta_n(d\mu_m) \quad n = 1, 2, 3, \dots , \; m = 0, 1, 2, \dots . \tag{2.68}$$

Proof. Using lemma 29 and definition 14 we find

$$\alpha_n(d\rho_m) = \alpha_n(d\rho_m / C_0(d\rho_m)) = \alpha_n(d\mu_m) \quad n = 0, 1, 2, \dots , m = 1, 2, 3 \dots , \tag{2.69}$$

$$\beta_n(d\rho_m) = \beta_n(d\rho_m / C_0(d\rho_m)) = \beta_n(d\mu_m) \quad n = 1, 2, 3, \dots , m = 1, 2, 3 \dots . \tag{2.70}$$

Hence taking into account theorem 30 we find

$$\alpha_{n+1}(d\mu_p) = \alpha_n(d\mu_{p+1}) \quad n, p = 0, 1, 2, \dots , \tag{2.71}$$

$$\beta_{n+1}(d\mu_p) = \beta_n(d\mu_{p+1}) \quad n = 1, 2, 3, \dots , \; p = 0, 1, 2, \dots . \tag{2.72}$$

We will now proceed to prove Eq. (2.67) by construction: by evaluating Eq. (2.71), for (n, p) at $(s-1, m)$, $(s-2, m+1)$, $(s-3, m+2)$,...,$(0, m+s-1)$ for any $m \geq 0$, $s \geq 1$ we have the following sequence of equations

$$\alpha_s(d\mu_m) = \alpha_{s-1}(d\mu_{m+1}) \tag{2.73}$$

$$\alpha_{s-1}(d\mu_{m+1}) = \alpha_{s-2}(d\mu_{m+2}) \tag{2.74}$$

$$\alpha_{s-2}(d\mu_{m+2}) = \alpha_{s-3}(d\mu_{m+3}) \tag{2.75}$$

$$\vdots$$

$$\alpha_1(d\mu_{m+s-1}) = \alpha_0(d\mu_{m+s}). \tag{2.76}$$

Thus by repeated substitution we arrive at

$$\alpha_s(d\mu_m) = \alpha_0(d\mu_{m+s}), \quad m = 0, 1, 2, \dots, s = 1, 2, 3, \dots . \tag{2.77}$$

We note that this equation is also valid for $s = 0$. If we make the change of variable $s = p + n$, $m = 0$ in Eq. (2.77) followed by relabeling indices, we find

$$\alpha_{m+s}(d\mu_0) = \alpha_0(d\mu_{m+s}) \quad m, s = 0, 1, 2, \dots . \tag{2.78}$$

Hence from Eq. (2.77) and (2.78), we arrive at (2.67). Similarly, we prove Eq. (2.68). □

We are now ready to state our second main result. The following objects, as we will soon see, are closely related to the sequence of normalised secondary measures Eq. (2.44) but have more interesting properties which are needed for our purposes.

Definition 32. *We call the sequence of gapless measures $d\nu_0(x)$, $d\nu_1(x)$, $d\nu_2(x)$, $d\nu_3(x)$, ...* beta normalised measures*, where $d\nu_0(x)$ defines the sequence*

$$\bar{\nu}_n(x) = \frac{\bar{\nu}_0(x)}{\left(P_{n-1}(d\nu_0; x)\frac{\varphi(d\nu_0;x)}{2} - Q_{n-1}(d\nu_0; x)\right)^2 + \pi^2\bar{\nu}_0^2(x)P_{n-1}^2(d\nu_0; x)} \tag{2.79}$$

$n = 1, 2, 3, \dots$, *and* $d\nu_n(x) = \bar{\nu}_n(x)dx \quad n = 0, 1, 2, \dots$.

Lemma 33. *For every sequence of beta normalised measures $\{d\nu_n\}_{n=0}^{n=\infty}$, there always exists a sequence of normalised secondary measures $\{d\mu_n\}_{n=0}^{n=\infty}$ such that*

$$\bar{\nu}_n(x) = \beta_n(d\nu_0)\bar{\mu}_n(x) \quad n = 0, 1, 2, \dots . \tag{2.80}$$

Proof. For $n = 0$ in Eq. (2.80) and taking into account Eq. (1.16), we have

$$\bar{\nu}_0(x) = C_0(d\nu_0)\bar{\mu}_0(x). \tag{2.81}$$

The only additional constraint on $d\mu_0$ as compared with any measure $d\mu$, is that $C_0(d\mu_0) = 1$. By calculating the zeroth moment of both sides, we see that relation Eq. (2.81) satisfies this additional constraint. Now we will proceed by finding an expression for the sequence of normalised measures generated from $d\mu_0$ in terms of $d\nu_0$. For this we need to find how the quantities $P_n(d\mu_0; x)$, $Q_n(d\mu_0; x)$, $\beta_{n+1}(d\mu_0)$, $n = 0, 1, 2, \dots$ and $\varphi(d\mu_0; x)$ can be written in terms

of $P_n(d\nu_0;x)$, $Q_n(d\nu_0;x)$, $\beta_{n+1}(d\nu_0)$, $n=0,1,2,\ldots$ and $\varphi(d\nu_0;x)$ respectively. Using relation Eq. (2.81) and definition 1.10, we find

$$P_n(d\mu_0;x) = \sqrt{C_0(d\nu_0)}P_n(d\nu_0;x) \quad n=0,1,2,\ldots . \tag{2.82}$$

Using this relation, and definitions 5 and 24, we find

$$Q_n(d\mu_0;x) = \frac{Q_n(d\nu_0;x)}{\sqrt{C_0(d\nu_0)}} \quad n=0,1,2,\ldots , \tag{2.83}$$

$$\varphi(d\mu_0;x) = \frac{\varphi(d\nu_0;x)}{C_0(d\nu_0)}. \tag{2.84}$$

Lemma 29 tells us

$$\beta_n(d\mu_0) = \beta_n(d\nu_0) \quad n=1,2,3,\ldots . \tag{2.85}$$

Hence using relation Eq. (1.20), we find

$$t^2_{n-1}(d\mu_0) = t^2_{n-1}(d\nu_0) = \beta_n(d\nu_0) \quad n=1,2,3,\ldots . \tag{2.86}$$

Now substituting Eqs. (2.82), (2.83), (2.84), and (2.86) into Eq. (2.44),

$$\bar{\mu}_n(x) = \frac{1}{\beta_n(d\nu_0)} \frac{\bar{\nu}_0(x)}{\left(P_{n-1}(d\nu_0;x)\frac{\varphi(d\nu_0;x)}{2} - Q_{n-1}(d\nu_0;x)\right)^2 + \pi^2\bar{\nu}_0^2(x)P^2_{n-1}(d\nu_0;x)} \tag{2.87}$$

$n=1,2,3,\ldots$. Hence by observing definition 32, we find Eq. (2.80) for $n=1,2,3,\ldots$. □

Theorem 34. *A sequence of beta normalised measures $d\nu_0(x)$, $d\nu_1(x)$, $d\nu_2(x)$, ..., satisfy*

$$\alpha_{m+n}(d\nu_0) = \alpha_n(d\nu_m) \quad n,m=0,1,2,\ldots , \tag{2.88}$$

$$\beta_{m+n}(d\nu_0) = \beta_n(d\nu_m) \quad n,m=0,1,2,\ldots . \tag{2.89}$$

Proof. From lemma 33 we see that $d\mu_n$ and $d\nu_n$ are related by a constant, hence using lemmas 29 and 31 we find

$$\alpha_{m+n}(d\nu_0) = \alpha_n(d\nu_m) \quad n,m=0,1,2,\ldots , \tag{2.90}$$

$$\beta_{m+n}(d\nu_0) = \beta_n(d\nu_m) \quad n=1,2,3,\ldots , m=0,1,2,\ldots . \tag{2.91}$$

For $\beta_0(d\nu_m)$ we find

$$\beta_0(d\nu_m) = \beta_0(\beta_m(d\nu_0)d\mu_m) = \beta_m(d\nu_0)C_0(d\mu_m) \quad m=0,1,2,\ldots , \tag{2.92}$$

where we have used Eq. (2.80) followed by Eq. (2.54) and then Eq. (1.16). But $C_0(d\mu_m) = 1 \quad m=0,1,2,\ldots$, by definition 14. □

Remark 35. *As we will see in section* 2.3*, for a wide range of* $d\nu_0$; $\alpha_{m+n}(d\nu_0)$, $\beta_{m+n}(d\nu_0)$ *and* $d\nu_m$ *can be determined analytically. Hence Eq.* (2.88) *and Eq.* (2.89) *can also be used to find analytical solutions to a wide range of integrals.*

The infinite tridiagonal matrix of a measure $d\mu(x)$

$$\mathcal{J}(d\mu) = \begin{bmatrix} \alpha_0(d\mu) & \sqrt{\beta_1(d\mu)} & & & 0 \\ \sqrt{\beta_1(d\mu)} & \alpha_1(d\mu) & \sqrt{\beta_2(d\mu)} & & \\ & \sqrt{\beta_2(d\mu)} & \alpha_2(d\mu) & \sqrt{\beta_3(d\mu)} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{bmatrix}, \tag{2.93}$$

is known as the *Jacobi matrix*. See [29] for more details. We will call the matrix

$$\mathcal{J}_n(d\mu) = \begin{bmatrix} \alpha_n(d\mu) & \sqrt{\beta_{n+1}(d\mu)} & & & 0 \\ \sqrt{\beta_{n+1}(d\mu)} & \alpha_{n+1}(d\mu) & \sqrt{\beta_{n+2}(d\mu)} & & \\ & \sqrt{\beta_{n+2}(d\mu)} & \alpha_{n+2}(d\mu) & \sqrt{\beta_{n+3}(d\mu)} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{bmatrix} \tag{2.94}$$

$n = 1, 2, 3, \ldots$, the *nth associated Jacobi matrix* of the Jacobi matrix $\mathcal{J}(d\mu)$. We are now ready to state our third main theorem:

Theorem 36. *For Jacobi matrices for which its corresponding measure defines a sequence of normalised secondary measures, there exist an infinite sequence of associated Jacobi matrices corresponding to the sequence of normalised secondary measures. These matrices are formed by crossing-out the first row and column of the previous Jacobi matrix in the sequence:*

$$\mathcal{J}_n(d\mu_0) = \mathcal{J}(d\mu_n) \quad n = 1, 2, 3, ... \tag{2.95}$$

Proof. By equating the matrix elements in Eq. (2.95), we find Eq. (2.67) and (2.68). Hence lemma 31 implies Eq. (2.95). □

Corollary 37. *Theorem* 36 *is also valid for any sequence of measures which are proportional to a sequence of normalised secondary measures such as the beta normalised measures.*

Proof. Given that the Jacobi matrix does not contain the β_0 coefficient, the result follows easily from lemma 29. □

2.2 Embeddings and Residual Spectral Densities

Now that we have developed the necessary mathematical tools in section 2.1, we will develop the physical theories of this chapter. These are the following theorems and corollaries. Theorem 42 shows how the results of [23] are a special case of the chain mapping developed here. Theorem 50 gives conditions under which a universal residual spectral density is asymptotically generated. Corollary 48 gives conditions for convergence of the chain mapping parameters. Corollaries 44 and 45 give explicit formula for the residual spectral densities.

To start with, we will now re-write the chain mapping (see theorem 9) in terms of Jacobi matrices, this is to illustrate the connection with Jacobi matrix theory and to write the Hamiltonian in a more compact form. We find

$$\begin{aligned} \hat{H} &= \hat{H}_S \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \sqrt{\beta_0(q)}\, \hat{A}_s \otimes (b_0^* + b_0) \\ &+ \mathbb{I}_{\mathcal{S}} \otimes \frac{q}{2} \left[\vec{b}_0^T \left(\mathcal{J}(d\lambda^q) - \frac{q}{4}\mathbb{I} \right) \vec{b}_0 + h.c. \right] + \mathbb{I}_{\mathcal{S}} \otimes \vec{b}_0^* \left(\mathcal{J}(d\lambda^q) + \frac{q}{4}\mathbb{I} \right) \vec{b}_0, \end{aligned} \tag{2.96}$$

where

$$\vec{b}_n^* = \vec{b}_n^*(q) := (b_n^*(q), b_{n+1}^*(q), b_{n+2}^*(q), b_{n+3}^*(q), \ldots)^T, \tag{2.97}$$

$$\vec{b}_n = \vec{b}_n(q) := (b_n(q), b_{n+1}(q), b_{n+2}(q), b_{n+3}(q), \ldots)^T \quad n = 0, 1, 2, \ldots . \tag{2.98}$$

Let us define (for every $q \in [0, 1]$) the orthonormal Fock basis

$$F_q := \left\{ \frac{b_0^{*m_0}(q)|0\rangle}{\sqrt{m_0!}} \otimes \frac{b_1^{*m_1}(q)|0\rangle}{\sqrt{m_1!}} \otimes \frac{b_2^{*m_2}(q)|0\rangle}{\sqrt{m_2!}} \otimes \ldots \right\}_{\{m_n\}_{n=0}^{\infty}=0}^{\infty}, \tag{2.99}$$

where the creation/annihilation operators (which we recall satisfy $[b_n(q), b_m^*(q)] = \delta_{n,m}$, $[b_n(q), b_m(q)] = [b_n^*(q), b_m^*(q)] = 0$) act on the kets $|n\rangle$ in the standard way: $b_m^*(q)|n\rangle = \sqrt{n+1}|n+1\rangle$, $b_m(q)|n\rangle = \sqrt{n}|n-1\rangle$. Since we can construct any state $\psi \in \Gamma(\mathfrak{h})$ by repetitive action of the creation operator on the vacuum state $\{1, 0, 0, \ldots\} \in \Gamma(\mathfrak{h})$, we can write any $\psi^{(n)}$ in terms of a linear combination of basis states F_q (see appendix B for more details). Hence we have $\Gamma(\mathfrak{h}) = \otimes_{n=0}^{\infty} \mathcal{K}_n$, where $\left\{ \frac{b_n^{*m}(q)|0\rangle}{\sqrt{m!}} \right\}_{m=0}^{\infty}$ is a basis for $\mathcal{K}_n$.

Definition 38. *We call* mth embedded system *to the new system-environment interaction produced when the new system is composed of the initial system plus the first* m *sites of the chain*

formed by the environment in the chain representation, this is to say, the quantum system described by the Hamiltonian $\hat{H}_{S_m^q}$ *on* $\mathcal{S} \otimes_{n=0}^{m-1} \mathcal{K}_n$,

$$\hat{H}_{S_m^q} := \hat{H}_S \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \sqrt{\beta_0(q)}\, \hat{A}_s \otimes (b_0^* + b_0) \tag{2.100}$$

$$+ \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=0}^{m-2} \sqrt{\beta_{n+1}(q)} \left(q(b_n^* b_{n+1}^* + b_n b_{n+1}) + (b_n^* b_{n+1} + b_n b_{n+1}^*) \right) \tag{2.101}$$

$$+ \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=0}^{m-1} \left(\frac{q}{2} \alpha_n(q) - \frac{q^2}{8} \right) (b_n^* b_n^* + b_n b_n) + \left(\alpha_n(q) + \frac{q}{4} \right) b_n^* b_n. \tag{2.102}$$

The mth environment *is formed by the remaining environment terms in the Hamilitonian, in other words the quantum system described by the Hamiltonian* $\hat{H}_{E_m^q}$ *on* $\otimes_{n=m}^{\infty} \mathcal{K}_n$,

$$\hat{H}_{E_m^q} = \frac{q}{2} \left[\vec{b}_m^T \left(\mathcal{J}_m(d\lambda^q) - \frac{q}{4} \mathbb{I} \right) \vec{b}_m + h.c. \right] + \vec{b}_m^* \left(\mathcal{J}_m(d\lambda^q) + \frac{q}{4} \mathbb{I} \right) \vec{b}_m \tag{2.103}$$

$$m = 1, 2, 3, \dots . \tag{2.104}$$

Hence we have $\hat{H} = \hat{H}_{S_m^q} + \hat{H}_{I_m^q} + \hat{H}_{E_m^q}$, where

$$\hat{H}_{I_m^q} := \sqrt{\beta_m(q)} \left(q(b_{m-1}^* b_m^* + b_{m-1} b_m) + (b_{m-1}^* b_m + b_{m-1} b_m^*) \right) \tag{2.105}$$

Lemma 39. *If the spectral density is gapless,*

$$\hat{H}_{E_m^q} = \int_{k_{min}}^{k_{max}} dk g(k) d_{k,m}^* d_{k,m}, \tag{2.106}$$

$$\hat{H}_{I_m^q} = \int_{k_{min}}^{k_{max}} dk \sqrt{M_m^q\big(G_q(g(k))\big) \left| \frac{dG_q(g(k))}{dk} \right|} \tag{2.107}$$

$$\Big(b_{m-1}^* \left[(qc_q(x) - s_q(x)) d_{k,m}^* + (c_q(x) - qs_q(x)) d_{k,m} \right] \tag{2.108}$$

$$+ b_{m-1} \left[(c_q(x) - qs_q(x)) d_{k,m}^* + (qc_q(x) - s_q(x)) d_{k,m} \right] \Big), \tag{2.109}$$

$m = 1, 2, 3, \dots$ *where* $c_q(k) := \cosh(r_q(g(k)))$, $s_q(k) := \sinh(r_q(g(k)))$, $d\lambda_m^q(k) = M_m^q(k) dk$ *and the sequence,* $d\lambda_0^q, d\lambda_1^q, d\lambda_2^q, \dots$ *is the sequence of beta normalised measures of* $d\lambda_0^q(k) = M^q(k) dk$ (*defined in* (1.55)). $[d_{k,m}, d_{k',m}^*] = \delta(k - k')$, *and* $d_{k,m}^* = \sum_{n=m}^{\infty} U_n(d\lambda_m^q; k)(c_q(k) b_n^*(q) + s_q(k) b_n(q))$, $d_{k,m} = \sum_{n=m}^{\infty} U_n(d\lambda_m^q; k)(c_q(k) b_n(q) + s_q(k) b_n^*(q))$,
$U_n(d\lambda_m^q; k) = \frac{\pi_{n-m}(\underline{d\lambda_m^q}; k)}{\sqrt{\langle \pi_{n-m}(d\lambda_m), \pi_{n-m}(d\lambda_m) \rangle_{M_m}}} \sqrt{\underline{M}_m^q(k)} \in \mathcal{L}^2([k_{min}, k_{max}])$, $n = m, m+1, m+2, \dots$ *and underlined measures are defined in lemma* 8.

Proof. The proof is by construction and will involve the properties of beta normalised measures developed in section 2.1.2. Theorem 36 tells us

$$\vec{b}_m^* \left(\mathcal{J}_m(d\lambda^q)\right) \vec{b}_m = \vec{b}_m^* \left(\mathcal{J}(d\lambda_m^q)\right) \vec{b}_m. \tag{2.110}$$

Let us define creation annihilation operators

$$a_{k,m} = \sum_{n=m}^{\infty} U_n(d\lambda_m^q; k) b_n^*(q), \tag{2.111}$$

$$a_{k,m} = \sum_{n=m}^{\infty} U_n(d\lambda_m^q; k) b_n(q) \tag{2.112}$$

with inverse relations

$$b_n^*(q) = \int_{k_{min}}^{k_{max}} dk U_n(d\lambda_m^q; k) a_{k,m}^*, \quad b_n(q) = \int_{k_{min}}^{k_{max}} dk U_n(d\lambda_m^q; k) a_{k,m}, \tag{2.113}$$

$n = m, m+1, m+2, \ldots$. Substituting these into the R.H.S. of (2.110), we have

$$\vec{b}_m^* \left(\mathcal{J}_m(d\lambda^q)\right) \vec{b}_m = \int_{k_{min}}^{k_{max}} dxdy \Big\{ \sum_{n=0}^{\infty} \underline{P}_n(\underline{d\lambda}_m^q; x) \underline{P}_n(\underline{d\lambda}_m^q; y) \alpha_n(d\lambda_m^q) \tag{2.114}$$

$$+ \underline{P}_{n+1}(\underline{d\lambda}_m^q; x) \underline{P}_n(\underline{d\lambda}_m^q; y) \sqrt{\beta_{n+1}(d\lambda_m^q)} \tag{2.115}$$

$$+ \underline{P}_n(\underline{d\lambda}_m^q; x) \underline{P}_{n+1}(\underline{d\lambda}_m^q; y) \sqrt{\beta_{n+1}(d\lambda_m^q)} \Big\} \tag{2.116}$$

$$\sqrt{\underline{M}_m^q(x) \underline{M}_m^q(y)} a_{x,m}^* a_{y,m}. \tag{2.117}$$

Noting that by definition $\underline{P}_{-1} = 0$, and using the three term recurrence relations (1.26), we now have

$$\vec{b}_m^* \left(\mathcal{J}_m(d\lambda^q)\right) \vec{b}_m = \tag{2.118}$$

$$\int_{k_{min}}^{k_{max}} dxdy G_q(g(x)) \sum_{n=0}^{\infty} \underline{P}_n(\underline{d\lambda}_m^q; x) \underline{P}_n(\underline{d\lambda}_m^q; y) \sqrt{\underline{M}_m^q(x) \underline{M}_m^q(y)} a_{x,m}^* a_{y,m}. \tag{2.119}$$

Hence using the orthogonality conditions,

$$\vec{b}_m^* \left(\mathcal{J}_m(d\lambda^q)\right) \vec{b}_m = \int_{k_{min}}^{k_{max}} dxdy G_q(g(x)) \delta(x-y) a_{x,m}^* a_{y,m} \tag{2.120}$$

$$= \int_{k_{min}}^{k_{max}} dk G_q(g(k)) a_{k,m}^* a_{k,m}. \tag{2.121}$$

We also find

$$\vec{b}_m^* \vec{b}_m = \int_{k_{min}}^{k_{max}} a_{k,m}^* a_{k,m}, \tag{2.122}$$

and similarly for the other terms in Eq. (2.103). Now define $d_{k,m} := c_q(k)a_{k,m} + s_q(k)a_{k,m}^*$, $d_{k,m}^* = c_q(k)a_{k,m}^* + s_q(k)a_{k,m}$ and substitute Eqs (2.113) into (2.105) and noting that $P_0(d\lambda_m^q; x) = 1/\sqrt{\beta_0(d\lambda_m^q)} = 1/\sqrt{\beta_m(d\lambda_0^q)}$, where we have used Eq (2.89), we find Eq. (2.109). The identity $[d_{k,m}, d_{k',m}^*] = \delta(k - k')$, follows from the orthogonality of the orthonormal polynomials. □

See **(a)** to **(c)** in figure (1.1) for a pictorial representation. As we will see in section 2.2.2, the chain coefficients converge for a wide range of spectral densities, and hence all the specific features of an environment appear in the first sites of the chain. Consequently, these can be progressively (or directly, all in one go) absorbed into the system by making an embedding; to reduce the complexity of the effective environment. We also point out that, due to a theorem by Farad (see *The Farad Theorem* p.167 of [49]), the existence of a positive measure $M_m^q(k)$ is guaranteed even if the spectral density is gapped in lemma 39. The only difference is that in this case $M_m(x)$ cannot be constructed using the sequence of beta normalised secondary measures formula (Theorem 32) and hence we cannot say anything about its asymptotic properties. This lemma also connects the chain mapping to the work of [35]. Imagine lemma 39 in the case that $m = 1$, $q = 1$, i.e. the phonon mapping with one mode of the bath extracted. In addition, imagine that the bath of oscillators consisted of discrete modes, rather than a continuum. This is the scenario presented in [35]. However, the author only derives an equation which the new spectral density of the bath must satisfy and resorts to solving it numerically for a few example cases. So lemma 39 can be view as a big generalisation of this result; not only do we give the explicit formula for the residual spectral density (in the continuous case), but we solve the iterated version of the problem, i.e. for when $m = 1, 2, 3, \ldots$ modes are extracted from the bath rather than just the first mode.

Definition 40. *We call the* nth residual spectral density $J_n(\omega)$ *to the spectral density corresponding to nth embedding* (*definition* 38). *We call the initial spectral density* $J_0(\omega)$ *such that* $J_0(\omega) \equiv J(\omega)$.

2.2.1 Connection Between the Phonon Mapping and previous work and the Sequence of Residual Spectral Densities

In [23], a similar mapping as in theorem 9 is developed. Starting from a Hamiltonian of the form Eq. (1.1), they show that it is equivalent to a Hamiltonian of the form

$$\hat{H}_S - D_0 s \otimes X'_1 + \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=1}^{\infty} \left(-D_n X'_n X'_{n+1} + \frac{\Omega_n^2}{2} X'^2_n + \frac{1}{2} P'^2_n \right), \tag{2.123}$$

where $\hat{H}_S = \frac{P^2}{2m} + V(s) + \Delta V(s)$ describes the quantum system dynamics and the self-adjoint operator s couples the quantum system to the bosonic bath. The domain of the operators $\{X'_n, P'_n\}_{n=1}^{\infty}$ is not defined by the authors nor the precise relation to the operators in the initial Hamiltonian. See [23] for more details. Here X_n and P_n are position and momentum operators satisfying $[X_n, P_m] = i\delta_{n,m}$. The derivation of the coefficients D_n, Ω_n involve repeated integration and apriori, seem unrelated to our method. However, given the apparent similarity between Eqs. (2.123) and (1.65), a more detailed analysis using some of the theorems developed in section 2 allows one to derive the following theorem which demonstrates that the the mapping of [23] is a special case of the phonon mapping, i.e. it is essentially the same as the phonon mapping for the case of a gapless spectral density. We will prove this after the next theorem

Theorem 41. *The sequence of residual gapless spectral densities in* [23] *are generated by*

$$J_n(\omega) = \frac{J_0(\omega)}{(P_{n-1}(d\lambda^1;\omega^2)\frac{\varphi(d\lambda^1;\omega^2)}{2} - Q_{n-1}(d\lambda^1;\omega^2))^2 + J_0^2(\omega) P_{n-1}^2(d\lambda^1;\omega^2)} \tag{2.124}$$

$n = 1, 2, 3, \ldots$.

Proof. As observed by Leggett [44], when the spectral density of an open quantum system has support on a real interval (in contrast to having support on disjoint intervals), one can easily obtain it from it's propagator $L_0(z)$. The authors of [23] have developed this to find a continued fraction representation for the case of the mapping of the propagator presented in their paper as

follows.

$$L_0(z) = -z^2 - w_0(z), \tag{2.125}$$

$$w_0(z) = \cfrac{D_0^2}{\Omega_1^2 - z^2 - \cfrac{D_1^2}{\Omega_2^2 - z^2 - \cfrac{D_2^2}{\Omega_3^2 - z^2 - \ldots}}}, \tag{2.126}$$

where

$$D_n^2 = \frac{2}{\pi}\int_0^\infty d\omega J_n(\omega)\omega \quad n = 0, 1, 2, \ldots , \tag{2.127}$$

$$\Omega_{n+1}^2 = \frac{2}{\pi D_n^2}\int_0^\infty d\omega J_n(\omega)\omega^3 \quad n = 0, 1, 2, \ldots , \tag{2.128}$$

and $z \in \mathbb{C} -$ support (J_0), where support (J_0) is an interval on the real line by definition [23]. Alternatively, we note that we can write the continued fraction Eq. (2.126) as a recurrence relation

$$w_n'(\sqrt{z}) = \frac{D_n^2}{z - \Omega_{n+1}^2 - w_{n+1}'(\sqrt{z})} \quad n = 0, 1, 2, \ldots , \tag{2.129}$$

where $w_n'(z) := -w_n(z)$. From [23], we have an alternative expression for w_n in terms of the residual spectral densities though the relation,

$$w_n(z) = \frac{2}{\pi}\int_0^\infty d\omega \frac{J_n(\omega)\omega}{\omega^2 - z^2} \quad n = 0, 1, 2, \ldots , \tag{2.130}$$

which by a change of variables and taking into account the definition of ω_n' in Eq. (2.129), can be written in the form

$$w_n'(\sqrt{z}) = \frac{1}{\pi}\int_0^\infty d\omega \frac{J_n(\sqrt{\omega})}{z - \omega} \quad n = 0, 1, 2, \ldots . \tag{2.131}$$

Furthermore, via a change of variables the integrals Eq. (2.127) and (2.128) can be written as

$$D_n^2 = \frac{1}{\pi}\int_0^\infty d\omega J_n(\sqrt{\omega}) \quad n = 0, 1, 2, \ldots , \tag{2.132}$$

$$\Omega_{n+1}^2 = \frac{1}{\pi D_n^2}\int_0^\infty d\omega J_n(\sqrt{\omega})\omega \quad n = 0, 1, 2, \ldots . \tag{2.133}$$

We note that in [23] the support of the spectral densities corresponds with the domain of the spectral densities defined by Eq. (1.7) and hence integrals Eq. (2.131), (2.132) and (2.133) are zero outside of the domain of $J_n(x)$, $\quad n = 0, 1, 2, \ldots$, therefore we can change the lower limit of 0

and upper limit of ∞ of the integrals by ω_{min}^2 and ω_{max}^2 respectively. Now let us define the set of measures

$$d\gamma_n(t) = dt\bar{\gamma}_n(t) \quad n = 0, 1, 2, \dots , \tag{2.134}$$

$$\bar{\gamma}_n(t) = \frac{J_n(\sqrt{t})}{\pi D_n^2} \quad n = 0, 1, 2, \dots . \tag{2.135}$$

This definition of the measure has some important consequences:

1) From Eq. (2.133) we note that Ω_{n+1}^2 are the first moments of the measures $d\gamma_n(t)$,

$$C_1(d\gamma_n) = \Omega_{n+1}^2 \quad n = 0, 1, 2, \dots . \tag{2.136}$$

2) From Eq. (2.131) and definition 6 we see that $w_n'(\sqrt{z})$ is proportional to the Stieltjes transformations of the measure $d\gamma_n(t)$

$$w_n'(\sqrt{z}) = D_n^2 S_n(z) \quad n = 0, 1, 2, \dots . \tag{2.137}$$

3) From Eq. (2.132) we see that the zeroth moments of the measures $d\gamma_n(t)$ are unity

$$C_0(d\gamma_n) = 1 \quad n = 0, 1, 2, \dots . \tag{2.138}$$

We are now able to re-write Eq. (2.129) in the form

$$S_{n+1}(z)D_{n+1}^2 = z - C_1(d\gamma_n) - \frac{1}{S_n(z)}, \quad n = 0, 1, 2, \dots , \tag{2.139}$$

where we have used the short hand $S_{m_n}(z) =: S_n(z)$. By comparing this recursion relation with Eq. (1.23), we deduce that $D_{n+1}^2 d\gamma_{n+1}$ is the secondary measure associated with $d\gamma_n$, for $n = 0, 1, 2, \dots$. We can also identify a sequence of normalised secondary measures. Noting that $C_0(d\gamma_0) = 1$ from Eq. (2.138), definition 14 tells us that the sequence of secondary normalised measures starting from $d\gamma_0$ is

$$d\gamma_0,\ D_1^2 d\gamma_1 / C_0(D_1^2 d\gamma_1),\ D_2^2 d\gamma_2 / C_0(D_2^2 d\gamma_2), \dots, D_m^2 d\gamma_m / C_0(D_m^2 d\gamma_m), \dots . \tag{2.140}$$

However,

$$C_0(D_n^2 d\gamma_n) = D_n^2 C_0(d\gamma_n) = D_n^2 \quad n = 1, 2, 3 \dots , \tag{2.141}$$

so the sequence of normalised secondary measures is $d\gamma_0(t)$, $d\gamma_1(t)$, $d\gamma_2(t)$, $d\gamma_3(t), \ldots$. Taking into account lemma 16 and theorem 22 we see that

$$D_n^2 = d_{n-1} = \beta_n(d\gamma_0) \quad n = 1, 2, 3 \ldots . \tag{2.142}$$

Due to Eqs. (1.16) and (2.138) we can also write D_0^2 in terms of β_0,

$$D_0^2 = \beta_0(d\eta_0) \tag{2.143}$$

where

$$d\eta_0 := D_0^2 d\gamma_0. \tag{2.144}$$

We can now construct a sequence of beta normalised measures from $d\eta_0$, denoted by $d\eta_0$, $d\eta_1$, $d\eta_2, \ldots$. From Eq. (2.143) and (2.144) we see that $d\eta_0$ satisfies Eq. (2.81) for $d\gamma_0$, hence lemma 33 tells us

$$\bar{\eta}_n(x) = \beta_n(d\eta_0)\bar{\gamma}_n(x) \quad n = 0, 1, 2, \ldots . \tag{2.145}$$

Taking into account that $\beta_n(d\eta_0) = \beta_n(d\gamma_0) \quad n = 1, 2, 3, \ldots$ due to lemma 29 and Eq. (2.144), from Eqs. (2.145) and (2.135) we gather

$$d\eta_n(t) = dt\, \bar{\eta}_n(t) \quad n = 0, 1, 2, \ldots , \tag{2.146}$$

$$\bar{\eta}_n(t) = \frac{J_n(\sqrt{t})}{\pi} \quad n = 0, 1, 2, \ldots , \tag{2.147}$$

hence we note that

$$d\eta_0 = d\lambda^1. \tag{2.148}$$

Substituting this into Eq. (2.79) gives us Eq. (2.124). □

Theorem 42. *Define* $X'_n := (-1)^n X_{n-1}$, $P'_n = (-1)^n P_{n-1}$, $s = \hat{A}_s$, $\mathcal{D}(X'_n) = \mathcal{D}(X_n)$, $\mathcal{D}(P'_n) = \mathcal{D}(P_n)$, $\mathcal{D}(s) = \mathcal{D}(\hat{A}_s)$, $n = 1, 2, 3, \ldots$, *and let the spectral density* J_0 *be gapless, then*

$$-D_0 s \otimes X'_1 + \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=1}^{\infty} \left(-D_n X'_n X'_{n+1} + \frac{\Omega_n^2}{2} X'^2_n + \frac{1}{2} P'^2_n \right) = \tag{2.149}$$

$$\sqrt{\beta_0(1)}\hat{A}_s \otimes X_0 + \mathbb{I}_{\mathcal{S}} \otimes \sum_{n=0}^{\infty} \left(\sqrt{\beta_{n+1}(1)} X_n X_{n+1} + \frac{\alpha_n(1)}{2} X_n^2 + \frac{1}{2} P_n^2 \right). \tag{2.150}$$

Proof. From Eq. (2.133) and (1.14) we see that we can write Ω_n^2 as

$$\Omega_{n+1}^2 = \alpha_0(d\eta_n) \quad n = 0, 1, 2, \dots . \tag{2.151}$$

Hence,

$$\Omega_{n+1}^2 = \alpha_n(d\eta_0) = \alpha_n(d\lambda^1) = \alpha_n(1) \quad n = 0, 1, 2, \dots , \tag{2.152}$$

where we have used Eq. (2.88) followed by Eq. (2.148). From Eqs. (2.132), and (1.16) we see that

$$D_n^2 = \beta_0(d\eta_n) \quad n = 0, 1, 2, \dots . \tag{2.153}$$

Hence using Eq. (2.89) followed by Eq. (2.148), we find

$$D_n^2 = \beta_n(d\eta_0) = \beta_n(d\lambda^1) = \beta_n(1) \quad n = 0, 1, 2, \dots . \tag{2.154}$$

Now using the definitions stated in the theorem, we conclude the proof. □

Remark 43. *We note that the three term recurrence relations Eq. (1.12) for gapped measures, still hold. Hence the generalised mapping (and therefore the phonon mapping) is still valid. However, the chain mapping presented in [23] is not valid under these conditions because the relation between the Stieltjes transformations of two consecutive measures, Eq. (1.23) is not valid anymore (see (E) in appendix for a proof) and hence one cannot calculate the chain coefficients from the sequence of residual spectral densities. In this sense, the phonon mapping presented here is a more general result. This is an important difference because if a spectral density is gapped, then the corresponding measure is also gapped. There are physical systems (such as photonic crystals and diatomic chains) which have these properties.*

We can also use the previous two theorems to prove a result about the phonon mapping. This is the fourth main result:

Corollary 44. *In the phonon mapping case, if the spectral density is gapless the sequence of residual spectral densities is given by*

$$J_n(\omega) = \frac{J_0(\omega)}{(P_{n-1}(d\lambda^1;\omega^2)\frac{\varphi(d\lambda^1;\omega^2)}{2} - Q_{n-1}(d\lambda^1;\omega^2))^2 + J_0^2(\omega)P_{n-1}^2(d\lambda^1;\omega^2)}, \tag{2.155}$$

$n = 1, 2, 3, \dots .$

Proof. Follows directly from theorems 41 and 42. Alternatively, we note that it is also a direct consequence of lemma 39 when $q = 1$. This has the advantage of being an independent derivation from the results of [23], but has the downside of not illustrating the connections between this result and their results. □

We can also derive this for the particle mapping case. This will be the fifth main result

Corollary 45. *In the particle mapping case, if the spectral density is gapless the sequence of residual spectral densities is given by*

$$J_n(\omega) = \frac{J_0(\omega)}{(P_{n-1}(d\lambda^0;\omega)\frac{\varphi(d\lambda^0;\omega)}{2} - Q_{n-1}(d\lambda^0;\omega))^2 + J_0^2(\omega)P_{n-1}^2(d\lambda^0;\omega)}, \tag{2.156}$$

$n = 1, 2, 3, \ldots$.

Proof. The proof is a direct consequence of Lemma 39. In Eqs. (2.106) and (2.109), set $q = 0$. Now by definiton of the spectral density (Eq. (1.7)), we have $J_m(x) = \pi M_m^0(x) \quad m = 1, 2, 3, \ldots$. Hence noting that $J_0(x) = \pi M_0^0(x)$ from Eq. (1.62) and applying definition 32, we find Eq. (2.156). □

2.2.2 Residual Spectral Densities Sequence Convergence

In this section we will prove convergence theorems for the asymptotic behaviour of the sequences of residual spectral densities.

Definition 46. *We say that the chain mapping for some q and a particular spectral density $J(x)$, will belong to the* Szegö class *if the measure $d\lambda^q(x) = M^q(x)dx$ satisfies*

$$\int_{G_q(\omega_{min})}^{G_q(\omega_{max})} \frac{\ln M^q(x)\, dx}{\sqrt{\big(G_q(\omega_{max}) - x\big)\big(x - G_q(\omega_{min})\big)}} > -\infty. \tag{2.157}$$

Examples of spectral densities which for any q do not belong to the Szegö class, are those which are gapped and those with unbounded support.

Theorem 47. *If for some q and spectral density $J(\omega)$, chain mapping belongs to the Szegö class, then the sequences $\alpha_0(q), \alpha_1(q), \alpha_2(q), \ldots$ and $\beta_0(q), \beta_1(q), \beta_2(q), \ldots$ converge to:*

$$\lim_{n\to\infty} \alpha_n(q) = \frac{G_q(\omega_{max}) + G_q(\omega_{min})}{2}, \tag{2.158}$$

$$\lim_{n\to\infty} \beta_n(q) = \frac{\big(G_q(\omega_{max}) - G_q(\omega_{min})\big)^2}{16}. \tag{2.159}$$

Proof. Follows from shifting the support region of the Szegö theorem in [19]. For the original theorem see chapter 12 of [45]. □

Corollary 48. *If for some q and spectral density $J(\omega)$ the chain mapping belongs to the Szegö class, the tail of the semi-infinite chain mapping tends to a translational invariant chain. In other words,*

$$\lim_{n\to\infty} E_{p,n}(q) = C_p(q) \quad p = 1, \ldots, 5\,, \tag{2.160}$$

where $C_p \in \mathbb{R}$ are finite constants for all constant $q \in [0,1]$ and $E_{p,n}$ are defined in theorem 9.

Proof. Follows from theorem 47 and Eq. (1.58). □

This last result would suggest that the sequence of residual spectral densities should converge under certain circumstances. Indeed this is the case. The next theorem will provide the necessary mathematical development from which we can easily derive the limiting residual spectral densities.

Theorem 49. *If for some gapless measure $d\mu(x)$ with finite support interval I the limits*

$$\lim_{n\to\infty} \alpha_n(d\mu) = \frac{a+b}{2}, \tag{2.161}$$

$$\lim_{n\to\infty} \beta_n(d\mu) = \frac{(b-a)^2}{16}, \tag{2.162}$$

exist, then the sequence of beta normalised and normalised secondary measures generated from $d\nu$ and $d\mu$ respectively, converge weakly to

$$\lim_{n\to\infty} \bar{\nu}_n(x) = \frac{\sqrt{(x-a)(b-x)}}{2\pi}, \tag{2.163}$$

$$\lim_{n\to\infty} \bar{\mu}_n(x) = \frac{8\sqrt{(x-a)(b-x)}}{\pi(b-a)^2}. \tag{2.164}$$

Proof. First we will show that the limit exists by construction (this is to say, by finding the fixed points of the sequence), then we will show that it corresponds to when the limits Eq. (2.161) and (2.162) are accomplished.
Substituting Eq. (2.40) into Eq. (2.34), we find

$$\varphi(d\rho; x) = 2\big[x - C_1(d\mu)\big] - \frac{\varphi(d\mu; x)\bar{\rho}(x)}{\bar{\mu}(x)}. \tag{2.165}$$

If the limit exists, then there must be at least one solution to $\bar{\rho}(x) = A\bar{\mu}(x)$ where $d\rho(x) = \bar{\rho}(x)dx$ is the secondary measure associated with the gapless measure $d\mu(x) = \bar{\mu}(x)dx$ and $A > 0$. From definitions 24 and 6 we see that $\varphi(d\rho; x) = A\varphi(d\mu; x)$ and hence from Eq. (2.165) we see that

$$\varphi(d\mu; x) = \frac{x - C_1(d\mu)}{A}. \tag{2.166}$$

Thus substituting this into Eq. (2.34), and solving for $\bar{\mu}(x)$ we find

$$\bar{\mu}^2(x) = \frac{4A - (x - C_1(d\mu))^2}{4\pi^2 A^2}. \tag{2.167}$$

Taking into account the definition of a gapless measure, we see that if the limit exits, then it must be bounded. Moreover, it must belong to the interval centered at $C_1(d\mu)$ and of length $4\sqrt{A}$. Making the change of variable $x - C_1(d\mu) = 2\sqrt{A}t$ gives us

$$d\mu(t) = \bar{\mu}(t)dt = \frac{2\sqrt{1-t^2}}{\pi}dt, \tag{2.168}$$

with support interval [-1,1]. We now can check that Eq. (2.168) exists by direct substitution. Using definition 6 we find that the Stieltjes Transform of Eq. (2.168) is $S_{\bar{\mu}}(z) = 2[z - \sqrt{z^2 - 1}]$ and hence from definition 24 we find $\varphi(d\mu; x) = 4x$. Thus using Eq. (2.34) we have $\bar{\rho}(x) = \bar{\mu}(x)/4$, hence the limit exists. By performing the change of variable $t = (2/(b-a))y + (b+a)/(a-b)$, we shift the support of Eq. (2.168) to the general case $[a, b]$ and the measure is now given by Eq. (2.164).

Now we will proceed to show that if Eq. (2.161) and (2.162) are satisfied, then the sequence of normalised secondary measures converge weakly to Eq. (2.164). By taking the nth moment of the measures in Eq. (2.3) and taking into account lemma 2.4 for $n = 0$, we have

$$C_n(d\rho_{n+1}) = \left[C_2(d\mu_n) - C_1(d\mu_n)^2\right] C_n(d\mu_{n+1}) \quad n, m = 0, 1, 2, \dots . \tag{2.169}$$

Writing Eq. (2.4) for a sequence of measures followed by substituting in our expression for $C_n(d\rho_{n+1})$ using Eq. (2.169), we find

$$\left(c_2^s - (c_1^s)^2\right) c_n^{s+1} = c_{n+2}^s - c_1^s c_{n+1}^s - \sum_{j=0}^{n-1} \left(c_2^s - (c_1^s)^2\right) c_j^{s+1} c_{n-j}^s \quad n, s = 0, 1, 2, \dots , \tag{2.170}$$

where $c_n^s := C_n(d\mu_s) \quad n, s = 0, 1, 2, \dots$. Let us define the limit $l_n = \lim_{s\to\infty} c_n^s$. We can now draw the following conclusions

1) Due to definition 14, we have $C_0(d\mu_n) = 1 \quad n = 0, 1, 2, \ldots$. Therefore $l_0 = 1$.

2) From Eq. (2.67) and (1.14) we see that

$$\alpha_n(d\mu_0) = \alpha_0(d\mu_n) = \frac{C_1(d\mu_n)}{C_0(d\mu_n)} = c_1^n. \tag{2.171}$$

Hence taking into account assumption Eq. (2.161), we have $l_1 = (a + b)/2$.

3) Noting the definition of d_n in theorem 16, theorem 22 tells us

$$\beta_{n+1}(d\mu_0) = c_2^n - (c_1^n)^2 \quad n = 0, 1, 2, \ldots . \tag{2.172}$$

Hence taking into account assumptions Eqs. (2.161) and (2.162), and Eq. (2.171) we have $l_2 = (5a^2 + 6ab + 5b^2)/16$.

We note that for any s, all the moments c_n^s in Eq. (2.170) are fully determined by the starting values c_0^s, c_1^s, and c_2^s, hence we conclude from the above points 1), 2) and 3), that under the assumptions Eqs. (2.161) and (2.162), all $l_n \quad n = 0, 1, 2, \ldots$ are finite and determined by

$$\left(l_2 - l_1^2\right) l_n = l_{n+2} - l_1 l_{n+1} - \left(l_2 - l_1^2\right) \sum_{j=0}^{n-1} l_j l_{n-j} \quad n, s = 0, 1, 2, \ldots , \tag{2.173}$$

with starting values $l_0 = 1$, $l_1 = (a + b)/2$, and $l_2 = (5a^2 + 6ab + 5b^2)/16$.
For the case of the normalised measure Eq. (2.164), we conclude that $c_n^s = c_n^{s+1} \quad n, s = 0, 1, 2, \ldots$ since its secondary normalised measure is equal to itself. Hence by denoting $m_n = c_n^s \quad n, s = 0, 1, 2, \ldots$ we can write Eq. (2.170) for this measure as

$$\left(m_2 - (m_1)^2\right) m_n = m_{n+2} - m_1 m_{n+1} - \left(m_2 - (m_1)^2\right) \sum_{j=0}^{n-1} m_j m_{n-j} \tag{2.174}$$

$n, s = 0, 1, 2, \ldots$. By direct calculation of the moments of Eq. (2.164), we find that $m_0 = l_0$, $m_1 = l_1$, $m_2 = l_2$, and hence by comparing Eq. (2.173) with Eq. (2.174) we conclude that $m_n = l_n \quad n = 0, 1, 2, \ldots$. Thus, since a measure with a finite support interval is uniquely determined by its moments (see *moment problem* [29]), we conclude Eq. (2.164) under the assumptions Eqs. (2.161) and (2.162). For Eq. (2.163), we note that Eqs. (2.80) and (2.85) tell us $\lim_{n\to\infty} \bar{\nu}_n(x) = \lim_{n\to\infty} \beta_n(d\mu_0)\bar{\mu}_n(x)$. Hence from Eqs. (2.162) and (2.164) we conclude Eq. (2.163). □

We will call *terminal spectral density* $J_T(\omega)$ the spectral density to which a sequence of residual spectral densities converge to weakly if such a limit exists: $J_T(\omega) = \lim_{n\to\infty} J_n(\omega)$. We are now ready to state our fourth main theorem:

Theorem 50. *If for the particle or phonon mapping the spectral density J belongs to the Szegö class, the sequence of residual spectral densities converge weakly to the Wigner semicircle distribution* see p191-198 of [46]

$$J_T(\omega) := \lim_{n\to\infty} J_n(\omega) = \frac{\sqrt{(\omega-\omega_{min})(\omega_{max}-\omega)}}{2}, \tag{2.175}$$

and the Rubin model spectral density [1]

$$J_T(\omega) := \lim_{n\to\infty} J_n(\omega) = \frac{\sqrt{(\omega^2-\omega_{min}^2)(\omega_{max}^2-\omega^2)}}{2}, \tag{2.176}$$

respectively, $\omega \in [\omega_{min}, \omega_{max}]$.

Proof. From Eq. (2.147) and theorem 49 we gather that if Eq. (2.161) and (2.162) are satisfied, then for the phonon case

$$J_T(\omega) = \frac{\sqrt{(\omega^2-a)(b-\omega^2)}}{2}. \tag{2.177}$$

From Eq. (1.66) we have that $a = \omega_{min}^2$ and $b = \omega_{max}^2$. Now taking into account theorem (47), we find Eq. (2.176). Proceeding in a similar manner, we find Eq. (2.175). □

In the Rubin model, the bath is represented by a semi-infinite translationally invariant nearest neighbour chain with phonon mapping type coupling between the oscillators. Hence with the knowledge of corollary 48, this result should not come as a surprise. Note however, that the derivation of the spectral density for the Rubin model is very different to the derivation of this limiting case presented here. The particle case is also interesting but for a different reason. Although, to the best of knowledge of the author, there is no known classic model in the literature with this spectral density, the semi-circle law function arises naturally in the field of random matrix theory. Therefore, one might wonder if there is a deeper connection between the particle mapping and random matrix theory. This might turnout be a fruitful line of investigation.

2.3 Examples

In this section, we will solve analytically the chain coefficients (see theorem 9) and sequences of residual spectral densities for the particle and phonon mapping (see corollaries 44 and 45) for particular examples of spectral densities.

2.3.1 Power Law Spectral Densities with Finite Support

The widely studied power law spectral densities are [10, 1]

$$J(x) = 2\pi\alpha\omega_c^{1-s}x^s, \tag{2.178}$$

with domain $[0, \omega_c]$ and $s > -1$. Let us start by calculating the sequence of residual spectral densities for the case of the particle mapping.
From Eq. (1.62) and (2.178) we have

$$M^0(x) = 2\alpha\omega_c^{1-s}x^s. \tag{2.179}$$

For simplicity, we will scale out the ω_c dependency and show how to put it back again afterwards. Let us start by defining the weight function $m_0^0(x) := \omega_c M^0(x\omega_c) = 2\alpha\omega_0^2 x^s$ with support interval $[0, 1]$. From lemma 72, we find that $m_n^0(x) = M_n^0(x\omega_c)/\omega_c \quad n = 1, 2, 3, \ldots$. where $m_n^0(x)$ and $M_n^0(x)$ are the sequence of beta normalised measures generated from $m_0^0(x)$ and $M^0(x)$ respectively. Now let us define the weight function

$$\tilde{m}_0^0(x) = x^s \tag{2.180}$$

with support interval $[0, 1]$. Given that this new measure is proportional to $m_0^0(x)$, from lemma 73 we conclude that it's sequence of beta normalised measures $\tilde{m}_n^0(x) \quad n = 1, 2, 3, \ldots$, are equal. Hence we have $M_n^0(x) = \omega_c\tilde{m}_n^0(x/\omega_c) \quad n = 1, 2, 3, \ldots$. Thus taking into account Eq. (1.62), we conclude

$$J_n(\omega) = \pi M_n^0(\omega) = \omega_c\pi\tilde{m}_n^0(\omega/\omega_c) \quad n = 1, 2, 3, \ldots . \tag{2.181}$$

The real polynomials orthogonal to the weight function $\tilde{m}_0^0(x)$ are $P_n^s(x) := P_n^{(0,s)}(2x-1)\sqrt{n+s+1}$ $n = 0, 1, 2, \ldots$; which are normalised shifted counterparts of the *Jacobi polynomials* $P_n^{(\alpha,\beta)}(x)$ $n = 0, 1, 2, \ldots$. The reducer for the case $s \geq 0$ is given by theorem 71

$$\varphi(d\tilde{m}^0; t) = 2\left[\ln\left(\frac{t}{1-t}\right) + s\int_0^1 x^{s-1}\ln\left|\frac{t-x}{t}\right| dx\right], \tag{2.182}$$

which has analytic solutions when a particular value of s is specified. For example, the first three in the sequence for the ohmic case ($s = 1$) are

$$\tilde{m}_1^0(x) = \frac{x}{2\left(\pi^2 x^2 + [1 + x\ln(\frac{1-x}{x})]^2\right)}, \tag{2.183}$$

$$\tilde{m}_2^0(x) = \frac{x}{4\pi^2(2-3x)^2x^2 + \left[1 - 6x + (4-6x)x\ln(\frac{1-x}{x})\right]^2}, \tag{2.184}$$

$$\tilde{m}_3^0(x) = \frac{6x}{36\pi^2x^2(3-12x+10x^2)^2 + \left[30x - 16 + (18 - 72x + 60x^2)(1 + x\ln(\frac{1-x}{x}))\right]^2}.$$

The chain coefficients are calculated in [19] to be

$$\alpha_n(0)(s) = \frac{\omega_c}{2}\left(1 + \frac{s^2}{(s+2n)(2+s+2n)}\right) \quad n = 0, 1, 2, \dots , \tag{2.185}$$

$$\sqrt{\beta_{n+1}(0)}(s) = \frac{\omega_c(1+n)(1+s+n)}{(s+2+2n)(3+s+2n)}\sqrt{\frac{3+s+2n}{1+s+2n}} \quad n = 0, 1, 2, \dots , \tag{2.186}$$

$$\tag{2.187}$$

where the (s) is to remind us of their s dependency. System environment coupling coefficient is [19]

$$\sqrt{\beta_0(0)} = \omega_c\sqrt{\frac{2\alpha}{s+1}}. \tag{2.188}$$

Now we will find the sequence of residual spectral densities for the case of the phonon mapping. From Eq. (1.66) and (2.178) we have

$$M^1(x) = 2\alpha\omega_c^{1-s}x^{s/2}, \tag{2.189}$$

with support $[0, \omega_c^2]$. Proceeding as in the particle mapping case and taking into account Eq. (2.147), we find

$$J_n(\omega) = \pi M_n^1(\omega^2) = \omega_c^2\pi\tilde{m}_n^1(\omega^2/\omega_c^2) \quad n = 1, 2, 3, \dots , \tag{2.190}$$

where $\tilde{m}_n^1(x) \quad n = 1, 2, 3, \dots$, are the sequence of beta normalised measures generated from

$$\tilde{m}_0^1(x) = x^{s/2}, \tag{2.191}$$

with support $[0, 1]$. Let us denote $\tilde{m}_0^1(x)$ and $\tilde{m}_0^0(x)$ by $\tilde{m}_{0s}^1(x)$ and $\tilde{m}_{0s}^0(x)$ respectively to remind us of their s dependency. By comparing eq. (2.191) with eq. (2.180), we have that $\tilde{m}_{0s}^1(x) = \tilde{m}_{0s/2}^0(x)$ for all $s > -1$ and hence from Eq. (2.181) and (2.190) we see that for the spin-boson models,

there is a simple relationship between the residual spectral densities of the particle and phonon mappings for different s values. For the same example as in the particle case ($s = 1$), we need to evaluate $m_n^0(x)$ $n = 1, 2, 3, \ldots$, for $s = 1/2$. The first one in the sequence is

$$\tilde{m}_1^1(x) = \frac{2\sqrt{x}}{3\left(\pi^2 x + (2 - 2\sqrt{x}\tanh^{-1}(\sqrt{x}))^2\right)}, \tag{2.192}$$

where $\tanh^{-1}(x)$ is the inverse hyperbolic tangent function. We can readily calculate the chain coefficients from the particle example. By comparing the expression for the α_n and β_n coefficients for the weight functions for the particle and phonon mappings, we find

$$\alpha_n(1)(s) = \omega_c \alpha_n(0)(s/2) \quad n = 0, 1, 2, \ldots , \tag{2.193}$$

$$\sqrt{\beta_{n+1}(1)}(s) = \omega_c \sqrt{\beta_{n+1}(0)}(s/2) \quad n = 0, 1, 2, \ldots , \tag{2.194}$$

and system environment coupling term to be

$$\sqrt{\beta_0(1)} = 2\omega_c \sqrt{\frac{\alpha\omega_c}{s+2}}. \tag{2.195}$$

For both the particle and phonon mappings, it is easy to verify that the chain coefficients and sequence of residual spectral densities will converge because Eq. (2.157) is satisfied in both cases as long as $s < \infty$. We also find that the sequence of residual spectral densities calculated in the above examples converge very rapidly to this limit after about the 3rd residual spectral density.

2.3.2 The Power Law Spectral Densities with Exponential Cut Off

The power law spectral densities with exponential cut off is [10, 1]

$$J(x) = 2\pi\alpha\omega_c^{1-s} x^s e^{-x/\omega_c}, \tag{2.196}$$

with domain $[0, \infty)$ and $s > -1$. Let us start by calculating the sequence of residual spectral densities for the case of the particle mapping.

From Eq. (1.62) and (2.196) we have

$$M^0(x) = 2\alpha\omega_c^{1-s} x^s e^{-x/\omega_c}. \tag{2.197}$$

Let us define the measure $m^0(x) := \omega_c M^0(x\omega_c) = 2\alpha\omega_0^2 x^s e^{-x}$ with support interval $[0,\infty)$. From lemma 72, we find that $m_n^0(x) = M_n^0(x\omega_c)/\omega_c \quad n = 1,2,3,\ldots.$ where $m_n^0(x)$ and $M_n^0(x)$ are the sequence of beta normalised measures generated from $m^0(x)$ and $M^0(x)$ respectively. We will now define a 3rd measure by $\tilde{m}^0(x) = x^s e^{-x}$. We note that it is proportional to the measure $m^0(x)$ and hence lemma 73 tells us that its sequence of beta normalised measures are equal. Thus we have the relation

$$M_n^0(x) = \omega_c \tilde{m}_n^0(x/\omega_c) \quad n = 1,2,3,\ldots. \tag{2.198}$$

The real polynomials orthogonal to the weight function $\bar{m}^0(x)$ are called the *associated Laguerre polynomials* $L_n^s(x) \quad n = 0,1,2,\ldots$. Their normalised counterparts are $P_n^s(x) := L_n^s(x)\ n!/\Gamma(n+s+1) \quad n = 0,1,2,\ldots$. The reducer in this case is given by theorem 71

$$\varphi(d\tilde{m}^0;x) = 2\int_0^{+\infty} (s-t)t^{s-1}e^{-t}\ln\left|\frac{t-x}{x}\right| dt, \tag{2.199}$$

which has analytic values when a particular value of s is specified. For example, if s is integer, we find

$$\varphi(d\tilde{m}^0;x) = 2\left[x^s e^{-x} Ei(x) - \sum_{k=0}^{k=s-1} (s-k-1)!\, x^k\right], \tag{2.200}$$

where $Ei(x)$ is the *exponential integral* function[47].

From Eq. (2.198) we have

$$J_n(\omega) = \pi M_n^0(\omega) = \omega_c \pi \tilde{m}_n^0(\omega/\omega_c) \quad n = 1,2,3,\ldots, \tag{2.201}$$

and Eq. (2.79) tells us

$$\tilde{m}_n^0(x) = \frac{x^s e^{-x}}{\left(P_{n-1}^s(x)\frac{\varphi(d\tilde{m}^0;x)}{2} - Q_{n-1}^s(x)\right)^2 + \pi^2 x^{2s} e^{-2x} P_{n-1}^s(x)^2} \quad n = 1,2,3,\ldots. \tag{2.202}$$

For example, the first two in the sequence for the ohmic case ($s = 1$) are

$$\tilde{m}_1^0(x) = \frac{xe^x}{e^{2x} + \pi^2 x^2 - 2xEi(x)e^x + x^2 Ei(x)^2}, \tag{2.203}$$

$$\tilde{m}_2^0(x) = \frac{2xe^x}{e^{2x}(1-x)^2 + \pi^2 x^2 (x-2)^2 - 2x(2-3x+x^2)Ei(x)e^x + x^2(x-2)^2 Ei(x)^2}. \tag{2.204}$$

We also have analytic expressions for the chain coefficients. From [19], we have that the chain coefficients are

$$\sqrt{\beta_{n+1}(0)} = \omega_c\sqrt{(n+1)(n+s+1)} \quad n = 0,1,2,\ldots, \tag{2.205}$$

$$\alpha_n(0) = \omega_c(2n+1+s) \quad n = 0,1,2,\ldots, \tag{2.206}$$

with the system-environment coupling coefficient given by

$$\sqrt{\beta_0(0)} = \omega_c \sqrt{2\alpha\Gamma(s+1)}. \tag{2.207}$$

Similarly, we can calculate the residual spectral densities and chain coefficients for the phonon mapping case.

Because the support interval is infinite, the spin-boson model with exponential cut off does not belong to the Szegö class for either the particle mapping nor the phonon mapping as can be easily verified from Eq. (2.157). This is reflected in the example above as the sequence of residual spectral densities do not converge[1].

Remark 51. *We note that for spectral densities for which the corresponding orthogonal polynomials are unknown analytically, we can easily calculate their coefficients using very stable numerical algorithms. See [29].*

2.4 Chapter Summary and Conclusion

In chapter 1 we have establish a general formalism for mapping an open quantum system of a specialized Pauli-Fierz Hamiltonian Eq. (1.1) onto chain representations. The different versions of chain mappings were generated by choosing particular values of 4 real constants which we parametrised by one real variable q. In this chapter, we used this to provide a very general connection between the theory of open quantum systems and Jacobi operator theory as the semi-infinite chains can be written in terms of Jacobi matrices as can be seen in Eq. (2.96). There has been a wealth of research into the properties of Jacobi operator theory [27], and hence this opens up the theorems of this field to the possibility of being applied to the theory of open quantum systems. Likewise, the theorem regarding Jacobi matrices (theorem 36) developed here, could turn out to be useful in the field of Jacobi operator theory.

There were two previously known exact chain mappings; the one of [19] which is the same as the particle mapping defined here (definition 11), and the mapping by [23]. We show that the phonon mapping derived in this article (see definition 13) has a wider range of validity (remark 43) than

[1]However, we do note that the ratio $\alpha_n(q)/\sqrt{\beta_{n+1}(q)}$ for $q = 0$ and $q = 1$ does converge. This suggests that there is a universal asymptotic expansion for large n for the nth residual spectral density.

the mapping of [23] and prove that they are formally equivalent in the range of validity of [23]; see theorem 42.

The concept of embedding degrees of freedom into the system has been around for some time [26, 23], however, we see that in chain representations, there is a natural way of shifting the system-environment boundary, that is to say, there is a natural and systematic way of embedding degrees of freedom into the system one by one (or all in one go). To solve quantitatively this problem, we have to first embark on finding the solution to an old problem in mathematics; an analytical solution to the sequence of secondary measures in terms of the initial measure, it's associated orthogonal polynomials and reducer; see theorem 28. Not only does this provide a means to find analytical expressions for the sequence of spectral densities corresponding to the new system-environment interaction after embedding environmental degrees of freedom into the system for the particle and phonon mappings in the gapless spectral densities case (corollary 45 and corollary 44 respectively), but it provides physical meaning to this abstract mathematical construct.

Using convergence theorems of Szegö and deriving the fixed point in the sequence of secondary measures; we have combined these results to obtain a convergence theorem of the sequence of residual spectral densities for the particle and phonon cases, theorem 50 (or equivalently, the sequence of secondary measures, theorem 49). What is more, because the criterion for convergence (definition 46) is solely in terms of the initial spectral density once the desired chain mapping is chosen, the convergence criterion is readily applicable to a particular problem. Furthermore, we see that any unbounded spectral density will not satisfy this criterion. This is reflected in the sequence generated in the examples section for the case of the family of power-law spectral densities with exponential cut off as the sequence does not converge, section 2.3.2.

We give two examples where we can find explicit analytical expressions for the chain coefficients and the sequence of residual spectral densities. These are the family of spectral densities used in the spin-boson model, which have spectral densities of the form x^s with finite support $I = [0, \omega_c]$ and $x^s e^{x/\omega_c}$ with semi-infinite support $I = [0, +\infty)$, where $s > -1$. Furthermore, we show how the residual spectral densities of the mapping for both phonon and particle cases are related for different families of the mapping as demonstrated by the identity $\tilde{m}^1_{0s}(x) = \tilde{m}^0_{0s/2}(x)$ and Eq. (2.181) and (2.196).

We note that when this convergence of the embeddings is achieved (i.e. inequality (2.157) is satis-

fied), the part of the chain corresponding to the new environment has a very universal property: all its couplings and frequencies become constant (Theorem 47). This is to say, they are translationally invariant. This suggests a universal way of simulating the environment as all the characteristic features of the environment are now embedded into the system. What is not so clear however, is what is the most effective chain mapping for simulating the environment.

Another way to view the chain mapping theorem (theorem 9), is that it takes us from a non-local Hamiltonian to a local Hamiltonian in which locality bounds for the system dynamics can be derived, this will be the approach of the following chapter.

Chapter 3

Locality Bounds

3.1 Introduction

In addition to many of the approaches used to try to find a simplified description of the environmental degrees of freedom of an open quantum system described in section 0.1, this problem fits into the wider context of understanding many-body dynamics which has been at the heart of many fundamental problems in mathematical physics. In this context, condensed matter and quantum computation theorists have a common interest in "complicated" states of many-body systems such as ground states. In such models, like their classical analogues, fortunately the interactions are either of finite range or their strength decays with a large inverse power (or even exponentially) in the distance between particles. From our everyday experience, we know that this local structure in classical systems is reflected in the dynamics by distant objects only being able to influence one another after a time proportional to the distance between them, such as the finite speed of sound in water or air. One might think, however, that this feature would not carry over to quantum mechanics since it has an additional layer of complexity due to entanglement not present in the classical theory. Especially since, as John Bell first pointed out in his seminal work of [50], that it is a highly non local phenomena and because these "complicated" states of many body quantum mechanical systems are, more often than not, also highly entangled. Luckily, while clearly the non-locality of entanglement is a powerful new feature and resource, it would not be just to say that the complexity implied by entanglement precludes a useful discussion of locality in quantum mechanics. One also may be thinking at this stage that such a result is obvious since even in

quantum mechanical theory there is always a known ultimate speed limit: the speed of light. However, it must be pointed out that this is a very different situation altogether than the one we are considering here. It applies to relativistic quantum field theory. This was constructed with the whole purpose in mind of being consistent with the theory of special relativity, and hence this theory was constructed in such a way that its very presence was there from the beginning. There is no "speed of sound" deliberately put into the non-relativistic theory of quantum mechanics, and the fact that such a speed exists, is a coincidental accident of the theory.

That this insight is true, was first made rigorous by Elliott H. Lieb and Derek W. Robinson in their seminal work [51] in 1972. In this work they prove that spin systems have a finite "speed of sound". The context is a spin system with Hilbert space $\mathcal{H} = \oplus_{k\in\mathcal{L}}\mathcal{H}_k$, $\mathcal{H}_k = \mathbb{C}^d$ on a lattice with $\mathcal{L}$ vertices and a finite range Hamiltonian $\hat{H} = \sum_{X\subset\mathcal{L}} \hat{\Delta}(X)$. Consider the Heisenberg evolution of a local operator $\hat{A}$ only acting non trivially on a subset of $\mathcal{L}$, under $\hat{H}$

$$\hat{A}(t) = e^{it\hat{H}}\hat{A}e^{-it\hat{H}}. \tag{3.1}$$

If we now consider its commutator with another local operator $\hat{B}$ only acting non trivially on another subset of $\mathcal{L}$, we have the bound

$$||[\hat{A}(t), \hat{B}]|| \leq C||\hat{A}||||\hat{B}||e^{-\mu(dist(A,B)-\nu|t|)}, \tag{3.2}$$

where $dist(A, B)$ is the shortest path between regions A and B, on the lattice, μ, C positive finite constants, and $||.||$ denotes the operator norm induced by the Euclidean vector norm. From now on this norm will simply be refered to as operator norm. The physical consequences of this bound are that outside of the so-called *causal light cone*, $\nu|t| < dist(A, B)$, one finds merely an exponential tail. In this sense we can only talk about a light cone in a vague way as compared with the strict light cones one encounters in relativistic quantum field theory; where the analogy with a light cone comes from. These bounds, and other bounds which allow for a similar causal light cone interpretation of the dynamics, are generically referred to as *Lieb Robinson bounds*, *Locality bounds*, or simply *proximity estimates* in the literature.

Since 1972, a vast amount of progress on the subject has been made and these bounds have been tightened [52, 53, 54], extended to more general graphs [55, 56] and to interacting fermionic systems [55]. Furthermore, many applications of the bounds have been found. They have been used to prove

area laws for entanglement [57] among many other things. However, progress has been much slower in the context of infinite dimensional Hilbert spaces such at bosonic systems. The main reason for this is that the proofs of Lieb-Robinson bounds almost always use a norm to bound the operators and for quantum systems on unbounded Hilbert spaces, the most interesting local operators are unbounded. In this context, Lieb Robinson bounds are known for Hamiltonians quadratic in its canonical position and momentum operators [59, 60] and certain anharmonic lattices [60]. In principle one could derive bounds of the form (3.2) for many different types of norms. The reason the operator norm is most commonly used, is because it is the physically relevant norm. Norms characterise the notion of length of vectors and by how much a vector can be amplified in the case of operators. The operator norm of a hermitian operator coincides with its largest eigenvalue in magnitude and hence for an observable, its largest value measured. Furthermore, one can write the norm using the well-known formula [61],

$$||B|| = \sup_{\hat{\rho}\in\mathcal{S}(\mathcal{H})} |tr[\hat{\rho}\hat{B}]|, \tag{3.3}$$

were $\mathcal{S}(\mathcal{H})$ denotes the set of all valid density operators for the Hilbert space. Therefore, if we consider the case where $\hat{B}$ is the difference between two observables $\hat{A}$ and $\hat{A}'$ we find

$$||\hat{A} - \hat{A}'|| = \sup_{\hat{\rho}\in\mathcal{S}(\mathcal{H})} |tr[\hat{\rho}\hat{A}] - tr[\hat{\rho}\hat{A}']|, \tag{3.4}$$

and hence if $||\hat{A}-\hat{A}'||$ is small the expectation value of the two observables will be almost the same for all states. In this chapter, we will derive bounds of this form with the difference that we will not maximise the quantity on the R.H.S. of Eq. (3.4) over all possible density operators, but instead, the bound will be dependent on the initial density operator. Doing so will, in principle, allow us to generate better bounds for particular initial states. The observables A and A' will take on the role of systems observables at time t i.e. operators which will only act non trivially on $\hat{H}_S$ at time t. They will differ by the fact that one evolves according to the full Hamiltonian and the other according to a truncated version of the full Hamiltonian. The reason for this is that the bath in Hamiltonian (1.1) when written in the form of the particle or phonon mapping Eqs. (10), (12), has infinitely many degrees of freedom and hence cannot be simulated exactly and hence truncating it is necessary (Unless one applies a Markovian approximation to the residual chain using some of the theories developed in Chapter 2). Here we will derive an error bound on system observables

when the Hamiltonian has been truncated in this way. For the sake of generality, we will derive the bounds for a more general Hamiltonian and then state the bounds for the case of the particle and phonon mappings as applications of the more general bound. The bounds we will derive will be new results and not direct consequences of any pre-existing bound found in the literature.

The content of this chapter is as follows. In section 3.2, we will introduce the Hamiltonian which will be considered. We will then proceed with deriving the Interaction and Schrödinger picture bounds. In section 3.2.1 we will make some additional assumptions of the form of the Hamiltonian. These will make the remaining results of the chapter easier to derive. In 3.2.2 we will make more explicit the interaction picture bound derived in section 3.2. In section 3.2.3 we show that the quantities which one would need to calculate in order to do a simulation in the interaction picture can be calculated with neglectable error. We will then proceed in section 3.2.4 to provide explicit bounds for the schrödinger picture bound derived in section 3.2 also. Then in section 3.3 we will work out some extensions to the bounds. In section 3.4 we will apply the results of the previous sections in this chapter to derive bounds for the particle and phonon mappings. Finally in section 3.5 we will summarise the results obtained in this chapter.

3.2 The Hamiltonian and Interaction and Schrödinger Main Bounds

The Hamiltonians considered in this chapter will be of the generic form

$$\hat{H} = \hat{H}_S \otimes \mathbb{I} + \hat{h}_s \otimes \hat{x}_0 + \mathbb{I} \otimes \frac{1}{2}\, \vec{r}^T H_B \vec{r} =: \hat{H}_S + \hat{I} + \hat{H}_B \tag{3.5}$$

where $\vec{r}^T = (\hat{x}_0, \hat{x}_1, \hat{x}_2, \ldots, \hat{p}_0, \hat{p}_1, \hat{p}_2, \ldots,)$ collects canonical position and momentum operators and $\hat{H}_S$ and $\hat{h}_s$ are hermitian operators acting on the system Hilbert space $\mathcal{S}$ as described in section 1.1. $\hat{H}_B$ is on $\oplus_{n=0}^{\infty}\mathfrak{h}_n$, where $\mathfrak{h}_n = L^2(\mathbb{R})$ is the Hilbert space of the bosonic modes. We will make the assumption that the Hamiltonain is well defined on some appropriate domain throughout this chapter. Let us introduce for notational convenience

$$\mathcal{L} = \begin{cases} \{\hat{x}_0, \hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{L-1}, \hat{p}_0, \hat{p}_1, \hat{p}_2, \ldots, \hat{p}_{L-1}\} & \text{if } L = 1, 2, 3, \ldots \\ \emptyset & \text{if } L = 0 \end{cases} \tag{3.6}$$

By and large, operators with super or subscripts $\mathcal{L}$ will have non trivial commutator relations with elements of the set $\mathcal{L}$ and commute with them if it has super or subscripts $\backslash\mathcal{L}$. In addition, we will omit the tensor product symbol $\otimes$ between operators and the identity operators for compactness of the expressions in this chapter. Throughout $\hat{O}_s$ will denote a system observable on $\mathcal{S}$. We will not need to assume $\hat{H}_S$ is bounded. We will develop bounds assuming that $\hat{O}_s$ and $\hat{h}_s$ are unbounded for generality, although the bounds will only be of much use when we make the additional assumption that they are bounded.

We will now derive a bound for then the truncation of the Hamiltonian is performed in a way that is reasonable if one is to calculate the dynamics in the interaction picture. Before we state the theorem, we will need to make a few definitions and concepts as follows. For the Hamiltonian in Eq. (3.5), let $\hat{\rho}_0$ be an initial state, and write $\hat{\rho}_s(t) := e^{-it\hat{H}}\hat{\rho}_0 e^{it\hat{H}}$ and define $\hat{O}_s(t) := e^{it\hat{H}_S}\hat{O}_s e^{-it\hat{H}_S}$, $\hat{h}_s(t) := e^{it\hat{H}_s}\hat{h}_s e^{-it\hat{H}_s}$, $\hat{x}_0(t) := e^{it\hat{H}_B}\hat{x}_0 e^{-it\hat{H}_B}$. We can simplify the last expression by noting it can be written as

$$\hat{x}_0(t) = e^{it\hat{H}_B}\hat{x}_0 e^{-it\hat{H}_B} =: \sum_{j=0}^{\infty} c_{j+1}(t)\hat{x}_j + \bar{c}_{j+1}(t)\hat{p}_j, \tag{3.7}$$

$c_j, \bar{c}_j \in \mathbb{C}$. We will use this form of $\hat{x}_0(t)$ to define how we will truncate the infinitely many degrees of freedom as follows

$$\hat{x}_0^{\mathcal{L}}(t) := \sum_{j=0}^{L-1} c_{j+1}(t)\hat{x}_j + \bar{c}_{j+1}(t)\hat{p}_j, \quad L = 0, 1, 2, \ldots \tag{3.8}$$

With these insights in mind, consider now

$$tr[\hat{O}_s\hat{\rho}_s(t)] = tr[\hat{O}_s(t)\hat{\rho}_I(t)], \tag{3.9}$$

where

$$\hat{\rho}_I(t) = e^{it(\hat{H}_S+\hat{H}_B)}\hat{\rho}_s(t)e^{-it(\hat{H}_S+\hat{H}_B)} = \hat{U}(t)\hat{\rho}_0\hat{U}^*(t) \tag{3.10}$$

solves

$$\begin{aligned} i\partial_t\hat{\rho}_I(t) &= [e^{it(\hat{H}_S+\hat{H}_B)}\hat{I}e^{-it(\hat{H}_S+\hat{H}_B)}, \hat{\rho}_I(t)] && (3.11)\\ &= [\hat{h}_s(t)\hat{x}_0(t), \hat{\rho}_I(t)] && (3.12) \end{aligned}$$

with initial condition $\hat{\rho}_I(0) = \hat{\rho}_0$ and $\hat{U}(t)$ solves

$$i\partial_t\hat{U}(t) = \hat{h}_s(t)\hat{x}_0(t)\hat{U}(t) \tag{3.13}$$

with initial condition $\hat{U}(0) = \mathbb{I}$. Now define $\hat{\rho}_0^{\mathcal{L}} := tr_{\setminus\mathcal{L}}[\hat{\rho}_0]$ and consider instead the solution $\hat{\rho}_I^{\mathcal{L}}(t) = \hat{U}_{\mathcal{L}}(t)\hat{\rho}_0^{\mathcal{L}}\hat{U}_{\mathcal{L}}^*(t)$ of

$$i\partial_t\hat{\rho}_I^{\mathcal{L}}(t) = [\hat{h}_s(t)\hat{x}_0^{\mathcal{L}}(t), \hat{\rho}_I^{\mathcal{L}}(t)] \tag{3.14}$$

with initial condition $\hat{U}_{\mathcal{L}}(0) = \mathbb{I}$. The following theorem was derived by Marcus Cramer.

Theorem 52. *The following bounds for the system observables of the truncated chain hold:*

$$\left|tr\left[\hat{O}_s\hat{\rho}_s(t)\right] - tr_{\mathcal{L}}\left[\hat{O}_s(t)\hat{\rho}_I^{\mathcal{L}}(t)\right]\right|^2 \leq 2\alpha(t)\int_0^t dx\beta(x)\sqrt{tr\left[(\hat{x}_0^{\setminus\mathcal{L}}(x))^2\hat{\rho}_0\right]}, \tag{3.15}$$

where,

$$\alpha(t) := \left(\sqrt{tr\left[\hat{U}_{\mathcal{L}}^*(t)\hat{O}_s^2(t)\hat{U}_{\mathcal{L}}(t)\hat{\rho}_0\right]} + \sqrt{tr\left[\hat{U}^*(t)\hat{O}_s^2(t)\hat{U}(t)\hat{\rho}_0\right]}\right)^2, \tag{3.16}$$

$$\beta(t) := \sqrt{tr\left[\hat{U}^*(t)\hat{h}_s^2(t)\hat{U}(t)\hat{\rho}_0\right]} \tag{3.17}$$

$$\hat{x}_0^{\setminus\mathcal{L}}(t) := \sum_{j=L}^{\infty} c_{j+1}(t)\hat{x}_j + \bar{c}_{j+1}(t)\hat{p}_j, \quad L = 0, 1, 2, \dots, \tag{3.18}$$

$$\tag{3.19}$$

Furthermore, if the system is finite-dimensional

$$\left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s(t)\hat{\rho}_I^L(t)]\right|^2 \leq 8||\hat{h}_s||\,||\hat{O}_s||^2\int_0^t ds\sqrt{tr\left[(\hat{x}_0^{\setminus\mathcal{L}}(s))^2\hat{\rho}_0\right]}. \tag{3.20}$$

Proof. Although quite tedious, the proof only involves very simple manipulations and the Cauchy Schwarz inequality plays the biggest role. We find

$$tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s(t)\hat{\rho}_I^{\mathcal{L}}(t)] = tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s(t)\hat{U}_{\mathcal{L}}(t)tr_{\setminus\mathcal{L}}[\hat{\rho}_0]\hat{U}_{\mathcal{L}}^*(t)] \tag{3.21}$$

$$=tr[\hat{O}_s(t)\left(\hat{\rho}_I(t) - \hat{\rho}_I^{\mathcal{L}}(t)\right)] \tag{3.22}$$

$$=tr[\hat{O}_s(t)\left(\hat{U}(t)\hat{\rho}_0\hat{U}^*(t) - \hat{U}_{\mathcal{L}}(t)tr_{\setminus\mathcal{L}}[\hat{\rho}_0]\hat{U}_{\mathcal{L}}^*(t)\right)] \tag{3.23}$$

$$=tr[\hat{O}_s(t)\left(\hat{U}(t)\hat{\rho}_0\hat{U}^*(t) - \hat{U}_{\mathcal{L}}(t)\hat{\rho}_0\hat{U}_{\mathcal{L}}^*(t)\right)] \tag{3.24}$$

$$=tr[\hat{O}_s(t)\left([\hat{U}(t) - \hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0\hat{U}_{\mathcal{L}}(t)\hat{\rho}_0[\hat{U}^*(t) - \hat{U}_{\mathcal{L}}^*(t)]\right)], \tag{3.25}$$

where applying the Cauchy-Schwarz inequality $tr[\hat{A}\hat{B}^*\hat{\rho}_0]^2 \leq tr[\hat{A}\hat{A}^*\hat{\rho}_0]tr[\hat{B}\hat{B}^*\hat{\rho}_0]$,

$$\left|tr[\hat{O}_s(t)[\hat{U}(t) - \hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0\hat{U}^*(t)]\right| = \left|tr[\hat{U}^*(t)\hat{O}_s(t)[\hat{U}(t) - \hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0]\right| \tag{3.26}$$

$$= \sqrt{tr\left[\hat{U}^*(t)\hat{O}_s^2(t)\hat{U}(t)\hat{\rho}_0\right]tr\left[[\hat{U}^*(t) - \hat{U}_{\mathcal{L}}^*(t)][\hat{U}(t) - \hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0\right]} \tag{3.27}$$

and, similarly,

$$\left|tr[\hat{O}_s(t)\hat{U}_{\mathcal{L}}(t)\hat{\rho}_0[\hat{U}^*(t)-\hat{U}^*_{\mathcal{L}}(t)]]\right| \tag{3.28}$$

$$\leq \sqrt{tr\left[\hat{U}^*_{\mathcal{L}}(t)\hat{O}^2_s(t)\hat{U}_{\mathcal{L}}(t)\hat{\rho}_0\right] tr\left[[\hat{U}^*(t)-\hat{U}^*_{\mathcal{L}}][\hat{U}(t)-\hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0\right]}. \tag{3.29}$$

Hence,

$$\left|tr[\hat{O}_s\hat{\rho}(t)]-tr_{\mathcal{L}}[\hat{O}_s(t)\hat{\rho}^{\mathcal{L}}_I(t)]\right|^2 \leq \alpha(t)tr\left[[\hat{U}^*(t)-\hat{U}^*_{\mathcal{L}}(t)][\hat{U}(t)-\hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0\right]. \tag{3.30}$$

Now,

$$tr\left[[\hat{U}^*(t)-\hat{U}^*_{\mathcal{L}}(t)][\hat{U}(t)-\hat{U}_{\mathcal{L}}(t)]\hat{\rho}_0\right] =tr\left[[\mathbb{I}+\mathbb{I}_{\mathcal{L}}-\hat{U}^*(t)\hat{U}_{\mathcal{L}}(t)-\hat{U}^*_{\mathcal{L}}(t)\hat{U}(t)]\hat{\rho}_0\right] \tag{3.31}$$

$$=2-2\mathrm{Re}tr\left[\hat{U}^*(t)\hat{U}_{\mathcal{L}}(t)\hat{\rho}_0\right] \tag{3.32}$$

$$=-2\mathrm{Re}\int_0^t dxtr\left[\partial_x\hat{U}^*(x)\hat{U}_{\mathcal{L}}(x)\hat{\rho}_0\right] \tag{3.33}$$

$$=-2\mathrm{Re}\int_0^t dx\left[\left([\partial_x\hat{U}^*(x)]\hat{U}_{\mathcal{L}}(x)+\hat{U}^*(x)\partial_x\hat{U}_{\mathcal{L}}(x)\right)\hat{\rho}_0\right], \tag{3.34}$$

where

$$[\partial_x\hat{U}^*(x)]\hat{U}_{\mathcal{L}}(x)+\hat{U}^*(x)\partial_x\hat{U}_{\mathcal{L}}(x) =i\hat{U}^*(x)\hat{h}_s(x)\hat{x}_0(x)\hat{U}_{\mathcal{L}}(x)-i\hat{U}^*(x)\hat{h}_s(x)\hat{x}^{\mathcal{L}}_0(x)\hat{U}_{\mathcal{L}}(x) \tag{3.35}$$

$$=i\hat{U}^*(x)\hat{h}_s(x)\hat{x}^{\backslash\mathcal{L}}_0(x)\hat{U}_{\mathcal{L}}(x) \tag{3.36}$$

$$=i\hat{U}^*(x)\hat{h}_s(x)\hat{U}_{\mathcal{L}}(x)\hat{x}^{\backslash\mathcal{L}}_0(x), \tag{3.37}$$

i.e.,

$$tr\left[[\hat{U}^*(x)-\hat{U}^*_{\mathcal{L}}(x)][\hat{U}(x)-\hat{U}_{\mathcal{L}}(x)]\hat{\rho}_0\right] \leq 2\int_0^t dx\left|tr\left[\hat{U}^*(x)\hat{h}_s(x)\hat{U}_{\mathcal{L}}(x)\hat{x}^{\backslash\mathcal{L}}_0(x)\hat{\rho}_0\right]\right|, \tag{3.38}$$

where (again, applying a Cauchy-Schwarz inequality)

$$\left|tr\left[\hat{U}^*(x)\hat{h}_s(x)\hat{U}_{\mathcal{L}}(x)\hat{x}^{\backslash\mathcal{L}}_0(x)\hat{\rho}_0\right]\right| \leq \beta(x)\sqrt{tr\left[(\hat{x}^{\backslash\mathcal{L}}_0(x))^2\hat{\rho}_0\right]}. \tag{3.39}$$

To summerise,

$$\left|tr\left[\hat{O}_s\hat{\rho}_s(t)\right]-tr_{\mathcal{L}}\left[\hat{O}_s(t)\hat{\rho}^{\mathcal{L}}_I\right]\right|^2 \leq 2\alpha(t)\int_0^t dx\beta(x)\sqrt{tr\left[(\hat{x}^{\backslash\mathcal{L}}_0(x))^2\hat{\rho}_0\right]}, \tag{3.40}$$

where, if $\hat{O}_s$, $\hat{h}_s$ are bounded we have $\alpha(t)\beta(t) \leq 4||\hat{O}_s||^2||\hat{h}_s||$, were we have used identity (3.3) and hence the bound reduces to Eq. (3.20). □

Definition 53. *We will refer to this bound as the* Interaction Picture Bound.

At this stage, it is probably not clear the significance of this bound, since it is not immediately obvious that the R.H.S. of Eq. (3.20) is small for sufficiently large L. In the next section, we will show that indeed this is the case. We should also point out that if one were to use this method to simulate $tr[\hat{O}_s\hat{\rho}_I^{\mathcal{L}}]$, then one would need to calculate the quantity $\hat{x}_0^{\mathcal{L}}(t)$ numerically. However, in order to do this, one must be able to calculate the coefficients $\{c_j(t), \bar{c}_j(t)\}_{j=1}^{L}$ (see Eq (3.8)). This requires exponentiation of the matrix $t\sigma H_B$, $\sigma_{ij} = [\hat{r}_i, \hat{r}_j]$. One will never be able to do this exactly, since H_B is an infinite dimensional matrix. In practice one would only be able to exponentiate its truncated finite dimensional counterpart. Later in lemma 60 we will derive bounds that show this can be done with neglectable error. Before we proceed to derive explicit bounds for (3.20), we will derive a similar bound as in theorem 52), but when the truncation is performed in the Schrödinger picture. In this case the way the Hamiltonian is truncated is much more direct and natural. Let us write $\hat{H}_B$ in the form $\hat{H}_B = \frac{1}{2}\sum_{i,j=0}^{\infty} \hat{x}_i X_{i+1,j+1}\hat{x}_j + \hat{p}_i P_{i+1,j+1}\hat{p}_j + \hat{x}_i Z_{i+1,j+1}\hat{p}_j + \hat{p}_i Z^*_{i+1,j+1}\hat{x}_j$. We can now define

$$\hat{H}_B^{\mathcal{L}} := \vec{r}_{\mathcal{L}}^{T} H_B^{\mathcal{L}} \vec{r}_{\mathcal{L}} \tag{3.41}$$

where

$$H_B^{\mathcal{L}} = \begin{bmatrix} [X]_{[1:L,1:L]} & [Z]_{[1:L,1:L]} \\ [Z^*]_{[1:L,1:L]} & [P]_{[1:L,1:L]} \end{bmatrix}, \tag{3.42}$$

and $\vec{r}_{\mathcal{L}}^{T} = (\hat{x}_0, \hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{L-1}, \hat{p}_0, \hat{p}_1, \hat{p}_2, \ldots, \hat{p}_{L-1})$

It is now appropriate for later use to introduce the quantities c_j^L, $\bar{c}_j^L$

$$e^{it\hat{H}_B^{\mathcal{L}}}\hat{x}_0 e^{-it\hat{H}_B^{\mathcal{L}}} =: \sum_{j=0}^{L-1} c_{j+1}^L(t)\hat{x}_j + \bar{c}_{j+1}^L(t)\hat{p}_j, \quad L = 0, 1, 2, \ldots \tag{3.43}$$

$c_j^L, \bar{c}_j^L \in \mathbb{C}$. c.f. Eq. (3.7).

Theorem 54. *Let* $\hat{\rho}_s^{\mathcal{L}}(t) := e^{-it(\hat{H}_s + \hat{H}_B^{\mathcal{L}} + \hat{h}_s\hat{x}_0)}\hat{\rho}_0^{\mathcal{L}} e^{it(\hat{H}_s + \hat{H}_B^{\mathcal{L}} + \hat{h}_s\hat{x}_0)}$. *Then*

$$\left| tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s\hat{\rho}_s^{\mathcal{L}}(t)] \right|^2 \leq \tag{3.44}$$

$$2\alpha(t)\left(\int_0^t dx\beta(x) \sqrt{\left(\sum_{i=0}^{2L-1} \nabla_i^L(x)\right)\left(\sum_{i=0}^{2L-1} \nabla_i^L(x) tr[\hat{r}_i^2\hat{\rho}_s(x)]\right)} \right. \tag{3.45}$$

$$\left. + \int_0^t dx\beta(x)\sqrt{tr[(\hat{x}_0^{\backslash\mathcal{L}}(x))^2\hat{\rho}_0]} \right). \tag{3.46}$$

where

$$\nabla_i^L(x) := \sum_{j=0}^{2L-1} |A_j^L(x) C_{j+1,i+1}^L(-x)|, \tag{3.47}$$

$$A_i^L(t) := C_{1,i+1}(t) - C_{1,i+1}^L(t), \tag{3.48}$$

and the $C_{i,j}, C_{i,j}^L \in \mathbb{C}$ *are define by*

$$\hat{r}_i^{\mathcal{L}}(t) = e^{it\hat{H}_B^{\mathcal{L}}} \hat{r}_i e^{-it\hat{H}_B^{\mathcal{L}}} = \sum_{j=0}^{2L-1} C_{i+1,j+1}^L(t) \hat{r}_j, \tag{3.49}$$

$$e^{it\hat{H}_B} \hat{r}_i e^{-it\hat{H}_B} = \sum_{j=0}^{\infty} C_{i+1,j+1}(t) \hat{r}_j. \tag{3.50}$$

As in theorem 52, if $\hat{O}_s$, $\hat{h}_s$ *are bounded we have* $\alpha(t)\beta(x) \leq 4||\hat{O}_s||^2||\hat{h}_s||$.

Proof. This follows practically the same steps as the proof of theorem 52, the only difference being we will define $\hat{U}_{\mathcal{L}}$ differently and denote it by $\hat{\tilde{U}}_{\mathcal{L}}$ to distinguish it. Let

$$\hat{\tilde{U}}_{\mathcal{L}}(t) := e^{it(\hat{H}_s + \hat{H}_B^{\mathcal{L}})} e^{-it(\hat{H}_s + \hat{H}_B^{\mathcal{L}} + \hat{h}_s \hat{x}_0)}. \tag{3.51}$$

We will also need a quantity which can be view as the difference between the two different ways we have truncated $\hat{H}_B$ in this section:

$$\delta\hat{x}_0^{\mathcal{L}}(t) := \sum_{i=0}^{L-1} (c_{i+1}(t) - c_{i+1}^L(t))\hat{x}_j + (\bar{c}_{i+1}(t) - \bar{c}_{i+1}^L(t))\hat{p}_j. \tag{3.52}$$

From the above definitions and the commutators $[\hat{H}_s, \hat{H}_B] = [\hat{O}_s, \hat{H}_B] = 0$ it follows

$$tr[\hat{O}_s \hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s \hat{\rho}_s^{\mathcal{L}}(t)] = tr[\hat{O}_s(t)(\hat{U}(t)\hat{\rho}_0\hat{U}^*(t) - \hat{\tilde{U}}_{\mathcal{L}}(t)\hat{\rho}_0\hat{\tilde{U}}_{\mathcal{L}}^*(t))] \tag{3.53}$$

$$= tr[\hat{O}_s(t)([\hat{U}(t) - \hat{\tilde{U}}_{\mathcal{L}}(t)]\hat{\rho}_0\hat{U}^*(t))] + tr[\hat{O}_s(t)\hat{\tilde{U}}_{\mathcal{L}}(t)\hat{\rho}_0[\hat{U}^*(t) - \hat{\tilde{U}}_{\mathcal{L}}^*(t)]] \tag{3.54}$$

where appling the Cauchy-Schwarz inequality $tr[\hat{A}\hat{B}^*\hat{\rho}_0]^2 \leq tr[\hat{A}\hat{A}^*\hat{\rho}_0]tr[\hat{B}\hat{B}^*\hat{\rho}_0]$,

$$\left|tr[\hat{O}_s(t)[\hat{U}(t) - \hat{\tilde{U}}_{\mathcal{L}}(t)]\hat{\rho}_0\hat{U}^*(t)]\right| = \left|tr[\hat{U}^*(t)\hat{O}_s(t)[\hat{U}(t) - \hat{\tilde{U}}_{\mathcal{L}}(t)]\hat{\rho}_0]\right| \tag{3.55}$$

$$= \sqrt{tr\left[\hat{U}^*(t)\hat{O}_s^2(t)\hat{U}(t)\hat{\rho}_0\right] tr\left[[\hat{U}^*(t) - \hat{\tilde{U}}_{\mathcal{L}}^*(t)][\hat{U}(t) - \hat{\tilde{U}}_{\mathcal{L}}(t)]\hat{\rho}_0\right]} \tag{3.56}$$

and, similarly,

$$\left|tr[\hat{O}_s(t)\hat{\bar{U}}_{\mathcal{L}}(t)\hat{\rho}_0[\hat{U}^*(t) - \hat{\bar{U}}^*_{\mathcal{L}}(t)]]\right| \tag{3.57}$$

$$\leq \sqrt{tr\left[\hat{U}^*_{\mathcal{L}}(t)\hat{O}^2_s(t)\hat{\bar{U}}_{\mathcal{L}}(t)\hat{\rho}_0\right] tr\left[[\hat{U}^*(t) - \hat{\bar{U}}^*_{\mathcal{L}}][\hat{U}(t) - \hat{\bar{U}}_{\mathcal{L}}(t)]\hat{\rho}_0\right]}. \tag{3.58}$$

Hence,

$$\left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s\hat{\rho}^{\mathcal{L}}_s(t)]\right|^2 \leq \alpha(t)\left|tr\left[[\hat{U}^*(t) - \hat{\bar{U}}^*_{\mathcal{L}}(t)][\hat{U}(t) - \hat{\bar{U}}_{\mathcal{L}}(t)]\hat{\rho}_0\right]\right| \tag{3.59}$$

where

$$\alpha(t) = \left(\sqrt{tr\left[\hat{\bar{U}}^*_{\mathcal{L}}(t)\hat{O}^2_s(t)\hat{\bar{U}}_{\mathcal{L}}(t)\hat{\rho}_0\right]} + \sqrt{tr\left[\hat{U}^*(t)\hat{O}^2_s(t)\hat{U}(t)\hat{\rho}_0\right]}\right)^2. \tag{3.60}$$

Now,

$$tr\left[[\hat{U}^*(t) - \hat{U}^*_{\mathcal{L}}(t)][\hat{U}(t) - \hat{\bar{U}}_{\mathcal{L}}(t)]\hat{\rho}_0\right] = tr\left[[\mathbb{I} + \mathbb{I}_{\mathcal{L}} - \hat{U}^*(t)\hat{\bar{U}}_{\mathcal{L}}(t) - \hat{\bar{U}}^*_{\mathcal{L}}(t)\hat{U}(t)]\hat{\rho}_0\right] \tag{3.61}$$

$$= 2 - 2\mathrm{Re}tr\left[\hat{U}^*(t)\hat{\bar{U}}_{\mathcal{L}}(t)\hat{\rho}_0\right] \tag{3.62}$$

$$= -2\mathrm{Re}\int_0^t dx tr\left[\partial_x\hat{U}^*(x)\hat{\bar{U}}_{\mathcal{L}}(x)\hat{\rho}_0\right] \tag{3.63}$$

$$= -2\mathrm{Re}\int_0^t dx tr\left[\left([\partial_x\hat{U}^*(x)]\hat{\bar{U}}_{\mathcal{L}}(x) + \hat{U}^*(x)\partial_x\hat{\bar{U}}_{\mathcal{L}}(x)\right)\hat{\rho}_0\right], \tag{3.64}$$

where

$$\begin{aligned}[\partial_x\hat{U}^*(x)]\hat{\bar{U}}_{\mathcal{L}}(x) + \hat{U}^*(x)\partial_x\hat{\bar{U}}_{\mathcal{L}}(x) =& i\hat{U}^*(x)\hat{h}_s(x)\hat{x}_0(x)\hat{\bar{U}}_{\mathcal{L}}(x) - i\hat{U}^*(x)\hat{h}_s(x)\hat{x}^{\mathcal{L}}_0(x)\hat{\bar{U}}_{\mathcal{L}}(x)\\ =& i\hat{U}^*(x)\hat{h}_s(x)(\delta\hat{x}^{\mathcal{L}}_0(x) + \hat{x}^{\backslash\mathcal{L}}_0(t))\hat{\bar{U}}_{\mathcal{L}}(x)\\ =& i\hat{U}^*(x)\hat{h}_s(x)\delta\hat{x}^{\mathcal{L}}_0(x)\hat{\bar{U}}_{\mathcal{L}}(x) + i\hat{U}^*(x)\hat{h}_s(x)\hat{x}^{\backslash\mathcal{L}}_0(t)\hat{\bar{U}}_{\mathcal{L}}(x).\end{aligned} \tag{3.65}$$

Hence,

$$\begin{aligned}\left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s\hat{\rho}^{\mathcal{L}}_s(t)]\right|^2 \leq& \alpha(t)2\Big|\int_0^t dx tr[\hat{U}^*(x)\hat{h}_s(x)\delta\hat{x}^{\mathcal{L}}_0(x)\hat{\bar{U}}_{\mathcal{L}}(x)\hat{\rho}_0]\\ &+ \int_0^t dx tr[\hat{U}^*(x)\hat{h}_s(x)\hat{\bar{U}}_{\mathcal{L}}(x)\hat{x}^{\backslash\mathcal{L}}_0(t)\hat{\rho}_0]\Big|.\end{aligned} \tag{3.66}$$

Now using Cauchy Schwarz inequality, we find

$$\left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s\hat{\rho}^{\mathcal{L}}_s(t)]\right|^2 \leq \tag{3.67}$$

$$2\alpha(t)\left(\int_0^t dx\beta(x)\sqrt{tr[\hat{\bar{U}}^*_{\mathcal{L}}(x)(\delta\hat{x}^{\mathcal{L}}_0(x))^2\hat{\bar{U}}_{\mathcal{L}}(x)\hat{\rho}_0]} + \int_0^t dx\beta(x)\sqrt{tr[(\hat{x}^{\backslash\mathcal{L}}_0(x))^2\hat{\rho}_0]}\right), \tag{3.68}$$

where β is defined in Eq. (3.17). We already have bounds for the second term in (3.68), so we will concentrate on the first term. Using the definition of $A_i^L(t)$ we have,

$$tr[\hat{\bar{U}}^*_{\mathcal{L}}(x)(\delta\hat{x}_0^{\mathcal{L}}(x))^2\hat{\bar{U}}_{\mathcal{L}}(x)\hat{\rho}_0] = \sum_{i,j=0}^{2L-1} A_i^L(x)A_j^L(x)tr[\hat{\bar{U}}^*_{\mathcal{L}}(x)\hat{r}_i\hat{r}_j\hat{\bar{U}}_{\mathcal{L}}(x)\hat{\rho}_0] \tag{3.69}$$

$$= \sum_{i,j=0}^{2L-1} A_i^L(x)A_j^L(x)tr[\hat{\bar{r}}_i^{\mathcal{L}}(-x)\hat{\bar{r}}_j^{\mathcal{L}}(-x)\hat{\rho}_s^{\mathcal{L}}(x)] \tag{3.70}$$

$$= \sum_{i,j,k,l=0}^{2L-1} A_i^L(x)A_j^L(x)C^L_{i+1,k+1}(-x)C^L_{j+1,l+1}(-x)tr[\hat{r}_k\hat{r}_l\hat{\rho}_s^{\mathcal{L}}(x)]. \tag{3.71}$$

After symmetrising, using $\hat{r}_k\hat{r}_l + \hat{r}_l\hat{r}_k \leq \hat{r}_k^2 + \hat{r}_l^2$ followed by the triangle inequality and taking into account Eq. (3.47),

$$tr[\hat{\bar{U}}^*_{\mathcal{L}}(x)(\delta\hat{x}_0^{\mathcal{L}}(x))^2\hat{\bar{U}}_{\mathcal{L}}(x)\hat{\rho}_0] \leq \left(\sum_{i=0}^{2L-1}\nabla_i^L(x)\right)\left(\sum_{i=0}^{2L-1}\nabla_i^L(x)tr[\hat{r}_i^2\hat{\rho}_s^{\mathcal{L}}(x)]\right). \tag{3.72}$$

Hence, from Eqs. (3.68), (3.71), and (3.72), it follows Eq. (3.44) □

Definition 55. *We will refer to this bound as the* Schrödinger Picture Bound.

As we can see from (3.44), the bound has two terms. The second term we have already seen. It is the quantity appearing on the R.H.S. of the bound in the interaction picture (theorem 52). The first term, is a new term which can be thought of as the difference between the two different ways of truncating the Hamiltonian $\hat{H}_B$ on $\mathcal{L}$ that we have considered. As we will see in section 3.2.4, this term can be upper bounded by a function that approaches zero as L gets larger. We will now make some additional assumptions before bounding these terms.

3.2.1 Some Additional Assumptions

For now on, unless stated otherwise, the following assumptions on $\hat{H}_B$ will be made:

1) $\hat{H}_B$ has only nearest neighbour coupling. In principle, one could probably generalise these results to arbitrary local coupling by a generalisation of theorem 59 beyond tridiagonal matrices, but since our main goal is to find bounds for the particle and phonon mappings which are nearest neighbour, we will not worry about this generalisation here.

2) $\hat{H}_B$ only has position-position and momentum-momentum coupling (if this is not the case, it is sometimes possible to satisfy this condition by local canonical transformations of the form $\{\hat{x}_i, \hat{p}_i\} \mapsto \{-\hat{p}_i, \hat{x}_i\}$).

With these two assumptions we have

$$\hat{H}_B = \frac{1}{2}\left(\sum_{i,j} \hat{x}_i X_{i,j} \hat{x}_j + \sum_{i,j} \hat{p}_i P_{i,j} \hat{p}_j\right) \tag{3.73}$$

where X and P are tridiagonal matrices. We will also assume for convenience that $t \geq 0$. Sometimes we will need to make some extra assumptions[1]. Assumption $A1$ will not be assumed unless stated otherwise:

Assumption $A1$**:** $P_{ii} \geq 0$, $X_{ii} \geq 0$, *and if* $P \neq \mathbb{I}$, *then* $sign(X_{i,i+1} + X_{i+1,i}) = sign(P_{i,i+1} + P_{i+1,i})$ $\forall i$.

3.2.2 Explicit Bounds for the Interaction Picture Bound

In this section we will find bounds for

$$\int_0^t dx \beta(x) \sqrt{tr[(\hat{x}_0^{\backslash \mathcal{L}}(x))^2 \hat{\rho}_0]} \tag{3.74}$$

with the assumption that $\hat{h}_s$ is bounded. This will allow us to find explicit values for the interaction picture bound (theorem 52) and one of the terms in the schrödinger picture bound (theorem 54). We will start with a lemma which bounds the coefficients c_j, $\bar{c}_j$ appearing in Eq. (3.74).

Lemma 56. *The coefficients* $c_j(t)$, $\bar{c}_j(t)$, $j = 1, 2, 3, \ldots$ (defined in Eq. 3.7) *are bounded by*

$$|c_j(t)| \leq \sum_{n=e(j)}^{\infty} \frac{t^{2n}}{(2n)!} ||PX||^n \tag{3.75}$$

$$|\bar{c}_j(t)| \leq \sum_{n=f(j)}^{\infty} \frac{t^{2n+1}}{(2n+1)!} ||PX||^n ||P||, \tag{3.76}$$

where

$$e(j) = \lfloor (j-1)/2 \rfloor, \quad f(j) = \lfloor (j-2)/2 \rfloor, \quad \forall X, P \tag{3.77}$$

[1]As with 1) above, it should be possible to get around these difficulties but they are automatically satisfied by the particle and phonon mappings anyway so we will not look into this here

$\lfloor . \rfloor$ *rounds up to the nearest integer and is defined by* $\lfloor x \rfloor = min(z \in \mathbb{Z}, x \leq z)$.
If $P = \mathbb{I}$*, then alternatively*

$$e(j) = f(j) = j - 1, \tag{3.78}$$

and $||P|| = 1$.

Proof. This proof follows very closely the proofs in [59] although the results here are not a direct consequnce of them.
From Eq. (3.73) we can write $H_B = X \oplus P$. Consider the time evolution of $\hat{r}_n$, the nth component of vector $\vec{r} = (\hat{x}_0, \hat{x}_1, \hat{x}_2, \ldots, \hat{p}_0, \hat{p}_1, \hat{p}_2, \ldots)$ under the Hamiltonian $\hat{H}_B$

$$\hat{r}_n(t) = e^{it\hat{H}_B} \hat{r}_n e^{-it\hat{H}_B}. \tag{3.79}$$

By solving Heisenburg's equations of motion, we find

$$\hat{r}_j(t) = \sum_{k=0}^{\infty} C_{j+1,k+1} \hat{r}_k, \quad j = 0, 1, 2, \ldots, \tag{3.80}$$

where

$$C_{ij}(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n+1}}{(2n+1)!} \begin{pmatrix} 0 & (PX)^n P \\ -(XP)^n X & 0 \end{pmatrix}_{ij} \tag{3.81}$$

$$+ \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n}}{(2n)!} \begin{pmatrix} (PX)^n & 0 \\ 0 & (XP)^n \end{pmatrix}_{ij} \tag{3.82}$$

$$i, j = 1, 2, 3, \ldots. \tag{3.83}$$

Hence for $\hat{x}_0(t)$, we have

$$\hat{x}_0(t) = \sum_{j=0}^{\infty} c_{j+1}(t) \hat{x}_j + \bar{c}_{j+1}(t) \hat{p}_j, \tag{3.84}$$

where

$$c_j(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n}}{(2n)!} [(PX)^n]_{1j} \tag{3.85}$$

$$\bar{c}_j(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n+1}}{(2n+1)!} [(PX)^n P]_{1j} \quad j = 1, 2, 3, \ldots. \tag{3.86}$$

We now note that for any real square matrices A, B, the operator norm satisfies

1) Is a sub multiplicative norm

$$||AB|| \leq ||A|||B|| \tag{3.87}$$

2) The absolute value of the components of the matrix A satisfy

$$|A_{ij}| \leq ||A|| \tag{3.88}$$

Taking into account the above identities and the triangle inequality, we can upper bound the magnitude of the coefficients in Eqs (3.85) and (3.86)

$$|c_j(t)| \leq \sum_{n=e(j)}^{\infty} \frac{t^{2n}}{(2n)!}||PX||^n \tag{3.89}$$

$$|\bar{c}_j(t)| \leq \sum_{n=f(j)}^{\infty} \frac{t^{2n+1}}{(2n+1)!}||PX||^n||P||, \tag{3.90}$$

where we assume $t \geq 0$ and $e(j)$ is any function which satisfies $[(PX)^n]_{1j} = 0$ for all non negative integers $n < e(j)$ and similarly for $f(j)$: $[(PX)^n P]_{1j} = 0$ for all non negative integers $n < f(j)$. Applying lemma 1 in sec 3.2 of [59], we can derive an expression for the functions e and f with X and P tridiagonal matrices we find (3.77). For P the identity we achieve (3.78). □

This lemma will be the main ingredient in the following two theorems

Theorem 57. *If all initial two point correlation functions are bounded by* $|tr[\hat{x}_j\hat{x}_k\hat{\rho}_0| \leq D$, $|tr[\hat{x}_j\hat{p}_k\hat{\rho}_0]| \leq D\frac{\sqrt{||PX||}}{||P||}$, $|tr[\hat{p}_j\hat{x}_k\hat{\rho}_0]| \leq D\frac{\sqrt{||PX||}}{||P||}$, $|tr[\hat{p}_j\hat{p}_k\hat{\rho}_0]| \leq D\frac{||PX||}{||P||^2}$, *for some* $D \geq 0$, *then*

$$\int_0^t ds\sqrt{tr[(\hat{x}_0^{\backslash\mathcal{L}}(s))^2\hat{\rho}_0]} \leq \begin{cases} \sqrt{\frac{D}{||PX||}}\sum_{j=1}^{\infty} j\frac{\tau^{j+L}}{(j+L)!} & \forall X, P \\ \sqrt{\frac{D}{||PX||}}\sum_{j=1}^{\infty} \lfloor j/2 \rfloor \frac{\tau^{j+2L}}{(j+2L)!} & \text{if } P = \mathbb{I} \end{cases} \tag{3.91}$$

$L = 0, 1, 2, \ldots$, *where* $\tau = \tau(t) := \sqrt{||PX||}\, t$. *We can further bound this by*

$$\sum_{j=1}^{\infty} j\frac{\tau^{j+L}}{(j+L)!} \leq \frac{(e^\tau - 1)}{(L-1)!}\tau^L \leq \frac{e^{\tau + \ln\tau + (L-1)(1+\ln\tau - \ln(L-1))}}{\sqrt{L-1}}, \tag{3.92}$$

$$\sum_{j=1}^{\infty} \lfloor j/2 \rfloor \frac{\tau^{j+2L}}{(j+2L)!} \leq \frac{1}{2}\left(1 + \frac{1}{L}\right)\frac{(e^\tau - 1)}{(2L-1)!}\tau^{2L} \tag{3.93}$$

$$\leq \frac{1 + 1/L}{\sqrt{2L-1}} e^{\tau + \ln\tau + (2L-1)(1+\ln\tau - \ln(2L-1))}, \tag{3.94}$$

for $L = 2, 3, 4, \ldots$

Proof. From the definitions in the lemma, taking into account that $\sqrt{x}$ is monotonically increasing for $x \geq 0$, and using the triangle inequality, we find

$$\int_0^t ds \sqrt{tr[(\hat{x}_0^{\setminus\mathcal{L}}(s))^2 \hat{\rho}_0]} \leq \sqrt{D} \int_0^t ds \sum_{k=L}^{\infty} \left(|c_{k+1}(s)| + \frac{\sqrt{||PX||}}{||P||} |\bar{c}_{k+1}(s)| \right) \tag{3.95}$$

$$\leq \sqrt{\frac{D}{||PX||}} \sum_{k=L+1}^{\infty} \left(\sum_{n=e(k)}^{\infty} \frac{\tau^{2n+1}}{(2n+1)!} + \sum_{n=f(k)+1/2}^{\infty} \frac{\tau^{2n+1}}{(2n+1)!} \right) \tag{3.96}$$

where in the last line we have used Eqs (3.75) and (3.76). Taking into account the values of e and f stated in Lemma 56 and the formula $\sum_{i,j=0} f(i+j) = \sum_{i=0}(i+1)f(i)$, appling simple manipulations to Eq. (3.96), we achieve (3.91). Applying Taylor's theorem with the Lagrange form of the reminder [62], to the Taylor expansion of the exponential function followed by using the indentity $1/d! \leq (e/d)^d d^{-1/2}$, $d \in \mathbb{N}$, we finally achieve Eqs. (3.92), (3.94). □

So we see that one gets faster than exponential decay for sufficiently large L. This will be a continuing theme through this chapter. If the initial two point correlation functions are unbounded, one can still achieve good bounds

Theorem 58.

$$\int_0^t ds \sqrt{tr[(\hat{x}_0^{\setminus\mathcal{L}}(s))^2 \hat{\rho}_0]} \tag{3.97}$$

$$\leq \frac{1}{\sqrt{||PX||}} \sum_{k=L}^{\infty} \left(d_k \sum_{n=e(k)}^{\infty} \frac{\tau(t)^{2n+1}}{(2n+1)!} + \frac{\bar{d}_k ||P||}{\sqrt{||PX||}} \sum_{n=f(k)+1/2}^{\infty} \frac{\tau(t)^{2n+1}}{(2n+1)!} \right) \tag{3.98}$$

$$\leq \sinh(\tau(t)) \sum_{k=L}^{\infty} \left(d_k \frac{\tau(t)^{2e(k)}}{(2e(k))!} + \frac{\bar{d}_k ||P||}{\sqrt{||PX||}} \frac{\tau(t)^{2f(k)+1}}{(2f(k)+1)!} \right), \tag{3.99}$$

$L = 1, 2, 3, \ldots,$ *where*

$$d_k = \begin{cases} 1 & \text{if } tr[\hat{x}_k^2 \hat{\rho}_0] \leq 1 \\ tr[\hat{x}_k^2 \hat{\rho}_0] & \text{otherwise,} \end{cases}; \quad \bar{d}_k = \begin{cases} 1 & \text{if } tr[\hat{p}_k^2 \hat{\rho}_0] \leq 1 \\ tr[\hat{p}_k^2 \hat{\rho}_0] & \text{otherwise.} \end{cases} \tag{3.100}$$

Proof. From definition Eq. (3.50),

$$\int_0^t ds\sqrt{tr[(\hat{x}_0^{\setminus\mathcal{L}}(s))^2\hat{\rho}_0]} \tag{3.101}$$

$$=\int_0^t ds\sqrt{\frac{1}{2}\sum_{j,k=L}^{\infty} C_{1,j+1}(s)C_{1,k+1}(s)tr[(\hat{r}_j\hat{r}_k+\hat{r}_k\hat{r}_j)\hat{\rho}_0]} \tag{3.102}$$

$$\leq\int_0^t ds\sqrt{\frac{1}{2}\sum_{j,k=L}^{\infty} |C_{1,j+1}(s)C_{1,k+1}(s)|tr[(\hat{r}_j^2+\hat{r}_k^2)\hat{\rho}_0]} \tag{3.103}$$

$$\leq\int_0^t ds\sqrt{\left(\sum_{j=L}^{\infty}|C_{1,j+1}(s)|\right)\left(\sum_{k=L}^{\infty}|C_{1,k+1}(s)|tr[\hat{r}_k^2\hat{\rho}_0]\right)} \tag{3.104}$$

$$\leq\sum_{k=1}^{\infty} D_k\int_0^t |C_{1,k+1}(s)|ds \tag{3.105}$$

where

$$D_k=\begin{cases}1 & \text{if } tr[\hat{r}_k^2\hat{\rho}_0]\leq 1\\ tr[\hat{r}_k^2\hat{\rho}_0] & \text{otherwise.}\end{cases} \tag{3.106}$$

Now substituting Eqs. (3.75), (3.76) into Eq. (3.104) we have

$$\int_0^t ds\sqrt{tr[(\hat{x}_0^{\setminus\mathcal{L}}(s))^2\hat{\rho}_0]} \tag{3.107}$$

$$\leq\frac{1}{\sqrt{||PX||}}\sum_{k=L}^{\infty}\left(d_k\sum_{n=e(k)}^{\infty}\frac{\tau(t)^{2n+1}}{(2n+1)!}+\frac{\bar{d}_k||P||}{\sqrt{||PX||}}\sum_{n=f(k)+1/2}^{\infty}\frac{\tau(t)^{2n+1}}{(2n+1)!}\right). \tag{3.108}$$

Applying Taylor's theorem with the Lagrange form of the reminder [62], to the Taylor expansion of the hyperbolic sin function we have

$$\sum_{n=k+1}^{\infty}\frac{x^{2n+1}}{(2n+1)!}\leq\sinh(x)\frac{x^{2k+2}}{(2k+2)!};\quad x\geq 0,\ k=0,1,2,\dots\ . \tag{3.109}$$

Hence we finally achieve (3.99). □

Therefore we see that if the two point correlation functions are not bounded, we can still achieve good bounds, even if $tr[\hat{x}_k^2\hat{\rho}_0], tr[\hat{p}_k^2\hat{\rho}_0]\propto K^k$ for some $K\in\mathbb{R}$. With the bounds in theorems 57 and 58, we have locality bounds for dynamics in the interaction picture by virtue of theorem 52.

3.2.3 Bounds for Approximating the Coefficients for Interaction Picture Numerics

We will start this section with the following preliminary lemma for tridiagonal matrices. The theorem after that will be the main result of this section.

Lemma 59. *Let $M(k)$, $k = 1, 2, 3, \ldots$ be infinite dimensional symetric tridiagonal matrices. Let $M_l(k)$, $k = 1, 2, 3, \ldots$ denote their $l \times l$ principle minors, $M_l(k) := [M]_{[1:l,1:l]}(k)$, $l = 1, 2, 3, \ldots$. Then the following holds*

$$[\Pi_{k=1}^{n} M(k)]_{1,j} - [\Pi_{k=1}^{n} M_l(k)]_{1,j} = 0 \text{ if } j + n \leq 2l, \tag{3.110}$$

$n, l = 1, 2, 3, \ldots \quad j = 1, 2, 3, \ldots, l$. *and the binary combination rule is that of matrix multiplication.*

Proof. First let us show that

$$[\Pi_{k=1}^{n} M(k)]_{1,j} - [\Pi_{k=1}^{n} M_l(k)]_{1,j} = 0 \tag{3.111}$$

if $[\Pi_{k=1}^{n} M(k)]_{1,j}$ does not contain coefficients in $[M(k)]_{[l+1:\infty,l+1:\infty]}$ $k = 1, \ldots, n$. To show this, we need the following two steps. First note that for any d by d matrices $A(k)$

$$[\Pi_{k=1}^{n} A(k)]_{i,j} = [\Pi_{k=1}^{n} (A(k) \oplus \mathbf{0})]_{i,j} \quad n = 1, 2, 3, \ldots \quad i, j = 1, 2, 3, \ldots, d. \tag{3.112}$$

where $\mathbf{0}$ is the infinite dimensional matrix with all components zero: $\mathbf{0}_{ij} = 0 \quad i, j = 1, 2, 3, \ldots$. (this is straightforward to prove). Next we use this observation and the definition of M_l to note

$$\begin{aligned} [\Pi_{k=1}^{n} M_l(k)]_{ij} &= [\Pi_{k=1}^{n} (M_l(k) \oplus \mathbf{0})]_{ij} && (3.113) \\ &= [\Pi_{k=1}^{n} (M(k) \mapsto M_{dm}(k) = 0, \forall d, m > l)]_{ij} && (3.114) \\ &= [\Pi_{k=1}^{n} M(k)]_{ij} \mapsto M_{dm}(k) = 0, \forall d, m > l \text{ and } k = 1, \ldots, n. && (3.115) \end{aligned}$$

$i, j = 1, 2, 3, \ldots, l \quad n = 1, 2, 3, \ldots$ where $\mapsto$ means evaluate the object on the left according to the rule on the right. Hence we conclude that $[\Pi_{k=1}^{n} M(k)]_{1,j} = [\Pi_{k=1}^{n} M_l(k)]_{1,j}$ if $([\Pi_{k=1}^{n} M(k)]_{1,j} \mapsto M_{id}(k) = 0, \forall i, d > l \text{ and } k = 1, \ldots, n) = [\Pi_{k=1}^{n} M(k)]_{1,j}$. This holds if $[\Pi_{k=1}^{n} M(k)]_{1,j}$ does not contain the non-zero coefficients in $[M(k)]_{[l+1:\infty,l+1:\infty]}$, $k = 1, \ldots, n$. Now we can show that this holds when $j + n \leq 2l; \quad n, l = 1, 2, 3, \ldots \quad j = 1, 2, 3, \ldots, l$ To do this, we will need to prove another identity by induction. But first we need the following three preliminary ingredients:

2.1) let us use the following notation for the matrix $M(k)$

$$M(k) := \begin{bmatrix} e[1](k) & t[2](k) & & & 0 \\ t[2](k) & e[2](k) & t[3](k) & & \\ & t[3](k) & e[3](k) & t[4](k) & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{bmatrix}, \tag{3.116}$$

With this notation, we note that $M_l(k)$ only contains coefficients $e[i](k), t[j](k)$ with $i, j \leq l$.

2.2) $M_{ij}(k) = \delta_{ij} e[i](k) + \delta_{i,j-1} t[i+1](k) + \delta_{i,j+1} t[j+1](k) \quad i, j = 1, 2, 3 \ldots .$

2.3) Let us make the following definition

$$\begin{aligned} V\left(M^n\right) :=& \left(\lceil [\Pi_{k=1}^n M(k)]_{1,1} \rceil, \lceil [\Pi_{k=1}^n M(k)]_{1,2} \rceil, \lceil [\Pi_{k=1}^n M(k)]_{1,3} \rceil, \ldots, \right. \\ & \left. \lceil [\Pi_{k=1}^n M(k)]_{1,n+1} \rceil \right) \end{aligned} \tag{3.117}$$

where $\lceil P(\{e,t\}) \rceil = \max\big(i \in \mathbb{Z}; e[i](k), t[i](k) \in \{e,t\}\big)$ and $P(\{e,t\})$ is a polynomial of a subset of the elements of $\{M(k)\}_{k=1}^n$.

We will now prove by induction the following rule:

$$\begin{aligned} & V\left(M^n\right) = \\ & \left(\frac{n-1}{2}+1, \frac{n-1}{2}+2, \frac{n-1}{2}+2, \frac{n-1}{2}+3, \frac{n-1}{2}+3, \frac{n-1}{2}+4, \ldots, \right. \\ & \left. \frac{n-1}{2}+\frac{n+1}{2}, \frac{n-1}{2}+\frac{n+1}{2}, n+1\right) \\ & \quad n = 1, 3, 5, \ldots \end{aligned} \tag{3.118}$$

$$\begin{aligned} & V\left(M^n\right) = \\ & \left(\frac{n}{2}+1, \frac{n}{2}+1, \frac{n}{2}+2, \frac{n}{2}+2, \frac{n}{2}+3, \frac{n}{2}+3, \ldots, \frac{n}{2}+\frac{n}{2}, \frac{n}{2}+\frac{n}{2}, n+1\right) \\ & \quad n = 2, 4, 6, \ldots \end{aligned} \tag{3.119}$$

Now we will prove that Eq. (3.118) implies Eq. (3.119). For $n = 1, 3, 5, \ldots$, we have that

$$\left[\Pi_{k=1}^{n+1} M(k)\right]_{1,j} = \sum_{p=1}^{\infty} \left[\Pi_{k=1}^{n} M(k)\right]_{1,p} M_{p,j}(n+1) = \sum_{p=1}^{n+1} \left[\Pi_{k=1}^{n} M(k)\right]_{1,p} M_{p,j}(n+1) \tag{3.120}$$

$$= \sum_{p=1}^{(n+1)/2} \left[\Pi_{k=1}^{n} M(k)\right]_{1,2p-1} M_{2p-1,j}(n+1) + \sum_{p=1}^{(n+1)/2} \left[\Pi_{k=1}^{n} M(k)\right]_{1,2p} M_{2p,j}(n+1) \tag{3.121}$$

$$= \sum_{p=1}^{(n+1)/2} \left[\Pi_{k=1}^{n} M(k)\right]_{1,2p-1} \left(\delta_{2p-1,j} e[i](n+1) + \delta_{2p-1,j-1} t[2p](n+1)\right. \tag{3.122}$$

$$\left. + \delta_{2p-1,j+1} t[j+1](n+1)\right) \tag{3.123}$$

$$+ \sum_{p=1}^{(n+1)/2} \left[\Pi_{k=1}^{n} M(k)\right]_{1,2p} \left(\delta_{2p,j} e[2p](n+1) + \delta_{2p,j-1} t[2p+1](n+1)\right. \tag{3.124}$$

$$\left. + \delta_{2p,j+1} t[j+1](n+1)\right). \tag{3.125}$$

Where in line (3.120) we have used $[\Pi_{k=1}^{n} M(k)]_{1p} = 0$ if $p > n+1$ to restrict the upper limit of the summation. This follows from lemma 1 in sec 3.2 of [59]. Now, from (3.118), we have that $\left\lceil [\Pi_{k=1}^{n} M(k)]_{1,2p-1} \right\rceil = \frac{n-1}{2} + p$, $\left\lceil [\Pi_{k=1}^{n} M(k)]_{1,2p} \right\rceil = \frac{n-1}{2} + p + 1$, $p = 1, 2, 3, \ldots, (n+1)/2$. We can use these identities to calculate $\lceil . \rceil$ for the even and odd sums in the above equation. For the odd sum we have

$$\left\lceil \sum_{p=1}^{(n+1)/2} \left[\Pi_{k=1}^{n} M(k)\right]_{1,2p-1} \left(\delta_{2p-1,j} e[i](n+1) + \delta_{2p-1,j-1} t[2p](n+1) + \right.\right. \tag{3.126}$$

$$\left.\left. \delta_{2p-1,j+1} t[j+1](n+1)\right)\right\rceil \tag{3.127}$$

$$= \begin{cases} \max\{\frac{n-1}{2} + \frac{j+1}{2}, \frac{j+1}{2}\} & j = 1, 3, 5, \ldots, n \\ \max\{\frac{n-1}{2} + \frac{j}{2}, j, \frac{n-1}{2} + \frac{j+2}{2}, j+1\} & j = 2, 4, 6, \ldots, n-1 \\ \max\{\frac{n-1}{2} + \frac{n+1}{2}, n+1\} & j = n+1 \end{cases} \tag{3.128}$$

For the even sum we have

$$\left\lceil \sum_{p=1}^{(n+1)/2} \left[\Pi_{k=1}^{n} M(k)\right]_{1,2p} \left(\delta_{2p,j} e[2p](n+1) + \delta_{2p,j-1} t[2p+1](n+1) + \right. \right. \tag{3.129}$$

$$\left. \left. \delta_{2p,j+1} t[j+1](n+1)\right)\right\rceil \tag{3.130}$$

$$= \begin{cases} \max\{\frac{n-1}{2} + \frac{j}{2} + 1, j\} & j = 2,4,6,\ldots,n+1 \\ \max\{\frac{n-1}{2} + 2, 2\} & j = 1 \\ \max\{\frac{n-1}{2} + \frac{j-1}{2} + 1, j, \frac{n-1}{2} + \frac{j+1}{2} + 1, j+1\} & j = 3,5,7,\ldots,n \\ \max\{\frac{n-1}{2} + \frac{n+1}{2} + 1, n+2\} & j = n+2 \end{cases} \tag{3.131}$$

We can now use Eqs. (3.128) and (3.131) together with Eq. (3.120) to calculate $\left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,j} \right\rceil$.

$$\left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,j} \right\rceil = \begin{cases} \frac{n-1}{2} + 2 & j = 1 \\ \frac{n+1}{2} + \frac{j+1}{2} & j = 3,5,7,\ldots,n \\ \frac{n+1}{2} + \frac{j}{2} & j = 2,4,6,\ldots,n-1 \\ n+1 & j = n+1 \\ n+2 & j = n+2 \end{cases} \tag{3.132}$$

for $n = 1,3,5\ldots$. We now have that

$$\left(\left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,1} \right\rceil, \left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,2} \right\rceil, \left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,3} \right\rceil, \ldots, \left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,n+1} \right\rceil \right) \tag{3.133}$$

$n+1 = 2,4,6,\ldots$, where $\left\lceil \left[\Pi_{k=1}^{n+1} M(k)\right]_{1,j} \right\rceil$ are given by Eq. (3.132), is equal to $V\left(M^{n+1}\right)$ given by Eq. (3.119). Hence Eq. (3.118) for n implies Eq. (3.119) for $n+1$, $n = 1,3,5,\ldots$. Similarly, we find that Eq. (3.119) for n implies Eq. (3.118) for $n+1$, for $n = 2,4,6,\ldots$. Now note that from Eq. (3.118) if follows $V\left(M^1\right) = (1,2)$. We can easily verify that this is correct by observing (3.116). Hence by induction we prove Eqs. (3.118) and (3.119). Finally to conclude the proof, we just have to note that from Eqs. (3.118) and (3.119) the identity $n + j \leq 2\left\lceil \left[\Pi_{k=1}^{n} M(k)\right]_{1,j} \right\rceil$, $n = 1,2,3,\ldots$, $j = 1,2,3,\ldots,n+1$. Hence from the definition of $\lceil . \rceil$, if follows that $\left[\Pi_{k=1}^{n} M(k)\right]_{1,j}$ does not contain elements from the set $\{\{e[i](k), t[i](k)\}_{k=1}^{n}\}_{i=l+1}^{\infty}$ if $n + j \leq 2l, \quad n, l = 1,2,3,\ldots,$

$j = 1, 2, 3, \ldots, n+1$. Hence taking into account (3.111) and observation 2.1), we conclude

$$[\Pi_{k=1}^{n} M(k)]_{1,j} - [\Pi_{k=1}^{n} M_l(k)]_{1,j} = 0 \text{ if } j + n \leq 2l, \tag{3.134}$$

$n, l = 1, 2, 3, \ldots, j = 1, 2, 3, \ldots, \min\{n+1, l\}$. From lemma 1 in sec 3.2 of [59], it follows that $[\Pi_{k=1}^{n} M(k)]_{1,j} = [\Pi_{k=1}^{n} M_l(k)]_{1,j} = 0$ for $l \geq j, \quad j > n+1$, $n = 1, 2, 3, \ldots$. Hence combining this with (3.134), we conclude the proof. □

If the bound in theorem 52 were to be used to upper bound the truncation error when calculating $tr[\hat{O}_s(t)\hat{\rho}_I^{\mathcal{C}}(t)]$ rather than $tr[\hat{O}_s(t)\hat{\rho}_I(t)]$, one would need to be able to calculate the coefficients $\{c_j(t), \bar{c}_j(t)\}_{j=1}^{L}$. However, from their definition (Eq. (3.7)), it follows that that requires exponentiating the matrix

$$t \begin{bmatrix} 0 & -P \\ X & 0 \end{bmatrix}. \tag{3.135}$$

Since X and P are infinite dimensional, in practice one would only ever be able to exponentiate a truncated version using $X_l := [X]_{[1:l,1:l]}$, $P_l := [P]_{[1:l,1:l]}$. However, if follows from the definitions of c_j^l, $\bar{c}_j^l$ (Eq. (3.43)) that they are given by exponentiating the truncated version of Eq. (3.135) too:

$$t \begin{bmatrix} 0 & -P_l \\ X_l & 0 \end{bmatrix}. \tag{3.136}$$

Therefore in the following theorem we will give bounds for approximating c_j by c_j^l, $\bar{c}_j$ by $\bar{c}_j^l$, and find that by making l large enough, we can achieve neglectable errors. We will assume $A1$ since this will be sufficient for later purposes, although one could prove a similar result even if $A1$ did not hold.

Theorem 60. *Assuming $A1$ we have the bounds*

$$-\sum_{n=g_1}^{\infty} \frac{\tau^{4n+2}}{(4n+2)!} \leq c_j(t) - c_j^l(t) \leq \sum_{n=h_1}^{\infty} \frac{\tau^{4n}}{(4n)!} \tag{3.137}$$

$$-\frac{||P||}{\sqrt{||PX||}} \sum_{n=g_2}^{\infty} \frac{\tau^{4n+3}}{(4n+3)!} \leq \bar{c}_j(t) - \bar{c}_j^l(t) \leq \frac{||P||}{\sqrt{||PX||}} \sum_{n=h_2}^{\infty} \frac{\tau^{4n+1}}{(4n+1)!}, \tag{3.138}$$

$j = 1, 2, 3, \ldots, l$, $\tau = \tau(t) = \sqrt{||PX||}t$ *where*

$$g_1 = \left\lfloor \frac{2l-j-1}{4} \right\rfloor, \; g_2 = \left\lfloor \frac{2l-j-2}{4} \right\rfloor, \; h_1 = \left\lfloor \frac{2l-j+1}{4} \right\rfloor, \; h_2 = \left\lfloor \frac{2l-j}{4} \right\rfloor \tag{3.139}$$

$\forall X, P,$ *and*

$$g_1 = g_2 = \left\lfloor \frac{2l-j}{2} \right\rfloor,\ h_1 = h_2 = \left\lfloor \frac{2l-j+1}{2} \right\rfloor \text{ If } P = \mathbb{I} \tag{3.140}$$

Proof. From Eqs. (3.81), we have for $t \geq 0$

$$c_j(t) - c_j^L(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n}}{(2n)!} \left([(PX)^n]_{1,j+1} - [(P_L X_L)^n]_{1,j+1} \right) \tag{3.141}$$

$$\bar{c}_j(t) - \bar{c}_j^L(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n+1}}{(2n+1)!} \left([(PX)^n P]_{1,j+1} - [(P_L X_L)^n P_L]_{1,j+1} \right) \tag{3.142}$$

$j = 0, 1, 2, \ldots, L-1$ Now assume that $P_{ij} \geq 0, X_{ij} \geq 0\ \forall i, j$ (We can do this w.l.o.g. since via transformations of the form $\{\hat{x}_i, \hat{p}_i\} \mapsto \{-\hat{x}_i, -\hat{p}_i\}$ this is always achievable) it follows $[(PX)^n]_{1,j+1} - [(P_L X_L)^n]_{1,j+1} \geq 0$, $[(PX)^n P]_{1,j+1} - [(P_L X_L)^n P_L]_{1,j+1} \geq 0$ and using (3.141), (3.142) we have for $j = 0, \ldots, L-1$

$$-\sum_{n=0}^{\infty} \frac{t^{4n+2}}{(4n+2)!} \left([(PX)^{2n+1}]_{1,j+1} - [(P_L X_L)^{2n+1}]_{1,j+1} \right) \leq c_j(t) - c_j^L(t)$$

$$\leq \sum_{n=0}^{\infty} \frac{t^{4n}}{(4n)!} \left([(PX)^{2n}]_{1,j+1} - [(P_L X_L)^{2n}]_{1,j+1} \right) \tag{3.143}$$

$$-\sum_{n=0}^{\infty} \frac{t^{4n+3}}{(4n+3)!} \left([(PX)^{2n+1}]_{1,j+1} - [(P_L X_L)^{2n+1}]_{1,j+1} \right) \leq \bar{c}_j(t) - \bar{c}_j^L(t)$$

$$\leq \sum_{n=0}^{\infty} \frac{t^{4n+1}}{(4n+1)!} \left([(PX)^{2n}]_{1,j+1} - [(P_L X_L)^{2n}]_{1,j+1} \right) \tag{3.144}$$

Now taking into account theorem 59 to neglect the zero terms in the summations followed by neglcting the remaining $[(P_L X_L)^q]_{ij}$ terms by noting that they are non-negative and finally taking into account identities Eqs (3.87) (3.88), from Eqs (3.143), (3.144) we achieve the results of the theorem □

3.2.4 Explicit Bounds for the Schrödinger Picture Bound

In what follows we will also develop locality bounds for the dynamics in the Schrödinger picture (bounds for theorem (52)) also. But before we state the bounds, we need to make a detour by stating one additional theorem. This theorem is based upon part of one of the proofs in[58]:

Theorem 61. *Given the Hamiltonain*

$$\hat{H} = \hat{H}_S \otimes \mathbb{I} + \hat{h}_s \otimes \hat{x}_0 + \mathbb{I} \otimes \frac{1}{2}\, \vec{r}^T H^B \vec{r} \tag{3.145}$$

where $\vec{r}^T = (\hat{x}_0, \hat{p}_0, \hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2, \dots,)$ *collects canonical position and momentum operators,* H^B *is a hermitian matrix and* $\hat{H}_S$, $\hat{h}_s$ *are hermitian operators acting on the system with* $\hat{h}_s$ *bounded (with no additional assumptions), then the auto two point bosonic correlations functions grow at most exponentially in time:*

$$\langle \hat{r}_k^2 \rangle(t) \leq \left(\sum_q \left[e^{|t|M} \right]_{k+1,q+1} \left(\langle \hat{r}_q^2 \rangle(0) + \delta_{1,q} \right) \right) - \delta_{1,k}, \quad k = 0, 1, 2, \dots \tag{3.146}$$

where $\langle \hat{r}_q^2 \rangle(t) := tr[\hat{r}_q^2 \hat{\rho}_s(t)]$, $\hat{\rho}_s(t) := e^{-it\hat{H}} \hat{\rho}_0 e^{it\hat{H}}$, $t \in \mathbb{R}$

$$M := \begin{bmatrix} \omega_0 + t_{0,0} & t_{1,0} & t_{2,0} & t_{3,0} & \dots \\ t_{0,1} & t_{1,1} + \omega_1 + ||\hat{h}_s|| & t_{2,1} & t_{3,1} & \dots \\ t_{0,2} & t_{1,2} & t_{2,2} + \omega_2 & t_{3,2} & \dots \\ t_{0,3} & t_{1,3} & t_{2,3} & t_{3,3} + \omega_3 & \dots \\ t_{0,4} & t_{1,4} & t_{2,4} & t_{3,4} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{3.147}$$

$$t_{q,k} = \begin{cases} |H^B_{k-1,q}| & \text{if } k = 1, 3, 5, \dots \\ |H^B_{k+1,q}| & \text{if } k = 0, 2, 4, \dots \end{cases} \quad \omega_k = \begin{cases} \sum_q |H^B_{k-1,q}| & \text{if } k = 1, 3, 5, \dots \\ \sum_q |H^B_{k+1,q}| & \text{if } k = 0, 2, 4, \dots \end{cases} \tag{3.148}$$

Proof. Define $\gamma_i = tr[\hat{r}_i^2 \hat{\rho}_s(t)]$ and denote the time derivative via "$\dot{}$". We have $\dot{\hat{\rho}_s}(t) = -i[\hat{H}, \hat{\rho}_s(t)]$, hence

$$\dot{\gamma_i}(t) = -itr[\hat{r}_i[\hat{H}, \hat{\rho}_s(t)]] = -itr[[\hat{r}_i, \hat{H}]\hat{\rho}_s(t)]. \tag{3.149}$$

Define the complex matrix entries $\sigma_{ij} = [\hat{r}_i, \hat{r}_j]$. Plunging in the expression for $\hat{H}$ and calculating the commutator $[\hat{r}_i, \hat{H}]$ explicitly in (3.149) followed by taking the absolute value applying the triangle inequality and using $|H^B_{ij}| = |H^B_{ji}|$, we have

$$|\dot{\gamma_k}| \leq 2|\sigma_{0k}|\, |tr[\hat{h}_s \hat{r}_k \hat{\rho}_s(t)]| + \sum_{ij} |\sigma_{kj}||H^B_{ji}| \left(|tr[\hat{r}_i \hat{r}_k \hat{\rho}_s(t)]| + |tr[\hat{r}_k \hat{r}_i \hat{\rho}_s(t)]| \right), \tag{3.150}$$

Now using Cauchy-Schwarz inequality to write $|tr[\hat{r}_i\hat{r}_k\hat{\rho}_s(t)]| \leq (tr[\hat{r}_i^2\hat{\rho}_s(t)]tr[\hat{r}_k^2\hat{\rho}_s(t)])^{1/2}$ followed by noting that $\sqrt{xy} \leq (x+y)/2$, $x, y \geq 0$ Eq. (3.150) gives us

$$|\dot{\gamma_k}| \leq |\sigma_{0k}|tr[\hat{h}_s^2\hat{\rho}_s(t)]^{1/2}(1 + tr[\hat{r}_0^2\hat{\rho}_s(t)]) + \sum_{ij} |\sigma_{kj}||H_{ji}^B| \left(tr[\hat{r}_i^2\hat{\rho}_s(t)] + tr[\hat{r}_k^2\hat{\rho}_s(t)]\right). \tag{3.151}$$

Noting that $|\sigma_{k0}| = \delta_{1,k}$, define $\gamma_k'(t) = \gamma_k(t) + \delta_{1,k}$. Since $\dot{\gamma_k'} = \dot{\gamma_k}$, it follows from (3.151)

$$|\dot{\gamma_k'}| \leq \delta_{1,k}tr[\hat{h}_s^2\hat{\rho}_s(t)]^{1/2}\gamma_k' + \sum_{ij} |\sigma_{kj}||H_{ji}^B| \left(\gamma_i' + \gamma_k'\right). \tag{3.152}$$

Using Eq. (3.4) to bound the 1st term on the R.H.S. of (3.152), and noting that $\dot{\gamma'}_k \leq |\dot{\gamma'}_k|$, since $\dot{\gamma}_k \in \mathbb{R}$ we have

$$\dot{\gamma_k'} \leq \delta_{1,k}||\hat{h}_s||\gamma_k' + \omega_k\gamma_k' + \sum_i t_{i,k}\gamma_i'. \tag{3.153}$$

where $\omega_k = \sum_{i,j} |\sigma_{kj}| \, |H_{ji}^B|$, $t_{i,k} = \sum_j |\sigma_{kj}| \, |H_{ji}^B|$. Writing the summation(s) in the expressions for ω_k and $t_{i,k}$ in odd and even terms and noting that

$$|\sigma_{ji}| = |\sigma_{ij}| = \begin{cases} \delta_{i,j-1} & \text{if } i = 0, 2, 4, \ldots \\ \delta_{i,j+1} & \text{if } i = 1, 3, 5, \ldots, \end{cases} \tag{3.154}$$

we get the definitions ω_k, $t_{i,k}$ found in the lemma. In order to find an upper bound to $\gamma_k(t)$ for non-negative t, it suffices to solve (3.153) for the case where the derivative takes on its maximally allowed value after time $t = 0$ .i.e. due to continuity, $\gamma_k(t) \leq \kappa_k(t)$, $k = 0, 1, 2, \ldots$ where

$$\dot{\kappa_k} = \delta_{1,k}||\hat{h}_s||\kappa_k + \omega_k\kappa_k + \sum_i t_{i,k}\kappa_i, \quad t \geq 0 \tag{3.155}$$

and $\gamma_k(0) = \kappa_k(0)$, $k = 0, 1, 2, \ldots$. This gives

$$\vec{\kappa}(t) = e^{tM}\vec{\gamma}'(0), \tag{3.156}$$

$\vec{\kappa}^T(t) := (\kappa_0(t), \kappa_1(t), \kappa_2(t), \ldots)^T$, $\vec{\gamma}'^T(t) := (\gamma_0'(t), \gamma_1'(t), \gamma_2'(t), \ldots)^T$. Thus we have (3.145) for $t \geq 0$. If $t < 0$, we do the same proof as above for non-negative t but with $\hat{H} \mapsto -\hat{H}$ yielding the same result. This justifies the appearance of the absolute value of t in (3.145). □

Note that M is a banded matrix for locally coupled Hamiltonians.

Now we will state a theorem which gives a locality bound for the dynamics in the Schrödinger picture which can easily be evaluated numerically (since all the quantities are finite real matrices) when taking into account the already derived bounds for $\int_0^t dx\sqrt{tr[(\hat{x}_0^{\backslash\mathcal{L}}(x))^2\hat{\rho}_0]}$:

Lemma 62. *If $\hat{h}_s$ is bounded, Eq. (3.44) is bounded by*

$$\left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr_{\mathcal{L}}[\hat{O}_s\hat{\rho}_s^{\mathcal{L}}(t)]\right|^2 \leq 2\alpha(t)\sqrt{2}||\hat{h}_s|| \tag{3.157}$$

$$\left(\int_0^t dx \sqrt{\left(\sum_{i=0}^{2L-1}\nabla_i^L(x)\right)\left(\sum_{i=0}^{2L-1}\nabla_{\varsigma(i)}^L(x)\left(\sum_{k=0}^{2L-1}[e^{xM_L}]_{i+1,k+1}\left(tr[r_{\varsigma(k)}^2\hat{\rho}_0]+\delta_{1,k}\right)-\delta_{1,i}\right)\right)}\right. \tag{3.158}$$

$$\left. + \int_0^t dx\sqrt{tr[(\hat{x}_0^{\setminus\mathcal{L}}(x))^2\hat{\rho}_0]}\right). \tag{3.159}$$

Where $\varsigma(k)$ re-orders the indices:

$$\varsigma(k) := \begin{cases} k/2, & k = 0, 2, 4, \dots \\ (k-1)/2 + L, & k = 1, 3, 5, \dots, \end{cases} \tag{3.160}$$

and M_L is defined by taking the $2L$ by $2L$ minor of M (defined in lemma 61) and setting to zero all remaining coefficients $|H_{ij}^B|$ which couple $\hat{r}_i, \hat{r}_j \in \setminus\mathcal{L}$.

Proof. follows from applying lemma 61 to Theorem 54. □

At this stage it is not clear that we have achieved that much, since although one can easily calculate numerically now a bound for line (3.157) given the initial two point correlation functions of the initial state, it is not clear that this quantity will be small. We will now show that line (3.158) is bounded from above by a function that decays with similar behaviour to that of Eqs. (3.92), (3.94). For this lemma, we will assume $A1$ (Note that we could derive slightly worse version of the bound for which this is not necessarily satisfied).

Lemma 63.

$$\int_0^t dx \sqrt{\left(\sum_{i=0}^{2L-1}\nabla_i^L(x)\right)\left(\sum_{i=0}^{2L-1}\nabla_{\varsigma(i)}^L(x)\left(\sum_{k=0}^{2L-1}[e^{xM_L}]_{i+1,k+1}\left(tr[\hat{r}_{\varsigma(k)}^2\hat{\rho}_0]+\delta_{1,k}\right)-\delta_{1,i}\right)\right)} \tag{3.161}$$

is bounded by:

- *(Bound 1)*

$$\leq \Phi(2L)^{5/2}\left(\sum_{n,m=4\theta}^{\infty}\frac{\tau(t)^{n+m+1}}{(n+m+1)(n!)(m!)}\right) \tag{3.162}$$

$$\sqrt{\frac{4\Delta^2-2\Delta||M_L||^2+e^{||M_L||t}(||M_L||^2(\cosh 2\Delta t+1)-4\Delta^2-2\Delta||M_L||\sinh 2\Delta t)}{2(1-4\Delta^2)||M_L||^3}} \tag{3.163}$$

$$\leq \Phi(2L)^{5/2}\left(\sum_{n,m=4\theta}^{\infty}\frac{\tau(t)^{n+m+1}}{(n+m+1)(n!)(m!)}\right)\sqrt{\frac{e^{t(2\Delta+||M_L||)}-1}{2\Delta+||M_L||}} \tag{3.164}$$

For $L=0,1,2,\ldots$

- *(Bound 2)*

$$\leq \frac{4\sqrt{6}\Phi}{\sqrt{4\theta-1}}\frac{e^{5\ln(L^5/(8\theta-1))+(1+\chi)\tau+(4\theta-1)(1+\ln\tau-\ln(4\theta-1))}}{\sqrt{2\Delta+||M_L||}} \tag{3.165}$$

$$\text{with}\quad \chi=(\sqrt{||PX||}+2\Delta+||M_L||)/\sqrt{||PX||} \tag{3.166}$$

For $L=3,4,5,\ldots$

where

$$\Phi=\frac{\max\{||X_L||,||P_L||\}}{\Delta(||PX||)^{1/4}}\max\Big\{1,\frac{||P||}{\sqrt{||PX||}}\Big\}\sqrt{\gamma^L_{\text{MAX}}} \tag{3.167}$$

and $\gamma^L_{\text{MAX}}:=\max\{tr[\hat{r}_k^2\hat{\rho}_0]+\delta_{1,k}\}_{k=0}^{2L-1}$, $\Delta:=\max\{\sqrt{||X_LP_L||},\sqrt{||P_LX_L||}\}$, $\tau(t):=\sqrt{||PX||}\,t$, $||M_L||$ *is defined in Lemma 62 and* $\theta:=\begin{cases}\lfloor\frac{L-2}{4}\rfloor & \forall X,P\\ \lfloor\frac{L}{2}\rfloor & \text{if } P=\mathbb{I}\end{cases}$. *Recall that* $\lfloor . \rfloor$ *rounds up its argument to the nearest integer. Furthermore if* $|X_{ij}|,\ |P_{ij}|\leq E<\infty$, $\forall i,j$, *for some* E *then there exists* D *finite such that* $||M_L||,||P_LX_L||,||X_LP_L||,||P||,||PX||\leq D\ \forall\ L$.

Proof. With the aid of theorem 60, the proof is quite simple and only involves straightforward manipulations and applying well-known inequalities such at the Cauchy Schwarz inequality

$$\int_0^t dx\sqrt{\left(\sum_{i=0}^{2L-1}\nabla_i^L(x)\right)\left(\sum_{i=0}^{2L-1}\nabla^L_{\varsigma(i)}(x)\left(\sum_{k=0}^{2L-1}[e^{xM_L}]_{i+1,k+1}\left(tr[\hat{r}^2_{\varsigma(k)}\rho_0]+\delta_{1,k}\right)-\delta_{1,i}\right)\right)} \tag{3.168}$$

$$\leq\int_0^t dx\left(\max_{j\in 0,\ldots,2L-1}\Big\{|A_j^L(x)|\Big\}\right)\left(\sum_{p,q=0}^{2L-1}|C^L_{p+1,q+1}(-x)|\right)\sqrt{\sum_{k=0}^{2L-1}[e^{xM_L}]_{i',k+1}\gamma^L_{\text{MAX}}} \tag{3.169}$$

where $i' = i'(x)$ is the value of i such that $\sum_{k=0}^{2L-1}[e^{xM_L}]_{i+1.k+1}(tr[\hat{r}_k^2\rho_0] + \delta_{1,i})$ is maximised at x. Similarly, we define k' as the value of k that maximises $tr[\hat{r}_k^2\rho_0] + \delta_{1,k}$ We will now bound every term in the integrand individually. From definition Eq. (3.49), Eq. (3.81) and identities Eqs. (3.87), (3.88) we have that

$$|C_{ij}^L(t)| \leq \begin{cases} \sum_{n=0}^{\infty} \frac{|t|^{2n}}{(2n)!} \left(||P_L X_L||\right)^n & \text{if } i,j = 1,2,3,\ldots,L \\ \sum_{n=0}^{\infty} \frac{|t|^{2n+1}}{(2n+1)!} \left(||P_L X_L||\right)^n ||P_L|| & \text{if } i = 1,\ldots,L; j = L+1,\ldots,2L \\ \sum_{n=0}^{\infty} \frac{|t|^{2n+1}}{(2n+1)!} \left(||X_L P_L||\right)^n ||X_L|| & \text{if } i = L+1\ldots,2L; j = 1,\ldots,L \\ \sum_{n=0}^{\infty} \frac{|t|^{2n}}{(2n)!} \left(||X_L P_L||\right)^n & \text{if } i,j = L+1,\ldots,2L. \end{cases} \tag{3.170}$$

Therefore defining $\Delta := \max\{\sqrt{||X_L P_L||}, \sqrt{||P_L X_L||}\}$ we conclude

$$\sum_{p,q=0}^{2L-1} |C_{p+1,q+1}^L(-x)| \leq (2L)^2 \max_{i,j\in 1,\ldots,2L} \Big\{|C_{ij}^L(-x)|\Big\} \tag{3.171}$$

$$\leq (2L)^2 \max\{1, \frac{||X_L||}{\Delta}, \frac{||P_L||}{\Delta}\} \max\{\cosh(\Delta|x|), \sinh(\Delta|x|)\} \tag{3.172}$$

$$= (2L)^2 \frac{\max\{||X_L||, ||P_L||\}}{\Delta} \cosh(\Delta|x|), \tag{3.173}$$

where in the last line we took into account that $\Delta \leq \sqrt{||X_L||\,||P_L||}$ and $\cosh(x)/\sinh(x) \geq 1$, for $x \geq 1$. Alternativerly, since $\cosh(x) \leq e^x$, for $x \geq 0$, we also have

$$\sum_{p,q=0}^{2L-1} |C_{p+1,q+1}^L(-x)| \leq (2L)^2 \frac{\max\{||X_L||, ||P_L||\}}{\Delta} e^{\Delta|x|}. \tag{3.174}$$

Furthermore for $x \geq 0$,

$$\sum_{k=0}^{2L-1} [e^{xM_L}]_{i',k+1}(tr[\hat{r}_k^2\rho_0] + \delta_{1,i}) \leq 2L[e^{xM_L}]_{i',k'+1}\gamma_{\text{MAX}}^L \tag{3.175}$$

$$= 2L|[e^{xM_L}]_{i',k'+1}|\gamma_{\text{MAX}}^L \tag{3.176}$$

$$\leq 2L||e^{xM_L}||\gamma_{\text{MAX}}^L \leq 2L\, e^{x||M_L||}\gamma_{\text{MAX}}^L. \tag{3.177}$$

Now we will bound $\max_{j\in 0,\ldots,2L-1} \Big\{|A_j^L(x)|\Big\}$. From definition 3.48 and lemma 60, it follows

$$\max_{j\in 0,\ldots,2L-1} |A_j^L(t)| \leq \max\Big\{1, \frac{||P||}{\sqrt{||PX||}}\Big\} \sum_{n=0}^{\infty} \frac{\tau^{4\theta+n}}{(4\theta+n)!} \tag{3.178}$$

Note that $\sum_{n=0}^{\infty} \frac{\tau^{4\theta+n}}{(4\theta+n)!}$ is simply the truncation of the power law expansion of the exponential function. Applying Taylor's theorem with the Lagrange form of the reminder [62], to the Taylor expansion of the exponential function we have

$$\sum_{n=k+1}^{\infty} \frac{x^n}{n!} \leq \frac{(e^x-1)x^k}{k!}, \quad x \geq 0 \quad k = 0, 1, 2, \dots \ . \tag{3.179}$$

Hence we finally achieve (3.99). Thus we achieve

$$\max_{j\in 0,\dots,2L-1} |A_j^L(t)| \leq \max\Big\{1, \frac{||P||}{\sqrt{||PX||}}\Big\} \frac{(e^{\tau(t)}-1)}{(4\theta-1)!} \tag{3.180}$$

Now substituting Eqs. (3.178), (3.173), (3.177), into Eq. (3.169), followed by applying a Cauchy Schwarz inequality and integrating the resultant expression, we find Eq. (3.163). The same procedure, but using (3.174) rather than (3.173) yields Eq. (3.164), and if we use Eq. (3.180) instead of Eq. (3.178), we get Eq. (3.165). The fact that the operator norms appearing in the bounds in the lemma are finite and bounded is a direct consequence of the definition of the operator norm for the $l = 2$ vector norm: Let K be a real square banded matrix of infinite dimension acting on a real vector space, then denoting the $l = 2$ vector norm by $||.||_2$, we find that for all vectors V in the domain of K,

$$||KV||_2^2 = \sum_{i,j,l} K_{ij}K_{il}V_jV_l \leq \sum_{i,j,l} |K_{ij}K_{il}V_jV_l| \leq \sum_{i,j,l} \frac{|K_{ij}K_{il}|}{2}(V_j^2 + V_l^2) \tag{3.181}$$

$$= \sum_j \left(\sum_{i,l} |K_{ij}K_{il}| \right) V_j^2 \leq C||V||_2^2 \tag{3.182}$$

where C is a finite constant due to the bandedness of K and the fact the $|K_{ij}| \leq F$ for some finite F. Now denote by K_L the L by L minor of K. Since for every finite L, $||K_L||$ is finite and we have just shown that $||K|| < \infty$ there must exist some finite D such that $||K_L|| \leq D$ for all non-negative integer L. □

From *Bound 1* it is not immediately clear how the bound behaves with L or $\tau(t)$. The point of it is simply that it can be evaluated numerically with less effort than expression (3.161) on a case by case basis. From *Bound 2* the behaviour in L and $\tau(t)$ becomes more apparent and interestingly, we see that for sufficiently large L we get faster than exponential decay where as only exponential growth in τ. We also see that if the harmonic oscillators are only coupled via their

position operators and not momentum (i.e. $P = \mathbb{I}$), then we get an improvement of approximately $L \mapsto 2L$. From Theorem 57, we see that the faster than exponential decay and the improvement when $(P = \mathbb{I})$ are also true for the other term on the R.H.S. of lemma 62 when the initial two point correlation functions are bounded. This better than exponential decay has also been found in harmonic lattice systems with locally coupled oscillators [59]. We will leave a discussion of the physical significance of the constants $||PX||$ and $||M_L||$ for section 3.4 where we will apply these results to the particle and phonon chain mappings. For the case that the initial two point correlation functions grow with distance L along the chain, then one could also say something about the behaviour in L of the bounds by using theorem 58.

3.3 Some Additional Bounds and Generalisations

In this section we will give a few generalisations of the results from the previous section and also a bound for when the local Hilbert space of each oscillator is truncated for a chain of finite length. Define the finite dimensional space $\mathcal{H}^m = \text{Span}(|n\rangle,\, n = 0, 1, \ldots, m)$ where $\{|n\rangle\}_{n=0}^{\infty}$ is an orthonormal Fock basis for $L^2(\mathbb{R})$. Now define the product space $\mathcal{H}_{\mathcal{L}}^{\vec{m}} = \otimes_{i=0}^{L-1}\mathcal{H}^{m_i}$, $\vec{m} = (m_0, m_1, \ldots, m_{L-1})$, $1 \leq L < \infty$. Let $\mathbb{I}_{\vec{m}}$ be the identity operator on $\mathcal{H}_L^{\vec{m}}$, $\mathbb{I}_{m_i}$ be the indentity on $\mathcal{H}_L^{m_i}$, $\mathbb{I}_{\setminus\vec{m}} := \mathbb{I}_{\vec{\infty}} - \mathbb{I}_{\vec{m}}$ and define the quantities

$$\hat{x}_0^{\vec{m}}(t) := e^{it\hat{H}_B^{\mathcal{L},\vec{m}}}\hat{x}_0 e^{-it\hat{H}_B^{\mathcal{L},\vec{m}}} \tag{3.183}$$

$$\bar{x}_0^{\vec{m}}(t) := \sum_{i=0}^{L-1} c_{i+1}^L(t)\hat{x}_i^{m_i+1} + \bar{c}_{i+1}^L(t)\hat{p}_i^{m_i+1} \tag{3.184}$$

$$\hat{U}_{\mathcal{L},\vec{m}}(t) := e^{it(\hat{H}_s+\hat{H}_B^{\mathcal{L},\vec{m}})}e^{-it(\hat{H}_s+\hat{H}_B^{\mathcal{L},\vec{m}}+\hat{h}_s\hat{x}_0^{\vec{m}})} \text{ on } \mathcal{S}\otimes\mathcal{H}_L^{\vec{m}} \tag{3.185}$$

where

$$\hat{H}_B^{\mathcal{L},\vec{m}} := \sum_{i=0}^{L-1}\hat{r}_i^{\vec{m}} H_{B_{i,j}}\hat{r}_j^{\vec{m}}, \tag{3.186}$$

$$\hat{r}_i^{\vec{m}} := \mathbb{I}_{\vec{m}}\hat{r}_i\mathbb{I}_{\vec{m}} \text{ i.e.} \tag{3.187}$$

$$\begin{cases} \hat{x}_i^{\vec{m}} & = \otimes_{j=0}^{i-1}\mathbb{I}_{m_j}\ \frac{1}{\sqrt{2}}\sum_{n=0}^{m_i-1}\sqrt{n+1}(|n+1\rangle_i\langle n| + |n\rangle_i\langle n+1|)\otimes_{j=i+1}^{\infty}\mathbb{I}_{m_j} \\ \hat{p}_i^{\vec{m}} & = \otimes_{j=0}^{i-1}\mathbb{I}_{m_j}\ \frac{1}{\sqrt{2}}\sum_{n=0}^{m_i-1}\sqrt{n+1}(|n+1\rangle_i\langle n| - |n\rangle_i\langle n+1|)\otimes_{j=i+1}^{\infty}\mathbb{I}_{m_j} \end{cases} \tag{3.188}$$

Now let $\mathcal{S}$ be finite dimensional and recall that $\hat{H}_S$ is on $\mathcal{S}$.

Lemma 64. *With* $\hat{\rho}_s^{\mathcal{L},\vec{m}}(t) := e^{-it(\hat{H}_s+\hat{H}_B^{\mathcal{L},\vec{m}}+\hat{h}_s\hat{x}_0^{\vec{m}})}(\mathbb{I}_{\vec{m}}\hat{\rho}_0^{\mathcal{L}}\mathbb{I}_{\vec{m}})e^{it(\hat{H}_s+\hat{H}_B^{\mathcal{L},\vec{m}}+\hat{h}_s\hat{x}_0^{\vec{m}})}$, *then we have*

$$\left|tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L}}(t)] - tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L},\vec{m}}(t)]\right|^2 \tag{3.189}$$

$$\leq 4||\hat{O}_s||^2\Bigg(tr[\hat{\rho}_{B,\vec{m}}] \tag{3.190}$$

$$+ 2||\hat{h}_s||\int_0^t dy\sqrt{tr[e^{-iy\hat{H}_B^{\mathcal{L},\vec{m}}}\left(\bar{x}_0^{\vec{m}}(y)-\hat{x}_0^{\vec{m}}(y)\right)^2 e^{iy\hat{H}_B^{\mathcal{L},\vec{m}}}\hat{\rho}_s^{\mathcal{L},\vec{m}}(y)]}\Bigg), \tag{3.191}$$

where

$$tr[\hat{\rho}_{B,\vec{m}}] := tr[\mathbb{I}_{\backslash\vec{m}}\hat{\rho}_0^{\mathcal{L}}\mathbb{I}_{\backslash\vec{m}}] = 1 - tr[\mathbb{I}_{\vec{m}}\hat{\rho}_0^{\mathcal{L}}\mathbb{I}_{\vec{m}}]. \tag{3.192}$$

Proof. This proof follows the same steps as the proof of Theorem 54. The differences in the final expressions come from the fact that we are not truncating a tensor product space, but rather the one particle spaces themselves which form the tensor product space. Throughout this proof, we will neglect tensor products with the identity when it is clear from the context where they should be to prevent the notation from becoming over cumbersome. For any state $\hat{\rho}_0^{\mathcal{L}}$ on $\mathcal{S}\otimes\mathcal{H}_{\mathcal{L}}^{\vec{\infty}}$, $\vec{\infty} := (\infty,\infty,\infty,\ldots)$ and operator $\hat{O}^{\vec{m}}$, on $\mathcal{S}\otimes\mathcal{H}^{\vec{m}}$ we have

$$tr[\hat{O}^{\vec{m}}\hat{\rho}_0^{\mathcal{L}}] = tr_{\mathcal{S}}\left[\sum_{\{n_i\}=0}^{\infty}\langle n_0,\ldots,n_{L-1}|\hat{O}^{\vec{m}}\hat{\rho}_0^{\mathcal{L}}|n_0,\ldots,n_{L-1}\rangle\right] \tag{3.193}$$

$$= tr_{\mathcal{S}}\left[\sum_{\{n_i\}=0}^{\{m_i\}}\langle n_0,\ldots,n_{L-1}|\hat{O}^{\vec{m}}\hat{\rho}_0^{\mathcal{L}}|n_0,\ldots,n_{L-1}\rangle\right] \tag{3.194}$$

$$= tr_{\mathcal{S}}\left[\sum_{\{n_i\}=0}^{\{m_i\}}\langle n_0,\ldots,n_{L-1}|\hat{O}^{\vec{m}}\mathbb{I}_{\vec{m}}\hat{\rho}_0^{\mathcal{L}}\mathbb{I}_{\vec{m}}|n_0,\ldots,n_{L-1}\rangle\right] \tag{3.195}$$

$$= tr[\hat{O}^{\vec{m}}\hat{\rho}_{\vec{m}}^{\mathcal{L}}], \tag{3.196}$$

where the trace in the last line is only over the finite dimensional subspace $\mathcal{S}\otimes\mathcal{H}^{\vec{m}}$ and $\hat{\rho}_{\vec{m}}^{\mathcal{L}} := \mathbb{I}_{\vec{m}}\hat{\rho}_0^{\mathcal{L}}\mathbb{I}_{\vec{m}}$. We note that $\mathbb{I}_{\vec{m}}$ when acting on $\hat{\rho}_0^{\mathcal{L}}$ is no longer the identity operator. Using this identity and proceeding in the same manner to the proof of theorem 52 up to Eq. (3.30), we find

$$\left|tr[\hat{O}_s\hat{\rho}^{\mathcal{L}}(t) - tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L},\vec{m}}(t)]\right|^2 \leq \alpha_{L,\vec{m}}(t)\left|2\sqrt{tr[(\hat{U}_{\mathcal{L}}^*(t)-\hat{U}_{\mathcal{L},\vec{m}}^*(t))(\hat{\tilde{U}}_{\mathcal{L}}(t)-\hat{U}_{\mathcal{L},\vec{m}}(t))\hat{\rho}_0^{\mathcal{L}}]}\right|^2, \tag{3.197}$$

where $\hat{\tilde{U}}_{\mathcal{L}}$ is defined in Eq. (3.51) and

$$\alpha_{L,\vec{m}} = \left(\sqrt{tr[\hat{U}^*_{\mathcal{L}}(t)\hat{O}_s^2\hat{\tilde{U}}_{\mathcal{L}}(t)\hat{\rho}_0^{\mathcal{L}}]} + \sqrt{tr[\hat{U}^*_{\mathcal{L},\vec{m}}(t)\hat{O}_s^2\hat{U}_{\mathcal{L},\vec{m}}(t)\hat{\rho}_0^{\mathcal{L}}]}\right). \tag{3.198}$$

and

$$\begin{aligned} &tr[(\hat{U}^*_{\mathcal{L}}(t) - \hat{U}^*_{\mathcal{L},\vec{m}}(t))(\hat{\tilde{U}}_{\mathcal{L}}(t) - \hat{U}_{\mathcal{L},\vec{m}}(t))\hat{\rho}_0^{\mathcal{L}}] \qquad (3.199)\\ =&1 + tr[\hat{U}^*_{\mathcal{L},\vec{m}}(t)\hat{U}_{\mathcal{L},\vec{m}}(t)\hat{\rho}_0^{\mathcal{L}}] - 2\Re\left(tr[\hat{U}^*_{\mathcal{L}}(0)\hat{U}_{\mathcal{L},\vec{m}}(0)\hat{\rho}_0^{\mathcal{L}}] + tr[\int_0^t dy \frac{d}{dy}\hat{U}^*_{\mathcal{L}}(y)\hat{U}_{\mathcal{L},\vec{m}}(y)\hat{\rho}_0^{\mathcal{L}}]\right). \end{aligned}$$

A simple calculation tells us $\hat{U}^*_{\mathcal{L},\vec{m}}(y)\hat{U}_{\mathcal{L},\vec{m}}(y) = \hat{U}^*_{\mathcal{L}}(0)\hat{U}_{\mathcal{L},\vec{m}}(0) = \mathbb{I}_{\mathcal{S}} \otimes \mathbb{I}_{\vec{m}}$ and hence

$$\begin{aligned} &tr[(\hat{U}^*_{\mathcal{L}}(t) - \hat{U}^*_{\mathcal{L},\vec{m}}(t))(\hat{\tilde{U}}_{\mathcal{L}}(t) - \hat{U}_{\mathcal{L},\vec{m}}(t))\hat{\rho}_0^{\mathcal{L}}] \qquad (3.200)\\ &= 1 - tr[\mathbb{I}_{\vec{m}}\hat{\rho}_B] - 2\Re\left(tr[i\int_0^t dy \hat{U}^*_{\mathcal{L}}(y)\hat{h}_s(y)(\hat{x}_0(y) - \hat{x}_0^{\vec{m}}(y))\hat{U}_{\mathcal{L},\vec{m}}(y)]\right) \qquad (3.201) \end{aligned}$$

where $\hat{\rho}_B := tr_{\mathcal{S}}\hat{\rho}_0^{\mathcal{L}}$ and noting that $\mathbb{I}_\infty = \mathbb{I}_{\vec{m}} + \mathbb{I}_{\setminus\vec{m}}$, we see that $1 - tr[\mathbb{I}_{\vec{m}}\hat{\rho}_B] = tr[\mathbb{I}_{\setminus\vec{m}}\hat{\rho}_B] = tr[\hat{\rho}_{B,m}]$, $\hat{\rho}_{B,m} := \mathbb{I}_{\setminus\vec{m}} tr_{\mathcal{S}}[\hat{\rho}_0^{\mathcal{L}}]\mathbb{I}_{\setminus\vec{m}}$. Hence using the triangle inequality and a Cauchy-Schwarz inequality, we find

$$\begin{aligned} &\alpha_{L,\vec{m}}(t)\left|2\sqrt{tr[(\hat{U}^*_{\mathcal{L}}(t) - \hat{U}^*_{\mathcal{L},\vec{m}}(t))(\hat{\tilde{U}}_{\mathcal{L}}(t) - \hat{U}_{\mathcal{L},\vec{m}}(t))\hat{\rho}_0^{\mathcal{L}}]}\right|^2 \leq \qquad (3.202)\\ &4\alpha_{L,\vec{m}}(t)\left(tr[\hat{\rho}_{B,m}] + 2\int_0^t \beta_L(y)\sqrt{tr[\hat{U}^*_{\mathcal{L},\vec{m}}(y)(\hat{x}_0(y) - \hat{x}_0^{\vec{m}}(y))^2\hat{U}_{\mathcal{L},\vec{m}}(y)\hat{\rho}_0^{\mathcal{L}}]}\right) \qquad (3.203) \end{aligned}$$

Furthermore, we can easily verify that

$$\hat{U}^*_{\mathcal{L},\vec{m}}(t)\left(\hat{x}_0(t) - \hat{x}_0^{\vec{m}}(t)\right)^2\hat{U}_{\mathcal{L},\vec{m}}(t)\hat{\rho}_0^{\mathcal{L}} = \hat{U}^*_{\mathcal{L},\vec{m}}(t)\left(\bar{x}_0^{\vec{m}}(t) - \hat{x}_0^{\vec{m}}(t)\right)^2\hat{U}_{\mathcal{L},\vec{m}}(t)\hat{\rho}_0^{\mathcal{L}} \tag{3.204}$$

where $\bar{x}_0^{\vec{m}}(t)$ is in Eq. (3.184). Hence from Eqs. (3.197), (3.202), and (3.204), it easily follows Eq. (3.189). □

This is not considered to be one of the important results of this thesis because its true value is not so clear. Since everything in the bound is on a finite space, in principle one would not need to truncate anything to calculate it numerically. However, although one could expect the second term on the R.H.S. of Eq. (3.204) to be small, it is not clear how small it would be without calculating it numerically. The other term on the R.H.S. can clearly be made zero if the initial state of the bath is a finitely many particle state. In the case of a thermal state, one could calculate it exactly

using the developments of appendix B. And since the contribution to higher energy states decays exponentially, one can imagine the quantity to decrease rapidly as one increments the m_i's.
We can now obtain a bound for the error in the expectation value of a local system observable when Hamiltonian (3.5) is truncated to finite length and the infinite dimensional Fock space of each harmonic oscillator corresponding to the operators $\{\hat{r}_i\}_{i=0}^{L-1}$ are truncated: $\hat{H}_S + \hat{H}_B^{\mathcal{L},\vec{m}} + \hat{h}_s\hat{x}_0^{\vec{m}}$.

Corollary 65.

$$\left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L},\vec{m}}(t)]\right| \leq \left|tr[\hat{O}_s\hat{\rho}_s(t)] - tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L}}(t)]\right| + \left|tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L}}(t)] - tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L},\vec{m}}(t)]\right| \quad (3.205)$$

where a bound for the first term on the R.H.S. is given by lemma 62 and a bound for the second term on the R.H.S. is given by lemma 64.

Proof. add and subtract $tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L}}(t)]$ to $tr[\hat{O}_s\hat{\rho}_s(t)] - tr[\hat{O}_s\hat{\rho}_s^{\mathcal{L},\vec{m}}(t)]$ and apply the trinangle inequality. □

It is noteworthy that many of these results readily apply to Hamiltonians with multiple chains, i.e. of the form

$$\hat{H}_{mul} = \hat{H}_S + \hat{h}_{s,1}\hat{x}_{0,1} + \frac{1}{2}\,\vec{r}_1^{T} H_{B,1}\vec{r}_1 + \hat{h}_{s,2}\hat{x}_{0,2} + \frac{1}{2}\,\vec{r}_2^{T} H_{B,2}\vec{r}_2 \quad (3.206)$$

$$+ \hat{h}_{s,3}\hat{x}_{0,3} + \frac{1}{2}\,\vec{r}_3^{T} H_{B,3}\vec{r}_3 + \ldots + \hat{h}_{s,l}\hat{x}_{0,l} + \frac{1}{2}\,\vec{r}_l^{T} H_{B,l}\vec{r}_l \quad (3.207)$$

where $\vec{r}_k^{T} = (\hat{x}_{0,k}, \hat{x}_{1,k}, \hat{x}_{2,k}, \ldots, \hat{p}_{0,k}, \hat{p}_{1,k}, \hat{p}_{2,k}, \ldots,)$, $k = 1, 2, 3, \ldots, l$ collects canonical position and momentum operators and $\hat{H}_S$ and $\{\hat{h}_{s,k}\}_{k=1}^{l}$ are hermitian operators acting on the system. That is to say, bounds on system observables when all the semi-infinite chains $\{\frac{1}{2}\,\vec{r}_k^{T} H_{B,k}\vec{r}_k\}_{k=1}^{l}$ are truncated:

Corollary 66. *define*

$$\hat{H}_{mul}^{\vec{\mathcal{L}}} = \hat{H}_S + \hat{h}_{s,1}\hat{x}_{0,1} + \frac{1}{2}\,\vec{r}_1^{T} H_{B,1}^{\mathcal{L}_1}\vec{r}_1 + \hat{h}_{s,2}\hat{x}_{0,2} + \frac{1}{2}\,\vec{r}_2^{T} H_{B,2}^{\mathcal{L}_2}\vec{r}_2 \quad (3.208)$$

$$+ \hat{h}_{s,3}\hat{x}_{0,3} + \frac{1}{2}\,\vec{r}_3^{T} H_{B,3}^{\mathcal{L}_3}\vec{r}_3 + \ldots + \hat{h}_{s,l}\hat{x}_{0,l} + \frac{1}{2}\,\vec{r}_l^{T} H_{B,l}^{\mathcal{L}_l}\vec{r}_l \quad (3.209)$$

with $\{\hat{h}_{sk}\}_{k=1}^{l}$ bounded operators. Then

$$\left|tr[\hat{O}_s\hat{\sigma}_s(t)] - tr[\hat{O}_s\hat{\sigma}_s^{\vec{\mathcal{L}}}(t)]\right| \leq \sum_{k=1}^{l} F(\hat{h}_{s,k}, H_{B,k}, \{tr[\hat{r}_{q,k}\hat{r}_{j,k}\hat{\sigma}_0]\}_{q,j=0}^{\infty}, L_k; t), \quad (3.210)$$

where

$$\hat{\sigma}_s(t) = e^{-it\hat{H}_{mul}}\hat{\sigma}_0 e^{it\hat{H}_{mul}} \tag{3.211}$$

$$\hat{\sigma}_s^{\vec{\mathcal{L}}}(t) = e^{-it\hat{H}^{\vec{\mathcal{L}}}_{mul}} tr_{\backslash\vec{\mathcal{L}}}[\hat{\sigma}_0] e^{it\hat{H}^{\vec{\mathcal{L}}}_{mul}} \tag{3.212}$$

$\hat{\sigma}_0$ being the initial state, and F is defined as the R.H.S. of Eq. (3.158) with its dependency on the operator $\hat{h}_s$, initial correlations $tr[\hat{r}_k\hat{r}_j\hat{\rho}_0]$, matrix H_B and cardinality of $\mathcal{L}$ made explicit:

$$F(\hat{h}_s, H_B, \{tr[\hat{r}_q\hat{r}_j\hat{\rho}_0]\}_{q,j=0}^{\infty}, L; t) = 2\alpha(t)\sqrt{2}||\hat{h}_s|| \tag{3.213}$$

$$\left(\int_0^t dx \sqrt{\left(\sum_{i=0}^{2L-1}\nabla_i^L(x)\right)\left(\sum_{i=0}^{2L-1}\nabla_{\varsigma(i)}^L(x)\left(\sum_{k=0}^{2L-1}[e^{xM_L}]_{i+1,k+1}\left(tr[r_{\varsigma(k)}^2\rho_0]+\delta_{1,k}\right)-\delta_{1,i}\right)\right)}\right. \tag{3.214}$$

$$\left. + \int_0^t dx\sqrt{tr[(\hat{x}_0^{\backslash\mathcal{L}}(x))^2\hat{\rho}_0]}\right). \tag{3.215}$$

Recall that if $\hat{O}_s$ is bounded, then $\alpha(t) \leq 4||\hat{O}_s||^2$ and definitions for the quantities in this equation can be found in lemma 62. We can also find more explicit bounds for F using lemmas 57, 58 and 63.

Proof. This follows a similar strategy to corrolary (65). Add and subtract l times the expectation value of the observable $\hat{O}_s$ at time t under the evolution of $\hat{H}_{mul}$ truncated in different ways to $tr[\hat{O}_s\hat{\sigma}_s(t)] - tr[\hat{O}_s\hat{\sigma}_s^{\vec{\mathcal{L}}}(t)]$ and apply the striangle inequality. Then noting crucially that F does not depend on the system Hamitonian, the result follows straightforwardly. □

3.4 An Application: Locality Bounds for the Particle and Phonon Mappings

Now we will finally apply the results of this chapter to the particle and phonon mappings derived in chapter 1. First we will need to define new position and momentum operators for the particle mapping case in terms of $b_n(0)$, $b_n(0)^*$: $b_n(0) = (\hat{x}_n(0) + i\hat{p}_n(0))/\sqrt{2}$, $b_n^*(0) = (\hat{x}_n(0) - i\hat{p}_n(0))/\sqrt{2}$. with these definitions, we can write Eqs. (10) and (12) in the form Eq. (3.5) by identifying.

- *for the particle representation*

$$X = P = \mathcal{J}(d\lambda^0), \quad \hat{h}_s = \sqrt{\beta_0(0)}\hat{A}_s \tag{3.216}$$

- *for the phonon representation*

$$X = \mathcal{J}(d\lambda^1), \quad P = \mathbb{I}, \quad \hat{h}_s = \sqrt{\beta_0(1)}\hat{A}_s \tag{3.217}$$

where $\mathcal{J}(d\lambda^0)$ and $\mathcal{J}(d\lambda^1)$ are Jacobi matrices defined in Eq. (2.93) and satisfy $A1$.

Lemma 67.

$$||\mathcal{J}(d\lambda^0)|| = \omega_{max}, \quad ||\mathcal{J}(d\lambda^1)|| = \omega_{max}^2 \tag{3.218}$$

$$||\mathcal{J}_l(d\lambda^0)|| \leq \omega_{max}, \quad ||\mathcal{J}_l(d\lambda^1)|| \leq \omega_{max}^2 \quad l = 1, 2, 3, \dots \,, \tag{3.219}$$

where $\mathcal{J}_l(d\lambda^q)$ *is the* l *by* l *minor of* $\mathcal{J}(d\lambda^q)$, $q = 0, 1$ *and* $\omega_{max} := \sup g$, g *defined in section* 1.1.

Proof. This consists of noting 3 things:

1.1) In addition to being tridiagonal, $\mathcal{J}(d\lambda^0)$ and $\mathcal{J}(d\lambda^1)$ are real symmetric matrices (this follows from definition 14 in [63]), and hence due to [64], we have that

$$||\mathcal{J}(d\lambda^q)|| = \max\{|E|, E \in \mathrm{Spec}(\mathcal{J}(d\lambda^q))\} \quad q = 0, 1\,. \tag{3.220}$$

1.2) It is also known that the spectrum of a Jacobi matrix is the (minimal closed) support interval of its corresponding measure [66].

1.3) From Corollary 4 and 5 of [63] and eq.(154) in [63], it follows that the support of $\mathcal{J}(d\lambda^0)$ is $[\omega_{min}, \omega_{max}]$ and the support interval of $\mathcal{J}(d\lambda^1)$ is $[\omega_{min}^2, \omega_{max}^2]$.

Hence from the above points, we conclude Eqs. (3.218). For Eq. (3.219) we note that the eigenvalues of the minors of Jacobi matrices lie in the interior of the Jacobi matrix support interval (this follows from theorems 1.19 and 1.31 of [65]) □

Now we will give conditions under which if the two point correlation functions of the initial second quantised bath are finite, then so will the two point correlation functions of the canonical position and momentum operators of the chain. We will formulate this in terms of D defined in lemma 57 being finite. Some of the notation we will use was introduced in section 1.1.

Lemma 68. *Assume $k_{max} - k_{min}$, $\omega_{max} < \infty$, and the two-point correlation function of the intial state $\hat{\rho}_0$ with the bath modes $\hat{x}_x := (a_x^* + a_x)/\sqrt{2}$, $\hat{p}_x := i(a_x^* - a_x)/\sqrt{2}$ are finite*

$$|tr[\hat{x}_x \hat{x}_y \hat{\rho}_0]|, |tr[\hat{x}_x \hat{p}_y \hat{\rho}_0]|, |tr[\hat{p}_x \hat{x}_y \hat{\rho}_0]|, |tr[\hat{p}_x \hat{p}_y \hat{\rho}_0]| < \infty \tag{3.221}$$

for all $x, y \in [k_{min}, k_{max}]$, then

- *For the particle representation case:*
  $D < \infty$.
- *For the phonon representation case:*
  Additionally assume that $\omega_{min} > 0$, then $D < \infty$.

Although the terminology is a bit misleading, the scenario $\omega_{min} > 0$ is known in the literature as *massive bosons* while the case $\omega_{max} = 0$ as *massless bosons*.

Proof. This is a straightforward consequence of previous results. One only has to apply a few well known inequalities. Evaluating Eq. (1.30) for the particular case of the particle and phonon mappings, we have respectively:

$$\hat{x}_n(0) = \frac{b_n^*(0) + b_n(0)}{\sqrt{2}} = \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^0; x) \hat{x}_x, \tag{3.222}$$

$$\hat{p}_n(0) = \frac{i(b_n^*(0) - b_n(0))}{\sqrt{2}} = \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^0; x) \hat{p}_x, \tag{3.223}$$

and

$$\hat{x}_n(1) = b_n^*(1) + b_n(1) = \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^1; x) \frac{1}{\sqrt{g(x)}} \hat{x}_x, \tag{3.224}$$

$$\hat{p}_n(1) = \frac{i(b_n^*(1) - b_n(1))}{2} = \int_{k_{min}}^{k_{max}} dx U_n(d\lambda^1; x) \sqrt{g(x)} \hat{p}_x, \tag{3.225}$$

where $\hat{x}_x$ and $\hat{p}_x$ are defined in the lemma, and

$$U_n(d\lambda^0; x) = \frac{\pi_n(d\lambda^0; g(x))}{\sqrt{\langle \pi_n(d\lambda^0), \pi_n(d\lambda^0) \rangle_{M^0}}} \sqrt{J(g(x)) \frac{1}{\pi} \left| \frac{dg(x)}{dx} \right|}, \tag{3.226}$$

$$U_n(d\lambda^1; x) = \frac{\pi_n(d\lambda^1; g^2(x))}{\sqrt{\langle \pi_n(d\lambda^1), \pi_n(d\lambda^1) \rangle_{M^1}}} \sqrt{2g(x) J(g(x)) \frac{1}{\pi} \left| \frac{dg(x)}{dx} \right|}. \tag{3.227}$$

recall that $\pi_n(d\lambda^0;x)$ and $\pi_n(d\lambda^1;x)$ are monic polynomias of degree n and J is the spectral density of the open quantum system. We can now use Eqs. (3.222), (3.223), (3.224), (3.225) to find relations between the two point correlations functions of the intial state $\hat{\rho}_0$ in the chain canonical conjugate valiables and those of the initial Hamiltonian. From these equations, we find

$$|tr[\hat{R}_n\hat{R}_m\hat{\rho}_0]| \leq \int_{k_{min}}^{k_{max}} dx \int_{k_{min}}^{k_{max}} dy |S_{R_n}(x)||S_{R_m}(y)||tr[\hat{r}_x\hat{r}_y\hat{\rho}_0]| \tag{3.228}$$

$$\leq \max_{x,y}\left(|tr[\hat{r}_x\hat{r}_y\hat{\rho}_0]|\right) \int_{k_{min}}^{k_{max}} dx|S_{R_n}(x)| \int_{k_{min}}^{k_{max}} dy|S_{R_m}(y)| \tag{3.229}$$

$n = 0, 1, 2, \dots$, where $\hat{R}_n = \{\hat{x}_n(q), \hat{p}_n(q)\}$. If $\hat{R}_n(q) = \hat{x}_n(q)$ then $\hat{r}_z = \hat{x}_z$, $S_{R_n}(z) = S_{x_n(q)}(z)$. If $\hat{R}_n(q) = \hat{p}_n(q)$ then $\hat{r}_z = \hat{p}_z$, $S_{R_n}(z) = S_{p_n(q)}(z)$, for $z = x, y$; $q = 0, 1$ and we define

$$S_{x_n(0)}(x) := S_{p_n(0)}(x) := U_n(d\lambda^0;x),$$
$$S_{x_n(1)}(x) := \frac{U_n(d\lambda^1;x)}{\sqrt{g(x)}}, \quad S_{p_n(1)}(x) := U_n(d\lambda^1;x)\sqrt{g(x)}. \tag{3.230}$$

We will now find upper bounds for the quantities (3.230). Let us start with $S_{x_n(0)}(x)$, $S_{p_n(0)}(x)$ the quatities relevant for the particle case. Using Eq. (3.226) we have:

$$\int_{k_{min}}^{k_{max}} |S_{x_n(0)}(x)|dx = \int_{k_{min}}^{k_{max}} |S_{p_n(0)}(x)|dx \tag{3.231}$$

$$= \int_{k_{min}}^{k_{max}} \frac{dx|\pi_n(d\lambda^0;g(x))|}{\sqrt{\langle\pi_n(d\lambda^0),\pi_n(d\lambda^0)\rangle_{M^0}}}\sqrt{J(g(x))\frac{1}{\pi}\left|\frac{dg(x)}{dx}\right|} \tag{3.232}$$

$$\leq \sqrt{\int_{k_{min}}^{k_{max}} \frac{dx\,\pi_n^2(d\lambda^0;g(x))J(g(x))}{\pi\langle\pi_n(d\lambda^0),\pi_n(d\lambda^0)\rangle_{M^0}}\left|\frac{dg(x)}{dx}\right|}\sqrt{\int_{k_{min}}^{k_{max}} dx} \tag{3.233}$$

$$= \sqrt{(k_{max}-k_{min})}. \tag{3.234}$$

where between 1st and 2nd lines, we used a Cauchy-Schwarz inequality, and in lines 2nd to 3rd we performaed a change of variable and noted $M^0(x) = J(x)/\pi$. This concludes the proof of lemma 68 for the particle mapping. Similarly,

$$\int_{k_{min}}^{k_{max}} |S_{p_n(1)}(x)|dx \leq \sqrt{\int_{k_{min}}^{k_{max}} g(x)dx} \tag{3.235}$$

$$\leq \sqrt{(k_{max}-k_{min})\omega_{max}}. \tag{3.236}$$

Similarly, for $S_{x_n(1)}$ we find

$$\int_{k_{min}}^{k_{max}} |S_{x_n(1)}(x)|dx \leq \sqrt{\frac{\int_{\omega_{min}^2}^{\omega_{max}^2} dx \pi_n^2(d\lambda^1; x)\frac{M^1(x)}{\sqrt{x}}}{\int_{\omega_{min}^2}^{\omega_{max}^2} dx \pi_n^2(d\lambda^1; x) M^1(x)}} \sqrt{(k_{max} - k_{min})}. \tag{3.237}$$

If $\omega_{min} > 0$, we then have

$$\int_{k_{min}}^{k_{max}} |S_{x_n(1)}(x)|dx \quad \leq \quad \sqrt{\frac{(k_{max} - k_{min})}{\omega_{min}}}. \tag{3.238}$$

and hence we conclude the proof for the phonon mapping. □

Now we will state the values of the constants appearing in lemma 63 in terms of the chain coefficients and ω_{max}, the maximum frequency in the bath.

Corollary 69. *For the phonon and particle representations, the constants appearing in lemmas 57, 58, 62, 63 can be replaced by:*

- *For the particle representation*

$$||P|| = \sqrt{||PX||} = \omega_{max}, \quad \tau(t) = \omega_{max} t, \quad \Delta \leq \omega_{max}, \quad \Phi \leq \sqrt{\frac{\gamma_{MAX}^L}{\omega_{max}}} \tag{3.239}$$

and defining $D_1(q) = ||\hat{A}_s||\sqrt{2\beta_0(q)} + \alpha_0(q) + \sqrt{\beta_1(q)}$, $D_i(q) = \alpha_{i-1}(q) + \sqrt{\beta_{i-1}(q)} + \sqrt{\beta_i(q)}$ *for* $i = 2, 3, 4, \ldots$ *we have*

$$M = \begin{bmatrix} \alpha_0 + \sqrt{\beta_1} & \alpha_0 & 0 & \sqrt{\beta_1} & 0 & 0 & 0 & 0 & \ldots \\ \alpha_0 & D_1 & \sqrt{\beta_1} & 0 & 0 & 0 & 0 & 0 & \ldots \\ 0 & \sqrt{\beta_1} & D_2 & \alpha_1 & 0 & \sqrt{\beta_2} & 0 & 0 & \ldots \\ \sqrt{\beta_1} & 0 & \alpha_1 & D_2 & \sqrt{\beta_2} & 0 & 0 & 0 & \ldots \\ 0 & 0 & 0 & \sqrt{\beta_2} & D_3 & \alpha_2 & 0 & \sqrt{\beta_3} & \ldots \\ 0 & 0 & \sqrt{\beta_2} & 0 & \alpha_2 & D_3 & \sqrt{\beta_3} & 0 & \ldots \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\beta_3} & D_4 & \alpha_3 & \ldots \\ 0 & 0 & 0 & 0 & \sqrt{\beta_3} & 0 & \alpha_3 & D_4 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{3.240}$$

for $D_n = D_n(0)$, $\beta_n = \beta_n(0)$, $\alpha_n = \alpha_n(0)$. $||M||$, $||M_L|| < \infty$ *for* $\omega_{max} < \infty$. *Furthermore, we use the versions of the bounds valid* $\forall\ X, P$.

- *For the phonon representation*

$$||P|| = 1, \quad \sqrt{||PX||} = \omega_{max}, \quad \tau(t) = \omega_{max}t, \quad \Delta \leq \omega_{max}, \quad \Phi \leq \sqrt{\frac{\gamma^L_{MAX}}{\omega^y_{max}}} \tag{3.241}$$

where $y = 1$ *if* $\omega_{max} \geq 1$ *and* $y = 5$ *if* $\omega_{max} < 1$.

$$M = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \alpha_0 & D_1 & \sqrt{\beta_1} & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & \dots \\ \sqrt{\beta_1} & 0 & \alpha_1 & D_2 & \sqrt{\beta_2} & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{\beta_2} & 0 & \alpha_2 & D_3 & \sqrt{\beta_3} & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{3.242}$$

for $D_n = D_n(1)$, $\beta_n = \beta_n(1)$, $\alpha_n = \alpha_n(1)$. $||M||$, $||M_L|| < \infty$ *for* $\omega_{max} < \infty$. *Furthemore, we can use the versions of the bounds valid when* $P = \mathbb{I}$.

Proof. A direct consequence of Eqs. (3.216), (3.217) and lemma 67. □

This should be considered the main result of this chapter and was the initial goal of the endeavour described here. We will therefore have a short discussion about this result. One of the first things we notice is that for both the particle and phonon mappings, $\tau = \omega_{max}t = (\sup g)t$, g being the dispersion relation of the bath. We see that the bath cannot compose of oscillators with unbounded frequencies. Furthermore, it suggests that high bath frequencies propagate faster down the chain. We can find more evidence for this when we recall Eqs. (2.158) and (2.159) which tells us that for Szegö Class spectral densities, the chain coefficients become translationally invariant and increase monotonically with ω_{max}. In the case that the frequencies are unbounded, i.e. that $\omega_{max} = \infty$, the chain coefficients are unbounded and grow along the chain. As a result, it is not even clear that there is a finite speed of sound and it is highly likely that signals accelerate as they go down the chain. More evidence for this possibility can be found in [67], where a minimum bound on the capacity of sending information down a harmonic chain was calculated. It was found that initial states with $tr[\hat{H}\hat{\rho}_0]$, $tr[\hat{H}^2\hat{\rho}_0]$, finite where $\hat{H}$ is the Hamiltonian and $\hat{\rho}_0$ is the initial state,

can transmit information with increasing speed down a harmonic chain if the chain coefficients are unbounded.

Another interesting point is that from the bounds we see that approximately, one has to have a chain of double the length in the particle mapping case to achieve the same value of the bound as in the phonon mapping case. From the maths point of view, the reason for this is because the particle chain has coupling in both position and momentum at each site to its nearest neighbour whereas the phonon mapping only has coupling in position. The question is whether it just happens that the phonon mapping has a tighter bound than the particle mapping or whether the difference is physical. We can find evidence which backs up that the difference is physical in the literature. In [68], the transport dynamics of entanglement is studied both numerically and analytically for harmonic systems. In section 5.4 *Speed of entanglement propagation*, they find that entanglement propagates faster in particle-like chains (they call these RWA chains) as opposed to in phonon-like chains (they call these hook-law chains)[2] suggesting that the difference really is physical.

3.5 Chapter Summary and Conclusion

In this chapter, we have developed locality bounds for local bounded observables acting on a local Hilbert space connected to a semi-infinite harmonic lattice with nearest neighbour coupling.

We have developed two different forms of the bound according to two different schemes, - one more appropriate if the simulation is performed in the interaction picture, the other more relevant if the simulation is done in the schrödinger picture. Depending of the properties for the initial state, we have developed difference forms of the bound. The bounds obtained decay in distance faster than exponential decay. These bounds are new results since previously the only bounds for infinite dimensional systems were harmonic lattices and certain types of anharmonic lattices. Very recently, Lieb Robinson bounds have been shown for the case of harmonic lattices coupled bi-linearly to spin systems [69]. However, the results here are still different since on the one hand

[2]In order to make a fair comparison between their hook and R.W.A. chains and the particle and phonon chains, one has to be careful how to find the correct relationship between their constant c and the corresponding constants for the phonon and particle chains. To do this one can use the translationally invariant limiting cases given by Eqs. (2.158) and (2.159) when the chain coefficients are known in terms of ω_{min}, and ω_{max} only. This yields the desired result

they only get algebraic decay (with an inverse power of around 3) with distance and their method could only be applied to the scenarios studied here if the system Hamiltonian $\hat{H}_S$ and the system operator coupling the system to the bath $\hat{h}_s$ are spanned by spin operators. For our proof, we only require that $\hat{h}_s$ be a bounded operator.

When we apply these results to the phonon and particle mappings, it provides an upper bound to the error induced if one truncates the semi-infinite chain. By doing so, we also prove that chain truncation is a numerically exact procedure. What's more, the error decreases faster than the standard Lieb-Robinson exponential decay in distance (or in the case of the chain, number of harmonic oscillators of the chain included in the simulation). The bounds suggest that the phonon mapping would be more efficient from the point of view of the truncation. Roughly speaking, it suggests that with a phonon mapping chain of half the length of a particle mapping chain, one could simulate the same observables for the same amount of time with the same error.

Chapter 4

Outlook

If time had permitted, there are many other interesting extensions one could have examined. A selection of these is the following:

1) The chain mapping theorem 9 is derived with the assumption that the bath of oscillators is bosonic. However, it should be straightforward to generalise this for fermionic baths. The derivation would differ in Eqs. (1.38), (1.39) where one would have to replace the cosh and sinh functions with sin and cos functions to satisfy the fermionic anti-commutation relations. This would lead to different versions of the equations (1.50) and (1.51). It would be interesting to see what kinds of chains can be generated, i.e. can one generate chains with the same type of coupling structure as in the bosonic particle and phonon mapping cases? Furthermore, a full investigation into all valid solutions for the parameters c_1, c_2, g_1, g_2, was not performed. Maybe other solutions exist where the chain has coupling between the nth site and $(n+1)$th site is of the form $b_n^* b_{n+1}^* + b_n b_{n+1}$. One could then find locality bounds for this case which may be better than for the particle and phonon mappings (we have already seen the the phonon mapping gives better bounds than the particle mapping) which may allow for more efficient simulations.

2) In the case that the support of the spectral density is on an unbounded interval, the sequence of secondary measures does not converge. However, the formula for them is still perfectly valid for gapless measures. One may be able to study their symptotic properties by looking at the symptonic properties of the orthogonal polynomials that appear in the formula. Symptotic

properties of orthogonal polynomials have been studied in great detail in [70]. Although it can be shown that there are no fixed points in the sequence, it is not unfeasible that the nth secondary measure has universal properties for large n and maybe measures of markovianity do converge and markovian approaches to treating the residual spectral density might be even more advantageous than in the bounded support interval case.

3) Lieb Robinson bounds for fermions are already known [55], so one can imagine that it would be simple to develop error bound for truncating the infinitely many degrees of freedom of the environment in the fermionic bath case.

4) One could make two generalisations of the results in chapter 3. One could extend it to Hamiltonians which do not have nearest neighbour to any local coupling. More precisely speaking, any Hamiltonian for which X and P appearing in Eq. (3.73) are any banded matrices. The results could also be extended to the case that the quantum system does not couple to the bath via the position operator $\hat{x}_0$ but rather any canonical position or momentum operator of the semi-infinite chain. The main ingredient in such a generalisation would be a generalisation of theorem 59 to any banded matrix (rather than just tridiagonal ones) and to all matrix components (rather than just the components of the first row. The inductive proof given for theorem 59 should be easily generalizable to cover these cases. One could also then use the generalised version of theorem 59 to derive error bounds for exponentiating a truncated banded matrix rather than exponentiating the matrix itself, i.e. generalisations of theorem 60.

5) One could use the results of the last chapter to work out a minimum time it takes the initial residual bath $tr_{\mathcal{L}}[\hat{\rho}_0]$ to have an effect on the system. Similar lines of investigation were studied in [71].

6) Since the particle and phonon mapping chains when truncated to include only L oscillators can be written as a discrete bath of oscillators with L modes, one should be able to use the results of the Schrödinger bound to derive error bounds for system observables of Hamiltonian Eq. (1.1) when the bath is discretised. One should be able to state the theorem in a way such that the particle and phonon mappings are not even mentioned. The way the spacing

of the discretisation would be chosen, would depend on whether we used the results of the particle mapping or the phonon mapping.

7) In [67] it was shown by example that there exist locally coupled Hamiltonians on infinite dimensional Hilbert spaces for which information can be transmitted at an accelerating speed thought the lattice under free evolution of initial states $\hat{\rho}_0$ which have $tr[\hat{H}\hat{\rho}_0]$, $tr[\hat{H}^2\hat{\rho}_0]$ finite, where $\hat{H}$ is the Hamiltonian of the lattice. In this example there was no maximum speed at which information can be transmitted. This raises a natural question: are their classes of initial states which do always have a locality bound with a finite speed of sound for all lattice models? My hunch is that for all locally coupled lattice models, all finitely many superpositions of energy eigenstates have a speed of sound i.e. maximum speed limit.

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Appendix A

The Hilbert Space of the Specialized Pauli-Fierz Hamiltonian presented in Eq (1.1)

Here we will brifly describe in a bit more detail the Hilbert space of Hamiltonian (1.1). Some of the concepts and definitions introduced here, will also be usefull in the next appendix section.
The Hilbert space of the Hamiltonian for this model $\mathcal{H}$, is the tensor product of the space of the quantum system wavefunctions and the Fock space for the bosonic bath. Formally, $\mathcal{H} = \mathcal{S} \otimes \Gamma(\mathfrak{h})$, where $\mathcal{S}$ is a separable Hilbert space describing the quantum system and $\Gamma(\mathfrak{h})$ is the bosonic Fock space[1] over the one particle space $\mathfrak{h} = L^2(\mathbb{R}^p, d\vec{k})$, where $\vec{k}$ is the boson momentum. This describes a field of bosons. An element Ψ of $\mathcal{H}$, is a vector $\{\Psi^{(n)}\}_{n=0}^{\infty}$ with $\Psi^{(n)} = \varphi \otimes \psi^{(n)}$, where $\psi = \{\psi^{(n)}\} \in \Gamma(\mathfrak{h})$, $\psi^{(n)}(\vec{k}_1, \ldots, \vec{k}_n) = \hat{S}\ \psi_1^{(n)}(\vec{k}_1) \otimes \psi_2^{(n)}(\vec{k}_2) \otimes \ldots \otimes \psi_n^{(n)}(\vec{k}_n)$ is on $\mathbb{R}^{p\,n}$. $\hat{S}$ is the *symmetrisation operator* which makes $\psi^{(n)}$ symmetric in $\vec{k}_1, \ldots, \vec{k}_n$ and $\psi_m^{(n)} \in \mathfrak{h}$ are known as *one particle wave functions*. The domain of $\varphi \in \mathcal{S}$ is to be specified with the details of the quantum system. The elements of $\mathcal{H}$ satisfy $||\Psi|| := ||\varphi||_{\mathcal{S}} ||\psi||_{\Gamma(\mathfrak{h})} < \infty$, where

$$||\Psi||^2 = ||\varphi||_{\mathcal{S}}^2 \left(|\psi^{(0)}|^2 + \sum_{n=1}^{\infty} \int_F \ldots \int dk_1 \ldots dk_n |\psi^{(n)}(k_1, \ldots, k_n)|^2 \right). \tag{A.1}$$

[1] also known as symmetric Fock space

As regards for Hamiltonian Eq. (1.1), reproduced here for convenince

$$\hat{H} = \hat{H}_{\mathcal{S}} \otimes \mathbb{I}_{\Gamma(\mathfrak{h})} + \mathbb{I}_{\mathcal{S}} \otimes \int dk g(k) a_k^* a_k + \hat{A}_s \otimes \int dk h(k)(a_k^* + a_k), \tag{A.2}$$

we have that $\hat{H}_S$ is a self-adjoint operator on $\mathcal{S}$ and describes the system dynamics, $\hat{H}_E := \int dx g(k) a_k^* a_k$ is the Hamiltonian of the bath where $g \geq 0$. This is also known in the literature as $d\Gamma(g)$, *the second quantisation* of g. a_k^*, a_k are creation and annihilation operators with cummutator $[a_k, a_{k'}^*] = \delta(k - k')$. They act on each $\psi^{(n)}$ by

$$(a_k \psi)^{(n)}(k_1, \ldots, k_n) = (n+1)^{1/2} \psi^{(n+1)}, (k, k_1, \ldots, k_n) \tag{A.3}$$

$$n = 0, 1, 2, \ldots \tag{A.4}$$

$$(a_k^* \psi)^{(n)}(k_1, \ldots, k_n) = n^{-1/2} \sum_{j=1}^{n} \delta(k - k_j) \psi^{(n-1)}, (k_1, \ldots, \hat{k}_j, \ldots, k_n) \tag{A.5}$$

$$n = 1, 2, 3, \ldots , \tag{A.6}$$

$$(a_k^* \psi)^{(0)} = 0, \tag{A.7}$$

where $\hat{k}_j$ indicates that k_j is omitted. Hence we have that $(\mathbb{I}_{\mathcal{S}} \otimes \hat{H}_E \Psi)^{(n)} = \sum_{j=1}^{n} g(k_j) \Psi^{(n)}$ on domain $\mathcal{D}(\mathbb{I}_{\mathcal{S}} \otimes \hat{H}_E)$ of all $\Psi \in \mathcal{H}$ such that $\{(\mathbb{I}_{\mathcal{S}} \otimes \hat{H}_E \Psi)^{(n)}\}$ is again in $\mathcal{H}$. Let $\mathfrak{n}$ be the number of bosons operator defined by

$$(\mathfrak{n}\psi)^{(n)} = n\psi^{(n)}, \quad n = 0, 1, 2, \ldots \tag{A.8}$$

on the domain $\mathcal{D}(\mathfrak{n})$ of all ψ in $\Gamma(\mathfrak{h})$ such that $\{n\psi^{(n)}\}$ is again in $\Gamma(\mathfrak{h})$. $\hat{H}_{int} := \hat{A}_s \otimes \int dk h(k)(a_k^* + a_k)$ describes the interaction between the quantum system and the bosonic environment. $h(k) \in \mathfrak{h}$ and $\int dk h(k)(a_k^* + a_k) = a_k^*(h) + a_k(h)$, where

$$\big(a_k(h)\psi\big)^{(n)}(k_1, \ldots, k_n) = (n+1)^{1/2} \int h(k) \psi^{(n+1)}(k, k_1, \ldots, k_n) dk, \tag{A.9}$$

$$n = 0, 1, 2, \ldots . \tag{A.10}$$

$$\big(a_k^*(h)\big)^{(n)}(k_1, \ldots, k_n) = n^{-1/2} \sum_{j=1}^{n} h(k_j) \psi^{(n-1)}(k_1, \ldots, \hat{k}_j, \ldots, k_n), \tag{A.11}$$

$$n = 1, 2, 3, \ldots . \quad \text{and } \big(a_k^*(h)\psi\big)^{(0)} = 0, \tag{A.12}$$

is a well-defined self-adjoint operator (also known in the literature as $\Phi_s(h)$, the *Segal field operator*) on $\mathcal{D}(\mathfrak{n}^{1/2})$. $\hat{A}_s$ is any bounded below self-adjoint operator with domain in $\mathcal{S}$ such that $\hat{H}$ is a well

defined Hamiltonian with domain in $\mathcal{H}$. The necesary conditions for $\hat{H}$ to be self-adjoint can be found in section 1.1.

Appendix B

The Initial State in the Chain Basis

In this section we will show how to write the second quantised Fock states of the bath of the Hamiltonian Eq (1.1) (i.e. states $\psi = \{\psi^{(n)}\}_{n=0}^{\infty} \in \Gamma(\mathfrak{h})$ written in terms of the one particle wave functions) in the chain Fock basis F_q defined in Eq. (2.99) and vice versa. We will use notation introduced in the previous appendix throughout this section. This should be implemented to write any initial state in a form which one can readily used to compute its dynamics in the chain basis. We do this by finding the relation between the vacuum state in the wave function representation and the vacuum state in the chain Fock basis. Then we apply creation operators to generate the relation between all the other states. We will exemplify this process for the particle mapping and assume that the one particle space is $\mathfrak{h} = L^2(\mathbb{R}, dk)$. Recall that if this is not already the case, we can assume this w.l.o.g. by applying a unitary transformation on the one-particle wave functions to bring them into the Standard Form discussed in section 1.1. The general procedure can also be implemented for the phonon mapping (although one must be careful in this case since the vacuum state of the phonon chain is shifted with respect to that of the second quantised wafe function vacuum state). The vacuum state in terms of one particle wave functions is $(1, 0, 0, \ldots)^T$ since $a(f)(1, 0, 0, \ldots)^T = (0, 0, 0, \ldots)^T$ for all test functions $f \in \mathfrak{h}$. In the chain Fock basis, the vacuum state is $|0, 0, 0, \ldots\rangle$. From Eq. (1.64), we have that $b_n(0) = a(F_n), b_n^*(0) = a^*(F_n)$ where $F_n(x) = P_n(d\lambda^0; g(x))\sqrt{J(g(x))/\pi\,|dg(x)/dx|}$ Hence we have $|0, 0, 0, \ldots\rangle = (1, 0, 0, \ldots)^T$. By applying the raising operator to both sides we find

$$|\underbrace{0, 0, \ldots, 0}_{q-\text{zeros}}, 1, 0, \ldots\rangle = (0, F_q(k_1), 0, \ldots)^T \; q = 0, 1, 2, \ldots. \tag{B.1}$$

Since for all $V \in \mathbb{P}$ we can write $V(x) = \sum_{i=0}^{\infty} c_i F_i(x)$, $c_i \in \mathbb{R}$, we see that any second quantised one-particle wave function is a superposition of one particle states in the chain Fock basis. If we apply the creation operator to both sides of this state, we find

$$|\underbrace{0,0,\ldots,0}_{q-\text{zeros}},2,0,\ldots\rangle = (0,0,F_q(k_1)\otimes F_q(k_2),0,\ldots)^T \tag{B.2}$$

$$|\underbrace{\overbrace{0,0,\ldots,0}^{p-\text{zeros}}}_{q-\text{zeros}},1,0,\ldots,0,1,\ldots\rangle = (1/\sqrt{2})(0,0,F_p(k_1)\otimes F_q(k_2)+F_p(k_2)\otimes F_q(k_1),0,\ldots)^T \tag{B.3}$$

We can continue this procedure to find how to write any chain Fock basis state in terms of second quantised one particle wave functions. By applying the raising operator N times, we find:

$$\Lambda_{p_1,\ldots,p_N}|\underbrace{0,0,\ldots,0}_{p_1-\text{slots}},1,0,\ldots,0,1,0,\ldots,0,1,\ldots,0,1,0,\ldots\rangle \tag{B.4}$$

$$\underbrace{\qquad\qquad}_{p_2-\text{slots}}$$

$$\underbrace{\qquad\qquad\qquad}_{p_3-\text{slots}}$$

$$\vdots$$

$$\underbrace{\qquad\qquad\qquad\qquad\qquad}_{p_N-\text{slots}}$$

$$= \Lambda_{p_1,\ldots,p_N}|l_0,l_1,l_2,\ldots,l_\gamma,0,0,0,\ldots\rangle \tag{B.5}$$

$$= \frac{1}{\sqrt{N!}}(\underbrace{0,\ldots,0}_{N-\text{zeros}},\hat{S}F_{p_1}(k_1)\otimes F_{p_2}(k_2)\otimes\ldots\otimes F_{p_N}(k_N),0,\ldots)^T \tag{B.6}$$

where $\Lambda_{p_1,\ldots,p_N} := \sqrt{\Pi_{i=\{p_1,p_2,\ldots,p_N\}} l_i}$, $l_i = \sum_{j=\{p_1,p_2,\ldots,p_N\}} \delta_{ij}$, $\gamma = \sup\{p_1,p_2,\ldots,p_N\}$, for $N,p_1,p_2,\ldots,p_N = 0,1,2,\ldots$ and $\hat{S}$ acts on $F_{p_1}(k_1)\otimes F_{p_2}(k_2)\otimes\ldots\otimes F_{p_N}(k_N)$ by summing over all permutations of the variables $k_1,k_2,\ldots,k_N$ so that it is invariant under exchange of any two variables k_i,k_j, e.g. $\hat{S}F_p(k_1)\otimes F_q(k_2) = F_p(k_1)\otimes F_q(k_2)+F_p(k_2)\otimes F_q(k_1)$. Using the orthogonality conditions of the polynomials and the linearity of the $\hat{S}$ operator, we can also derive the inverse relation: Let $W_i(x)\in\mathfrak{h}$ be a one-particle wave function, then

$$\frac{1}{\sqrt{N!}}(\underbrace{0,\ldots,0}_{N-\text{zeros}},\hat{S}W_1(k_1)\otimes W_2(k_2)\otimes\ldots\otimes W_N(k_N),0,0,0,\ldots)^T = \tag{B.7}$$

$$\sum_{p_1=0}^{\infty}\sum_{p_2=0}^{\infty}\ldots\sum_{p_N=0}^{\infty} C_{1,p_1}C_{2,p_2}\ldots C_{N,p_N}\Lambda_{p_1,\ldots,p_N}|l_0,l_1,l_2,\ldots\rangle \tag{B.8}$$

where

$$C_{i,j} := \int W_i(x) F_j(x) dx. \tag{B.9}$$

Hence we can write any second quantised wave functions in terms of the chain Fock basis. What is more, since $\sum_{i=0}^{\infty} l_i = N$, we conclude from Eqs. (B.5)-(B.6) and (B.7)-(B.8) that all n-particle wave functions are linear superposition's of n-particle chain Fock states and vice versa. This should not come as a surprise, given that the coupling between harmonic oscillators of the chain mapping is also particle preserving. Furthermore, we can readily check that $\langle m|n\rangle = \delta_{mn}$ courtesy of the orthogonally conditions of the orthonormal polynomials used to construct $F_q(x)$. For the numerics, we can justify the approximation

$$\frac{1}{\sqrt{N!}}(\underbrace{0,\ldots,0}_{N-\text{zeros}}, \hat{S}W_1(k_1)W_2(k_2)\ldots W_N(k_N), 0, 0, 0, \ldots)^T \tag{B.10}$$

$$\approx \sum_{p_1=0}^{M_1}\sum_{p_2=0}^{M_2}\ldots\sum_{p_N=0}^{M_N} C_{1,p_1}C_{2,p_2}\ldots C_{N,p_N}\Lambda_{p_1,\ldots,p_N}|l_0, l_1, l_2, \ldots\rangle \tag{B.11}$$

$$= \sum_{p_1=0}^{M_1}\sum_{p_2=0}^{M_2}\ldots\sum_{p_N=0}^{M_N} C_{1,p_1}C_{2,p_2}\ldots C_{N,p_N}\Lambda_{p_1,\ldots,p_N}|l_0, l_1, l_2, \ldots, l_\kappa, 0, 0, \ldots\rangle, \tag{B.12}$$

$\kappa = \max\{M_1, M_2, \ldots, M_N\}$ by noting that this corresponds to approximating $W_i(x)/\sqrt{J(g(x))|dg(x)/dx|/\pi}$ to order M_i in $g(x)$. Since k is the momentum space variable, this will be a good approximation if the ith one particle wave function has low probability of having high momenta.

Appendix C

Methods for Calculating the Reducer

In this section we will give a few different methods for calculating the reducer (see Eq. 24) when the measure satisfies some special properties

Theorem 70. *If for a measure $d\mu(x) = \bar{\mu}(x)dx$, $\bar{\mu}(x)$ satisfies a Lipschitz condition over its support interval $[a, b]$, then*

$$\varphi(d\mu; x) = 2\bar{\mu}(x) \ln\left(\frac{x-a}{b-x}\right) - 2\int_a^b \frac{\bar{\mu}(t) - \bar{\mu}(x)}{t-x} dt. \tag{C.1}$$

Proof. From definitions 24 and 6 we have

$$\varphi(d\mu; x) = \lim_{\epsilon \to 0^+} 2\int_a^b \frac{(x-t)\bar{\mu}(t)dt}{(x-t)^2 + \epsilon^2}. \tag{C.2}$$

Writing this as

$$\varphi(d\mu; x) = \lim_{\epsilon \to 0^+} 2\int_a^b \frac{(x-t)\bar{\mu}(x)}{(x-t)^2 + \epsilon^2} dt + \lim_{\epsilon \to 0^+} 2\int_a^b \frac{(x-t)(\bar{\mu}(t) - \bar{\mu}(x))}{(x-t)^2 + \epsilon^2} dt \tag{C.3}$$

$$= \lim_{\epsilon \to 0^+} 2\int_a^b \frac{(x-t)\bar{\mu}(x)}{(x-t)^2 + \epsilon^2} dt - 2\int_a^b \frac{\bar{\mu}(t) - \bar{\mu}(x)}{t-x} dt \tag{C.4}$$

$$- \lim_{\epsilon \to 0^+} \int_a^b \left(\frac{2\epsilon^2}{(x-t)^2 + \epsilon^2}\right) \frac{\bar{\mu}(t) - \bar{\mu}(x)}{x-t} dt. \tag{C.5}$$

1) The first integral in line (C.4) reduces to

$$\lim_{\epsilon \to 0^+} 2\int_a^b \frac{(x-t)\bar{\mu}(x)}{(x-t)^2 + \epsilon^2} dt = \lim_{\epsilon \to 0^+} \bar{\mu}(x) \left[\ln((a-x)^2 + \epsilon^2) - \ln((b-x)^2 + \epsilon^2)\right] \tag{C.6}$$

$$= 2\bar{\mu}(x) \ln\left(\frac{x-a}{b-x}\right). \tag{C.7}$$

2) Now imposing the Lipschitz condition on $\bar{\mu}(x)$: $|\bar{\mu}(x) - \bar{\mu}(t)| \leq K|t - x|$ for some K over interval $[a, b]$, the absolute value of the expression on line (C.5) reduces to

$$\lim_{\epsilon \to 0^+} \int_a^b \left(\frac{2\epsilon^2}{(x-t)^2 + \epsilon^2} \right) \frac{|\bar{\mu}(t) - \bar{\mu}(x)|}{|t - x|} dt \tag{C.8}$$

$$\leq \lim_{\epsilon \to 0^+} \int_a^b \frac{2K\epsilon^2}{(x-t)^2 + \epsilon^2} dt \tag{C.9}$$

$$= \lim_{\epsilon \to 0^+} 2K\epsilon \left[\arctan\left(\frac{b-x}{\epsilon} \right) - \arctan\left(\frac{a-x}{\epsilon} \right) \right] \tag{C.10}$$

$$= 0. \tag{C.11}$$

Hence expression on line (C.5) vanishes.

□

Theorem 71. *If for a measure $d\mu(x) = \bar{\mu}(x)dx$, $\bar{\mu}(x)$ possesses a bounded continuous first derivative on its support interval I and $\bar{\mu}(x)$ can be evaluated on the limits a, b, then*

$$\varphi(d\mu; x) = 2 \left[\bar{\mu}(a) \ln \left| \frac{x-a}{x} \right| + \bar{\mu}(b) \ln \left| \frac{x}{b-x} \right| + \int_a^b \bar{\mu}'(t) \ln \left| \frac{t-x}{x} \right| dt \right], \tag{C.12}$$

where $\bar{\mu}'(t)$ is the first derivative of $\bar{\mu}(t)$.

Proof. Follows from integrating Eq. (C.1) by parts and noting that if a function $f(x)$ possesses a bounded continuous first derivative on its domain, then it also satisfies a Lipschitz condition on its domain (this last statement is proven in [48]). □

Appendix D

Scaling Properties of the Sequence of Beta Normalised Measures

Here we present a few simple lemmas which are useful for section 2.3.

Lemma 72. *Suppose we have two measures $d\nu^1(x) = \bar{\nu}^1(x)dx$ and $d\nu^2(x) = \bar{\nu}^2(x)dx$ with support intervals I^1, I^2 bounded by $\lambda a, \lambda b$ and a, b respectively. If they are related by*

$$\bar{\nu}^1(x) = \frac{\bar{\nu}^2(x/\lambda)}{\lambda}, \qquad \lambda > 0, \tag{D.1}$$

then their sequence of beta normalised measures have the relation

$$\bar{\nu}^1_n(x) = \lambda \bar{\nu}^2_n(x/\lambda) \quad n = 1, 2, 3, \ldots . \tag{D.2}$$

Proof. Using the definition of inner product, Eq. (1.9), and relation eq. (D.1), we find

$$\langle f, g \rangle_{\bar{\nu}^2} = \int_a^b f(\lambda t) g(\lambda t) d\nu^1(t). \tag{D.3}$$

Hence we conclude

$$P_n(d\nu^1; x) = P_n(d\nu^2; x/\lambda) \quad n = 0, 1, 2, \ldots . \tag{D.4}$$

Using this relation and definition 5, we find

$$Q_n(d\nu^1; x) = \frac{Q_n(d\nu^2; x/\lambda)}{\lambda} \quad n = 0, 1, 2, \ldots . \tag{D.5}$$

Similarly, we have from definition 24

$$\varphi(d\nu^1; x) = \frac{\varphi(d\nu^1; x/\lambda)}{\lambda}. \tag{D.6}$$

Finally, substituting Eq. (D.4), (D.5), and (D.6) into definition 32 we arrive at Eq. (D.2). □

Lemma 73. *The sequence of beta normalised measures generated from a measure $d\nu(x) = \bar{\nu}(x)dx$ are invariant under the mapping $d\nu(x) \to \lambda d\nu(x)$, $\lambda > 0$ while keeping the support interval I unchanged.*

Proof. Follows with a similar line of reasoning as for lemma 72. □

Appendix E

Proof that the Relation between the Stieltjes Transforms of two Consecutive Measures is invalid for Gapped Measures

In the case of a gapless interval $I = [a, b]$, the relation between the Stieltjes transforms of subsequent measures, Eq (1.23): $S_\rho(z) = z - C_1(d\mu) - 1/S_\mu(z)$, $z \in \mathbb{C} - I$ is well defined because $S_\mu(z)$ does not vanish on $\mathbb{C} - I$:

Proof. Let $z = x + iy \quad x, y \in \mathbb{R}$;

$$S_\mu(z) = \int_a^b \frac{\mu(t)dt}{x + iy - t} = \int_a^b \frac{(x-t)\mu(t)dt}{(x-t)^2 + y^2} - iy \int_a^b \frac{\mu(t)dt}{(x-t)^2 + y^2}. \tag{E.1}$$

Hence for $S_\mu(z) = 0$ we need $y = 0$, thus $z = x \in \mathbb{C} - I$, however, under these conditions $(x-t)\mu(t)$ cannot change sign in $t \in I$, therefore $S_\mu(z) \neq 0$. □

In the case of a gapped interval $I = [a, b] \cup [c, d]$, $S_\mu(z)$ the Stieltjes transformation is defined by

$$S_\mu(z) = \int_a^b \frac{\mu(t)dt}{z - t} + \int_c^d \frac{\mu(t)dt}{z - t}. \tag{E.2}$$

Unfortunately, this expression vanishes on a point in $[b, c]$

Proof. Taking real and imaginary parts of $S_\mu(z)$ followed by setting the imaginary part to zero,

we find

$$S_\mu(x) = \int_a^b \frac{(x-t)\mu(t)dt}{(x-t)^2} + \int_c^d \frac{(x-t)\mu(t)dt}{(x-t)^2}, \tag{E.3}$$

where $z = x \in \mathbb{R} - I$. However, the numerators of the first and second integrals have a different sign for $x \in [b, c]$. Thus due to the continuity of $S_\mu(x)$ in $]b, c[$ and the existence of the limits $\lim_{x\to b} S_\mu(x) = +\infty$, $\lim_{x\to c} S_\mu(x) = -\infty$, there exists a point z_0 in $\mathbb{C} - I$ such that $S_\mu(z_0) = 0$. □

Consequently, one cannot define a secondary measure which satisfies theorem 7, through this relation because the Stieltjes transform must be holomorphic.