DIFFUSION FOR MARKOV WAVE EQUATIONS

By

Bernard Clark Musselman II

A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

Applied Mathematics

2012

ABSTRACT

DIFFUSION FOR MARKOV WAVE EQUATIONS

By

Bernard Clark Musselman II

We consider the long time evolution of solutions to a Schrödinger-type wave equation on a lattice, with a divergence-form, Markov, random generator. We show that solutions to this problem diffuse. That is, the amplitude converges to the solution of a diffusion equation, in the diffusive scaling limit.

Additionally, we expand upon a similar result due to Kang and Schenker for a Markov-Schrödinger wave equation by computing higher moments of position, also in the diffusive scaling limit.

In memory of my father, Dr. Bernard C. Musselman.

ACKNOWLEDGMENT

First and foremost, I wish to thank my advisor, Jeffrey Schenker. Without his patience and depth of knowledge, this work would not be possible. His generosity in supporting my graduate work made the task of completing this thesis much more manageable. I am also deeply indebted to my wife, Alexandria, for her unwavering encouragement and faith in my abilities. I am most thankful to my mother for her unconditional support; to John Theakston for interesting conversations related to this work; to Shari Ultman for encouragement early on, when I needed it the most; to Liam Finlay for giving me an outlet and for putting things in perspective; to Dr. Hill for giving me the opportunity, year after year, to be a part of something really important; to my students for giving me purpose; to P.T. for teaching me to live in the moment; and to Tom Bellsky, Matt St. Peter, and Sara Vredevoogd for their friendship and collaboration. Additionally, I wish to thank Luke Williams and Dr. Weil for their help in preparing this document. I am also grateful to the Erwin Schrödinger Institute for their support and hospitality.

TABLE OF CONTENTS

LIST OF FIGURES

Chapter 1

Introduction to Diffusion for Markov Wave Equations

In the classic study of *deterministic* partial differential equations, the phenomena of *wave propagation* and *diffusion* are treated separately. The derivations of the heat and wave equations are distinct and rely on observations of different physical behavior. Important properties such as the maximum principle, regularity and the domain of dependence, also called the wave cone [2], have no analog on the other side. While both models have existence/uniqueness theorems, the methods of proof are vastly different and a deep understanding of one does not necessarily provide any intuition about the other. Waves in nature, however, do not satisfy such a distinction. Indeed, a vibrating guitar string will eventually come to rest as do the waves on water's surface, in the absence of wind or further vibration.

It is not the immediate goal here to include every aspect of nature in a particular wave model. Instead, we show that when noise or disorder is included, one can see a departure from the classic understanding of wave propagation. The resulting more natural model allows for the diffusion of wave packets. Specifically, we show that for two particular examples, if the environment through which a wave packet propagates is governed by a Markov process, then the wave packet will eventually diffuse.

Related to the above, the first question we address is "How does one detect diffusion?". In chapter 2, we develop a mathematical *characterization* of diffusion by beginning with the diffusion equation. After all, whatever characterization we decide upon must be consistent with the classic diffusion equation. From this, we derive a natural *scaling* and define diffusion for a wave equation to be the convergence (under this *scaling-limit*) of its square-amplitude to the solution of a diffusion equation.

In chapter 3 and with this understanding of diffusion, we discuss a model with a *divergence-form* generator that includes randomness. This begins by studying the semi-group generated by a Markov process and its underlying probability measure. This semi-group gives rise to a *generator* which encapsulates the process in a *maximally-dissipative* operator on a Hilbert space. A few further assumptions on the generator give us enough leverage to control the spectrum of the *overall* problem: the Markov generator together with the divergence-form generator. We then demonstrate the (slightly weakened) diffusion criterion by computing the diffusive-scaling limit of norm-squared solutions.

The weakening of this criterion is essential to our method. (A procedure for strengthening this weakened criterion, as well as a complete example, is given in chapter 4.) By averaging the diffusive criterion over all realizations of the disorder, instead of computing the criterion for arbitrary realizations, we reformulate it in terms of a *particular matrix element* of the complete generator. This reduces the problem to controlling the spectrum. That is, we write the semi-group in terms of its resolvent by way of the *holomorphic functional calculus*.

We control the resolvent, in the diffusive scaling limit, by controlling its constituent parts individually. This choice of a decomposition is motivated in a natural way by the generator itself; we use the Schur complement (see Appendix E) according to the *projections* onto the kernel and range.

In chapter 4, we elaborate on a similar problem addressed by Kang and Schenker [3]. In their paper, the weakened criterion is demonstrated for a Markov-Schrödinger equation. We provide further evidence of diffusion by showing that *higher moments* of position also possess a diffusive scaling limit and that this limit is a derivative of the heat kernel. We do this by analytically continuing the diffusion criterion and recognizing that higher moments are merely derivatives in the complex variable. Convergence then follows from the theory of complex variables. It should be noted that this procedure will apply to the problem considered in chapter 3 if sufficient control of the *perturbed* spectrum can be obtained. This is a topic for further study.

Chapter 2

A Mathematical Characterization of Diffusion

To detect diffusion in solutions to a Markov wave equation, we require a rigorous characterization of diffusion. For consistency, this characterization must also be a property of the classic heat equation. That shall be our starting point.

Consider the solution to the classic heat equation with Dirac initial data:

$$\begin{cases} \partial_t u(x,t) = \Delta u(x,t), & (x,t) \in \mathbb{R}^d \times \mathbb{R}_+ \\ u(x,0) = \delta_0(x), & x \in \mathbb{R}^d \end{cases},$$

which we may write explicitly as

$$u(x,t) = \frac{1}{(2\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}}.$$

The function $x \mapsto cu(x,t)$ is then a probability density function on $\mathbb{R}^d$, where we let

$$c = \left(\int_{\mathbb{R}^d} u(x,t)\, dx \right)^{-1} = 2^{d/2}$$

be the normalizing constant. For $p \in \mathbb{N}$, the p^{th} moment of position is given by

$$\int_{\mathbb{R}^d} |x|^p cu(x,t)\, dx = \frac{c\omega_d}{(2\pi t)^{d/2}} \int_0^\infty r^{p+d-1} e^{-\frac{r^2}{4t}}\, dr,$$

where we have switched to polar coordinates. Here, ω_d is the surface area of the unit ball in $\mathbb{R}^d$. We then see that the integrand on the right-hand side obtains its maximum, regardless of the value of p, when the position r is proportional to $\sqrt{t}$. This leads us to consider the *diffusive scaling*

$$\begin{cases} t \mapsto t/\eta \\ x \mapsto x/\sqrt{\eta} \end{cases},$$

in the small η limit, as in reference [3].

The models we wish to study are on the lattice, so we must find a way to apply this scaling in a discretized context. To this end, we use a mollifier $h \in C_c^\infty(\mathbb{R}^d)$ with $\int h\, dx = 1$ which we convolve with a lattice function to obtain a smooth approximation. Ultimately, our characterization of diffusion should be independent of the choice of h. We may accomplish this by using a Fourier transform. To see this, suppose $\psi_t \in \ell^2(\mathbb{Z}^d)$ satisfies

$$\begin{cases} \partial_t \psi_t(x) = H_{\omega(t)} \psi_t(x), \quad x \in \mathbb{Z}^d, t \in \mathbb{R}_+ \\ \psi_0 = \delta_0 \end{cases}, \tag{2.1}$$

a wave equation with a random, time-dependent generator. We say ψ_t exhibits *diffusion* (see [3]) if

$$h * |\psi_t|^2(x) = \sum_{\xi \in \mathbb{Z}^d} h(x-\xi)|\psi_t(\xi)|^2$$

satisfies

$$\frac{1}{\eta^{d/2}} \int_{\mathbb{R}^d} h * |\psi_{t/\eta}|^2(x/\sqrt{\eta})\, \phi(x)\, dx \quad \overset{\eta \to 0}{\longrightarrow} \quad \int_{\mathbb{R}^d} \frac{1}{(\pi D t)^{d/2}} e^{-\frac{|x|^2}{Dt}}\, \phi(x)\, dx \tag{2.2}$$

for all suitable test functions ϕ, and some $D > 0$. That is, under the diffusive scaling, $h * |\psi_t|^2$ converges weakly to a solution of the heat equation. Using the Fourier transform, we see that (2.2) is satisfied if

$$\sum_{x \in \mathbb{Z}^d} e^{-i\sqrt{\eta} k \cdot x} |\psi_{t/\eta}(x)|^2 \quad \overset{\eta \to 0}{\longrightarrow} \quad e^{-Dt|k|^2}.$$

This is the characterization we seek.

Note that the disorder parameter here is suppressed. The solution $\psi_t \in \ell^2(\mathbb{Z}^d)$ depends implicitly on which realization of the disorder actually occurs. The method we establish in chapter 3 and Kang and Schenker discuss in [3] require us to weaken this condition to

$$\sum_{x \in \mathbb{Z}^d} e^{-i\sqrt{\eta} k \cdot x} \mathbb{E}\left(|\psi_{t/\eta}(x)|^2\right) \quad \overset{\eta \to 0}{\longrightarrow} \quad e^{-Dt|k|^2}, \tag{2.3}$$

where we have averaged over all realizations of the disorder. Later, we will establish the existence of a diffusive-scaling limit to higher moments of position (see chapter 4).

Chapter 3

Diffusion for a Markov, Divergence-form Generator

Here we demonstrate that the amplitude of the solution to a wave equation with a Markov, Divergence-form generator satisfies the diffusion characterization (2.3). We begin with the assumptions necessary to precisely state the wave model under consideration. These include the construction of a Markov generator and differential operators on the lattice.

Having stated the theorem, we prove it in several steps. First, an equivalent problem is derived which is more appropriate for the diffusion characterization (2.3). We then transform (2.3) into a statement about the holomorphic functional calculus of a particular matrix element of the generator. We then reduce the integral in the functional calculus to its substantive part in the diffusive scaling limit. The remainder is then dissected by way of the Schur Complement Formula and projections which are natural to the problem. The components are then controlled by a spectral analysis and we are then free to compute the diffusive scaling limit, establishing the theorem.

3.1 Assumptions

For the purposes of this chapter, we assume that we are given a probability space (Ω, μ) and a Markov Generator[1] B with domain $\mathcal{D}(B) \subseteq L^2(\Omega)$. We assume that the numerical range[2] of B is sectoral:

$$\mathcal{N}(B) \subseteq \{z = x + iy \in \mathbb{C} : x \geq 0, \ |y| \leq mx\},$$

for some $m > 0$, and that B satisfies a *gap condition.* That is, if we restrict B to it's range, then the numerical range of this restriction is bounded away from zero:

$$Re\langle \psi, B\psi \rangle \geq \frac{1}{T}||\psi||^2$$

for some $T > 0$ and all $\psi \in Rng(B)$. Also, assume that there are μ-measure preserving maps $\sigma_x : \Omega \to \Omega$, for each $x \in \mathbb{Z}^d$, such that $\sigma_x \circ \sigma_y = \sigma_{x+y}$. These maps shift the process by x and will be used as part of a Fourier transform[3] which partially diagonalizes the generator for the overall problem.

Next, we construct the generator for the wave model. We start with "differential operators" on the lattice (finite difference operators) and include a function of a random variable so that we may include the Markov process in the generator.

Let $\mathbb{E}^d$ be the space of directed edges connecting nearest neighbors in $\mathbb{Z}^d$ and $\nabla : \ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{E}^d)$ be the discrete gradient $\nabla f(x, e) = f(x + e) - f(x)$. It's adjoint is given by $\nabla^\dagger f(x) = \sum_e (f(x + e, -e) - f(x, e))$. Suppose that $\theta : \mathbb{E}^d \times \Omega \to \mathbb{R}$ is positive,

[1] See appendix B for the complete construction of B.

[2] See appendix A for the definition of the numerical range and its implications.

[3] See section 3.4.1 for the Fourier transform and the operator to be partially diagonalized.

bounded, non-constant, and *translation covariant*: $\theta(x, e, \omega) = \theta(x - \xi, e, \sigma_\xi(\omega))$. That is, θ is invariant under shifts of the process in $\mathbb{Z}^d$. Further assume that $||\theta - \bar{\theta}||_{L^2(\mathbb{E}^d \times \Omega)} \neq 0$ where $\bar{\theta}$ is the average

$$\bar{\theta}(e) := \int_\Omega \theta(x, e, \omega) d\mu(\omega) = \int_\Omega \theta(0, e, \omega) d\mu(\omega),$$

independent of x since θ is translation covariant and σ_x is μ-measure preserving. Lastly, assume that θ is constant across directions on a given edge: $\theta(x, e, \omega) = \theta(x + e, -e, \omega)$.

We are now able to state the initial-value problem under consideration and make the goal of this chapter explicit. Before doing so, we give a brief example of such a Markov process.

3.2 The Flip Process

A particular example of the Markov process constructed above is the so-called "flip process", similar to [3]. For this process, we envision each (non-directed) edge in $\mathbb{E}^d$ as the site for a process which takes values in $\{1, 2\}$. Let $\tilde{\mathbb{E}}^d$ be the space of edges, irrespective of direction, connecting nearest neighbors in $\mathbb{Z}^d$. Then, the probability space is $\Omega = \tilde{\mathbb{E}}^d \otimes \{1, 2\}$. Now, suppose that for each site $(x, e) \in \tilde{\mathbb{E}}^d$, $0 \leq t_1(x, e) \leq t_2(x, e) \leq \ldots$ is a collection of random times given by independent, identically distributed Poisson processes. At each of these times, the process at the corresponding site will change sign. The Markov process ω is then a point in the path space $\Omega^{[0,\infty)}$. With this process, we may choose θ to be point evaluation of the process at the given edge. That is, $\theta(x, e, \omega(t)) \in \{1, 2\}$, the value the process takes at time t on the edge (x, e).

3.3 Statement of the Problem

The goal is to show that mean-squared solutions to $-i\partial_t \psi_t = \nabla^\dagger \theta_{\omega(t)} \nabla \psi_t$ on the lattice, diffuse. That is, under the diffusive scaling limit,

$$\begin{cases} x \mapsto x/\sqrt{\eta} \\ t \mapsto t/\eta \end{cases} \quad \text{as } \eta \to 0^+, \tag{3.1}$$

the quantity $\mathbb{E}(|\psi_t|^2)$ converges to the solution of a heat equation. A criterion for diffusion was derived in chapter 2, however, we use an equivalent statement. We establish the criterion on the Fourier transform side as this allows for the partial diagonalization of the key generator for the problem. The task before us is stated in the following theorem.

Theorem 1. *If $\psi_t \in \ell^2(\mathbb{Z}^d)$ is a solution to the discrete Schrödinger initial-value problem*

$$\begin{cases} i\partial_t \psi_t(x) = \nabla^\dagger \theta_{\omega(t)} \nabla \psi_t(x), & t > 0,\ x \in \mathbb{Z}^d \\ \psi_0(x) = \delta_0(x), & x \in \mathbb{Z}^d \end{cases}, \tag{3.2}$$

then there exists a symmetric matrix D such that

$$\lim_{\eta \to 0^+} \sum_{x \in \mathbb{Z}^d} e^{i\sqrt{\eta} k \cdot x} \mathbb{E}\left(|\psi_{t/\eta}(x)|^2 \right) = e^{-t\langle k, Dk \rangle} \tag{3.3}$$

for $k \in \mathbb{T}^d$.

3.4 Proof of the Theorem

First, we derive an equivalent problem which is more appropriate to our goal. We then reformulate (3.3) in terms of a particular matrix element of the resolvent of the semigroup generator by using a Feynman-Kac-Pillet formula. A symmetry in the new formulation allows us to bound the resolvent and take the limit.

3.4.1 A More Appropriate Problem

Since the diffusion criterion (3.3) requires only information about the amplitude of the solution, a linear problem for $|\psi_t|^2$ is more suitable. We will use a *random density matrix* $\rho(x,y) = \psi_t(x)\psi_t(y)^*$ so that $|\psi_t(x)|^2 = \rho_t(x,x)$. It follows that ρ_t defined in this way satisfies

$$\begin{cases} i\partial_t \rho_t(x,y) = L(\omega)\rho_t(x,y), & t>0,\ (x,y)\in\mathbb{Z}^d\times\mathbb{Z}^d \\ \rho_0(x,y) = \delta_0(x)\otimes\delta_0(y) & (x,y)\in\mathbb{Z}^d\times\mathbb{Z}^d \end{cases}$$

where $L(\omega) = \nabla_x^\dagger \theta_{x,\omega}\nabla_x - \nabla_y^\dagger \theta_{y,\omega}\nabla_y$. For each $\omega\in\Omega$, $L(\omega)$ is then a bounded, symmetric operator on $\ell^2(\mathbb{Z}^d\times\mathbb{Z}^d)$. Now, the Fourier transform

$$\mathcal{F}f(x,\omega,k) = \sum_{\xi\in\mathbb{Z}^d} e^{-ik\cdot\xi} f(x-\xi,-\xi,\sigma_\xi(\omega)), \tag{3.4}$$

acting on the augmented space $L^2(\mathbb{Z}^d \times \mathbb{Z}^d \times \Omega)$, *partially* diagonalizes L. That is, the transformed operator, which we will refer to as $\hat{L}_k$, depends on k as a parameter.

$$\begin{aligned}\hat{L}_k \psi(x,\omega) = \quad & 2\sum_e \theta(x,e,\omega)\left(\psi(x,\omega) - \psi(x+e,\omega)\right) \\ & -2\sum_e \theta(0,e,\omega)\left(\psi(x,\omega) - e^{-ik\cdot e}\psi(x-e,\sigma_e(\omega))\right)\end{aligned}$$

In light of this observation, we will now operate solely on the space $L^2(\mathbb{Z}^d \times \Omega)$ for arbitrary $k \in \mathbb{T}^d$.

3.4.2 The Resolvent of the Generator

To reduce the problem to a resolvent analysis, we will need a Feynman-Kac-Pillet formula [6], derived as follows. The conditional expectation we wish to understand can be differentiated and thus can be seen as the solution to an initial-value problem. The derivative invokes both the Markov generator and the wave model generator. So it follows that the conditional expectation – that is, the solution to the initial value problem – can be written as an exponential of this operator.

$$\begin{aligned}\partial_t \mathbb{E}(\rho_t : \omega(t) = \alpha) \quad &= \quad \lim_{h\to 0^+} \frac{1}{h}(\mathbb{E}(\rho_{t+h} : \omega(t+h) = \alpha) - \mathbb{E}(\rho_t : \omega(t) = \alpha)) \\ &= \quad \lim_{h\to 0^+} \frac{1}{h}(\mathbb{E}(\rho_{t+h} : \omega(t+h) = \alpha) - \mathbb{E}(\rho_t : \omega(t+h) = \alpha)) \\ &\quad + \lim_{h\to 0^+} \frac{1}{h}(\mathbb{E}(\rho_t : \omega(t+h) = \alpha) - \mathbb{E}(\rho_t : \omega(t) = \alpha)) \\ &= \quad \mathbb{E}(\partial_t \rho_t : \omega(t) = \alpha) - B\mathbb{E}(\rho_t : \omega(t) = \alpha) \\ &= \quad (-iL(\alpha) - B)\mathbb{E}(\rho_t : \omega(t) = \alpha))\end{aligned}$$

That B is the derivative of a conditional expectation is illustrated in appendix B. This is the deterministic Cauchy problem with exponential solution

$$\mathbb{E}(\rho_t : \omega(t) = \alpha)) \;=\; e^{-t(iL(\alpha)+B)}\rho_0,$$

since the initial data is assumed to be non-random. Integrating over $\alpha \in \Omega$, we may now express the left-hand side of (3.3) as a particular matrix element of the semigroup generated by the Markov process and the revised problem.

$$\begin{aligned}\mathbb{E}(\rho_t(x,y)) &= \int_\Omega e^{-t(iL(\alpha)+B)}\rho_0 \otimes 1(x,y)\, d\mu(\alpha) \\ &= \langle \delta_x \otimes \delta_y \otimes 1,\, e^{-t(iL+B)}\rho_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\mathbb{Z}^d\times\Omega)} \end{aligned} \tag{3.5}$$

Using the unitarity of the Fourier transform, we will exploit the partial diagonalization of L. That is, we are fortunate that the matrix element under consideration is the one which corresponds to the function $\delta_0 \otimes 1$ on $\mathbb{Z}^d \times \Omega$ and that this function is in the kernel of $\hat{L}_k$. This will allow us to pick projections according to the kernel of $\hat{L}_k$, allowing us to decompose $\hat{L}_k$ in a natural way. This is the subject of section 3.4.4. For a brief tutorial on these ideas, see section E.2. With this in mind, and using the fact that $\mathcal{F}\rho_0 = \delta_0$, we write:

$$\begin{aligned}\mathbb{E}(\rho_t(x,x)) &= \langle \delta_x \otimes \delta_x \otimes 1, e^{-t(iL+B)}\rho_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\mathbb{Z}^d\times\Omega)} \\ &= \langle \mathcal{F}\delta_x \otimes \delta_x \otimes 1,\, \left(\mathcal{F}e^{-t(iL+B)}\mathcal{F}^\dagger\right)\mathcal{F}\rho_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\Omega\times\mathbb{T}^d)} \\ &= \langle e^{ik\cdot x}\delta_0 \otimes 1,\, e^{-t(i\hat{L}_k+B)}\delta_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\Omega\times\mathbb{T}^d)} \\ &= \int_{\mathbb{T}^d} e^{-ik\cdot x}\langle \delta_0 \otimes 1,\, e^{-t(i\hat{L}_k+B)}\delta_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\Omega)}\, d\ell(k) \end{aligned} \tag{3.6}$$

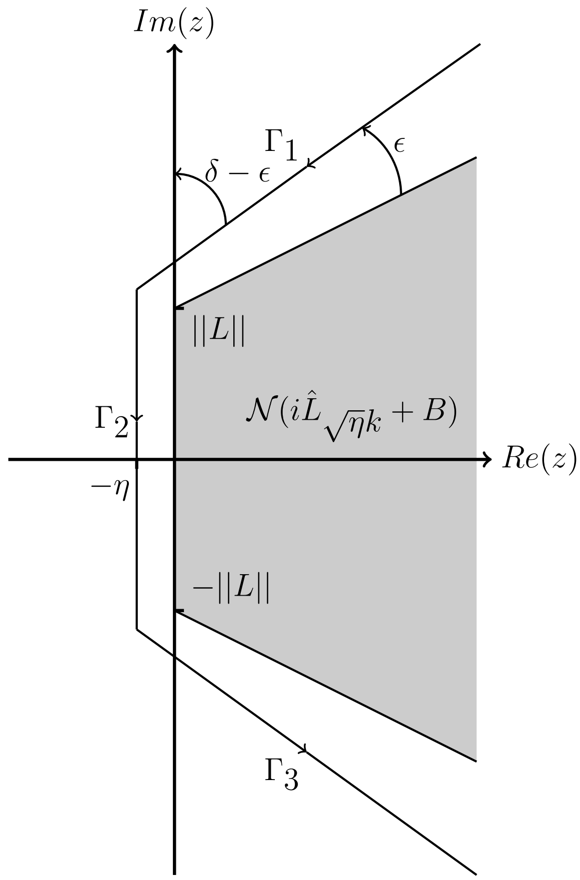

Figure 3.1: The contour Γ in (3.7) and the numerical range of $i\hat{L}_{\sqrt{\eta}k} + B$.

and we interpret the exponential of an unbounded operator by using the holomorphic functional calculus in [5]. This will allow us to write the semigroup in terms of the resolvent of its generator. Under the diffusive scaling (3.1), we arrive at

$$e^{-(t/\eta)(i\hat{L}_{\sqrt{\eta}k}+B)} = \frac{1}{2\pi i}\int_\Gamma e^{-\frac{1}{\eta}tz}\frac{1}{z-(i\hat{L}_{\sqrt{\eta}k}+B)}\,dz. \tag{3.7}$$

Our motivation for the particular choice of the contour $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$,

$$\begin{aligned}
\Gamma_1 &:= \{z = x + iy \in \mathbb{C} \;:\; y = 1 + ||L|| + \cot(\delta - \epsilon)(x + \eta) \}\\
\Gamma_2 &:= \{z = -\eta + iy \in \mathbb{C} \;:\; |y| \leq 1 + ||L|| \}\\
\Gamma_3 &:= \{z = x + iy \in \mathbb{C} \;:\; y = -1 - ||L|| + \cot(\delta - \epsilon)(x + \eta) \}
\end{aligned}$$

with $\epsilon \in (0, \delta)$, subject to the constraints in [5], is as follows. By bounding the resolvent in terms of the distance to the numerical range, we will show that in the small η limit, the integral along $\Gamma_1 \cup \Gamma_3$ vanishes. The substantive part of the integral is then along Γ_2. We will show that this contribution is exactly what was stated in (3.3). To this end, we apply the functional calculus (3.7) to (3.6). In doing so, we have reduced the problem to understanding the limiting behavior of one matrix element of the resolvent.

$$\begin{aligned}
&\sum_{x \in \mathbb{Z}^d} e^{i\sqrt{\eta}k\cdot x}\mathbb{E}\left(|\psi_{t/\eta}(x)|^2\right)\\
&= \sum_{x \in \mathbb{Z}^d} e^{i\sqrt{\eta}k\cdot x} \int_{\mathbb{T}^d} e^{-i\tilde{k}\cdot x}\langle \delta_0 \otimes 1,\, e^{-(t/\eta)(i\hat{L}_{\tilde{k}}+B)}\delta_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\Omega)}\, d\ell(\tilde{k})\\
&= \int_{\mathbb{T}^d} \sum_{x \in \mathbb{Z}^d} e^{i(\sqrt{\eta}k - \tilde{k})\cdot x}\langle \delta_0 \otimes 1,\, e^{-(t/\eta)(i\hat{L}_{\tilde{k}}+B)}\delta_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\Omega)}\, d\ell(\tilde{k})\\
&= \int_{\mathbb{T}^d} \delta_0(\sqrt{\eta}k - \tilde{k})\langle \delta_0 \otimes 1,\, e^{-(t/\eta)(i\hat{L}_{\tilde{k}}+B)}\delta_0 \otimes 1\rangle_{L^2(\mathbb{Z}^d\times\Omega)}\, d\ell(\tilde{k})\\
&= \left\langle \delta_0 \otimes 1, e^{-(t/\eta)(i\hat{L}_{\sqrt{\eta}k}+B)}\delta_0 \otimes 1 \right\rangle_{L^2(\mathbb{Z}^d\times\Omega)}\\
&= -\frac{1}{2\pi i}\int_{\Gamma} e^{-\frac{1}{\eta}tz}\left\langle \delta_0 \otimes 1, \frac{1}{i\hat{L}_{\sqrt{\eta}k} + B - z}\delta_0 \otimes 1 \right\rangle dz
\end{aligned}$$

We proceed by showing that the contribution to the integral from the unbounded portion of the contour is small.

3.4.3 The Substantive Part of the Integral

Given our sectorality assumption on the Markov generator B, our choice of the contours Γ_1 and Γ_3, and the above lemma, it is easy to see the integral over $\Gamma_1 \cup \Gamma_3$ vanishes. For $z = x + iy \in \Gamma_1$, the distance from z to $\mathcal{N}(i\hat{L}_{\sqrt{\eta}k} + B)$ is at least 1. Let $\ell = 1 + ||L||$ and $m = \cot(\delta - \epsilon)$. Then $y = \ell + m(x + \eta)$ for $-\eta < x < \infty$.

$$\begin{aligned}
& \left\| \frac{1}{2\pi i} \int_{\Gamma_1} e^{-\frac{t}{\eta} z} \frac{1}{z - (i\hat{L}_{\sqrt{\eta}k} + B)} \, dz \right\| \\
= & \left\| \frac{-(1+im)}{2\pi i} \int_{-\eta}^{\infty} e^{-\frac{t}{\eta}(x+iy)} \frac{1}{x + iy - (i\hat{L}_{\sqrt{\eta}k} + B)} \, dx \right\| \\
\leq & \frac{\sqrt{1+m^2}}{2\pi} \int_{-\eta}^{\infty} e^{-\frac{t}{\eta} x} \frac{1}{dist(x+iy, \mathcal{N}(i\hat{L}_{\sqrt{\eta}k} + B))} \, dx \\
\leq & \frac{\sqrt{1+m^2}}{2\pi} \int_{-\eta}^{\infty} e^{-\frac{t}{\eta} x} \, dx = \mathcal{O}(\eta)
\end{aligned}$$

Likewise for Γ_3. We then have

$$\begin{aligned}
\sum_{x \in \mathbb{Z}^d} e^{i\sqrt{\eta}k \cdot x} \mathbb{E}\left(|\psi_{t/\eta}(x)|^2 \right) = & -\frac{1}{2\pi i} \int_{\frac{1}{\eta}\Gamma_2} \\
& e^{-tw} \left\langle \delta_0 \otimes 1, \frac{\eta}{i\hat{L}_{\sqrt{\eta}k} + B - \eta w} \delta_0 \otimes 1 \right\rangle dw + \mathcal{O}(\eta)
\end{aligned} \tag{3.8}$$

after the substitution $z = \eta w$.

To proceed, we wish to take the small η limit of the resolvent. It is unlikely that this limit exists as a bounded operator, given that heuristically, L is a second order derivative.

Indeed, L will map large, slowly varying functions to functions with small norm. However, we need not address the entire resolvent. We will be satisfied with the particular matrix element in (3.8). We continue by dissecting the resolvent according to projections which are natural to the generator.

3.4.4 Natural Projections and the Schur Complement Formula

Let P_0 be the orthogonal projection on $L^2(\Omega)$ to non-random functions: $P_0 f = \int_\Omega f \, d\mu$. Then $P_0^\perp$ is the projection onto mean-zero functions. Also, let $Q_0 = (\delta_0 \otimes 1)\langle \delta_0 \otimes 1, \cdot \rangle$. We will use these projections with the Schur complement (see appendix E.2) to estimate the resolvent in (3.8). These projections are the natural choice for the resolvent in question, given that $Ker(\hat{L}_0) = Rng(Q_0)$, $Ker(B) = Rng(P_0)$, and the gap condition on the Markov generator gives us that $B^{-1}P_0^\perp$ is norm bounded by $1/T$ (see appendix D).

A first iteration of the Schur complement formula yields

$$\begin{aligned}
&\left\langle \delta_0 \otimes 1, \, Q_0 \frac{\eta}{i\hat{L}_{\sqrt{\eta}k} + B - \eta w} Q_0 \, \delta_0 \otimes 1 \right\rangle \qquad (3.9) \\
&= \left\langle \delta_0 \otimes 1, \, \left[-w + \left(Q_0 \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0^\perp \right) \frac{1}{iQ_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + BQ_0^\perp - \eta w Q_0^\perp} \right.\right. \\
&\left.\left. \left(Q_0^\perp \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0 \right) \right]^{-1} \delta_0 \otimes 1 \right\rangle \\
&= \left[-w + Bigg\langle \delta_0 \otimes 1, \, \left(Q_0 \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0^\perp \right) \frac{1}{iQ_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + BQ_0^\perp - \eta w Q_0^\perp} \right. \\
&\left. \left(Q_0^\perp \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0 \right) \delta_0 \otimes 1 \right\rangle \Bigg]^{-1} .
\end{aligned}$$

The last equality follows from the fact the operator has a one-dimensional domain and range and thus may be treated as scalar multiplication. The factor on either side of the resolvent in (3.9) will play a special role (see (3.12) below and appendix C). This leads us to define

$$\begin{aligned} f_{\eta,k} &:= P_0 \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} \delta_0 \otimes 1 \\ &= e^{-i\frac{\sqrt{\eta}k}{2}\cdot x} \left(\frac{-2i\bar{\theta}}{\sqrt{\eta}}\right) \sum_{|e|=1} \sin\left(\frac{\sqrt{\eta}k}{2}\cdot e\right)(\delta_e - \delta_{-e}). \end{aligned} \tag{3.10}$$

We now apply the Schur complement a second time. In this instance, we apply it to the resolvent in (3.9) according to the projection P_0. We will then take the limit of the $P_0 \cdots P_0$ term in (3.9) and later we will use this to compute the other three terms, $P_0 \cdots P_0^{\perp}$, $P_0^{\perp} \cdots P_0$, and $P_0^{\perp} \cdots P_0^{\perp}$. A second iteration of the Schur complement gives us:

$$\begin{aligned} &P_0 \frac{1}{iQ_0^{\perp}\hat{L}_{\sqrt{\eta}k}Q_0^{\perp} + BQ_0^{\perp} - \eta w Q_0^{\perp}} P_0 \\ &\quad = \Bigg[iP_0 Q_0^{\perp}\hat{L}_{\sqrt{\eta}k}Q_0^{\perp}P_0 - \eta w Q_0^{\perp}P_0 \\ &\qquad + (P_0Q_0^{\perp}\hat{L}_{\sqrt{\eta}k}P_0^{\perp}) \frac{1}{iP_0^{\perp}\hat{L}_{\sqrt{\eta}k}P_0^{\perp} + BP_0^{\perp} - \eta w P_0^{\perp}} (P_0^{\perp}\hat{L}_{\sqrt{\eta}k}Q_0^{\perp}P_0) \Bigg]^{-1}. \end{aligned} \tag{3.11}$$

Note that the validity of these two applications of the Schur complement formula hinge on the inversion in the right-hand side of (3.11). Indeed, the inner-most resolvent on the right hand side of (3.11) is norm bounded by $1/T$, so by the Schur complement formula, the left hand side is a bounded operator if the right hand side is invertible. Therefore, to proceed, we must find a lower bound for operator being inverted on the right hand side of (3.11).

It is important to note that we need not compute the limit of (3.11) in its entirety. We need only compute the limit of the particular matrix element $\langle f_{\eta,k}, (P_0 \cdots P_0) f_{\eta,k}\rangle$ because of the factor $\left(Q_0^{\perp} \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0 \right)$ in (3.9).

3.4.5 In Search of a Lower Bound

For simplicity, we define

$$\begin{aligned} C_{\sqrt{\eta}k} &= (P_0^{\perp} \hat{L}_{\sqrt{\eta}k} Q_0^{\perp} P_0) \\ F_{\eta,k}(w) &= iP_0^{\perp} \hat{L}_{\sqrt{\eta}k} P_0^{\perp} + BP_0^{\perp} - \eta w P_0^{\perp} \\ M_{\eta,k}(w) &= iP_0 Q_0^{\perp} \hat{L}_{\sqrt{\eta}k} Q_0^{\perp} P_0 - \eta w Q_0^{\perp} P_0 + C^{\dagger}_{\sqrt{\eta}k} \frac{1}{F_{\eta,k}} C_{\sqrt{\eta}k}. \end{aligned}$$

A reasonable next step might be to show that $Re\, M_{\eta,k}(w)$ is bounded below, away from zero, uniformly in η. We could then take the limit of a uniformly bounded sequence of operators. In attempting to compute this lower bound, we find instead that $Re\, M_{\eta,k}(w)$ is bounded below by another operator, which we will call $R_{\sqrt{\eta}k/2}$, and that this operator has spectrum near zero. While the ideal lower bound does not exist, we may show nonetheless that $R^{-1/2}_{\sqrt{\eta}k/2} Re\, M_{\eta,k}(w) R^{-1/2}_{\sqrt{\eta}k/2}$ is uniformly bounded below on the range of $R^{1/2}_{\sqrt{\eta}k/2}$. To show that $R^{-1/2}_{\sqrt{\eta}k/2} M_{\eta,k}(w) R^{-1/2}_{\sqrt{\eta}k/2}$ is appropriate for our problem, we must also show that $f_{\eta,k}$ is in the domain of $R^{-1/2}_{\sqrt{\eta}k/2}$. This compels us to find a more explicit representation for $R_{\sqrt{\eta}k/2}$.

As a first step to this goal, define

$$D_k := (B^{-1} P_0^{\perp} \hat{L}_k P_0 Q_0^{\perp})^{\dagger} (B^{-1} P_0^{\perp} \hat{L}_k P_0 Q_0^{\perp}) \tag{3.12}$$

for $k \in \mathbb{T}^d$, a bounded operator on $L^2(\mathbb{Z}^d \times \Omega)$. This operator has the more explicit form

$$D_k = 8\chi \triangle_0^N + 8\chi \triangle_k^N + 4\chi \sum_e (\delta_e - e^{ik\cdot e}\delta_{-e})\langle \delta_e - e^{ik\cdot e}\delta_{-e}, \cdot\rangle, \tag{3.13}$$

the derivation of which is the subject of Appendix C. Here Δ_0^N is the "Neumann Laplacian"

$$\triangle_0^N \psi(x) = (1 - \delta_0(x)) \sum_{\substack{x+e\neq 0 \\ |e|=1}} (\psi(x) - \psi(x+e))$$

and Δ_k^N is it's Gauge transform:

$$\begin{aligned} \triangle_k^N &= e^{-ik\cdot X} \triangle_0^N e^{ik\cdot X} \\ \triangle_k^N \psi(x) &= (1 - \delta_0(x)) \sum_{\substack{x+e\neq 0 \\ |e|=1}} \Big(\psi(x) - e^{ik\cdot e}\psi(x+e)\Big). \end{aligned}$$

We shall soon see that $D_{\sqrt{\eta}k}$ is a lower bound for the operator in question. However $f_{\eta,k}$, the function which forms the key matrix element, also varies with η. This makes some of the required calculations difficult. To remedy this, we use a Gauge transform to "push" the k and η dependence from the function to the operator. To see this, we first transform the finite-rank part of D_k,

$$4\chi e^{i\frac{k}{2}\cdot x} \sum_{|e|=1} (\delta_e - e^{ik\cdot e}\delta_{-e})\langle \delta_e - e^{ik\cdot e}\delta_{-e}, \psi\rangle = 4\chi \sum_{|e|=1} (\delta_e - \delta_{-e})\langle \delta_e - \delta_{-e}, e^{i\frac{k}{2}\cdot X}\psi\rangle$$

so that we may write

$$D_k = 8\chi e^{-i\frac{k}{2}\cdot X}\left(\triangle^N_{-k/2} + \triangle^N_{k/2} + \frac{1}{2}\sum_e (\delta_e - \delta_{-e})\langle \delta_e - \delta_{-e}, \cdot\rangle\right) e^{i\frac{k}{2}\cdot X}.$$

We then obtain a lower bound as follows. For $|k| < \frac{2\pi}{3}$, $2\cos\left(\frac{k}{2}\cdot e\right) > 1$ and

$$\begin{aligned}
&\left\langle \psi, \left(\triangle^N_{-k/2} + \triangle^N_{k/2}\right)\psi\right\rangle \\
= \;& \sum_{x\neq 0}\psi^*(x)\sum_{\substack{x+e\neq 0\\ |e|=1}}\left(2\psi(x) - \left(e^{-i\frac{k}{2}\cdot e} + e^{i\frac{k}{2}\cdot e}\right)\psi(x+e)\right) \\
\geq \;& \sum_{x\neq 0}\psi^*(x)\sum_{\substack{x+e\neq 0\\ |e|=1}}\left(2\cos\left(\frac{k}{2}\cdot e\right)\psi(x) - 2\cos\left(\frac{k}{2}\cdot e\right)\psi(x+e)\right) \\
\geq \;& \sum_{x\neq 0}\psi^*(x)\sum_{\substack{x+e\neq 0\\ |e|=1}}\left(\psi(x) - \psi(x+e)\right) \\
= \;& \left\langle \psi, \triangle^N_0\psi\right\rangle
\end{aligned}$$

and thus $\triangle^N_{-k/2} + \triangle^N_{k/2} \geq \triangle^N_0$ and $D_k \geq e^{-i\frac{k}{2}\cdot X} R_0 e^{i\frac{k}{2}\cdot X} =: R_{k/2}$, where we have defined

$$R_0 = 8\chi\triangle^N_0 + 4\chi\sum_e (\delta_e - \delta_{-e})\langle \delta_e - \delta_{-e}, \cdot\rangle. \tag{3.14}$$

Notice that the factor $\delta_e - \delta_{-e}$ appears in (3.14). Also, the same function is present in the definition (3.10) of $f_{\eta,k}$ which was inspired by the $P_0\cdots P_0$ term of (3.9). With the following lemma, we may conclude that $f_{\eta,k}$ is in the domain of $R^{-1/2}_{\sqrt{\eta}k/2}$ which means that $R^{-1/2}_{\sqrt{\eta}k/2} M_{\eta,k}(w) R^{-1/2}_{\sqrt{\eta}k/2}$ is indeed appropriate for our problem.

Lemma 2. *Let* $A \geq 0$ *on a Hilbert space* $\mathcal{H}$ *and let* $f \in \mathcal{H}$. *Then, for* $\alpha > 0$, $f \in \mathcal{D}\left(A_\alpha^{-1/2}\right)$ *where* $A_\alpha = A + \alpha f\langle f, \cdot\rangle$.

Proof. First note that the following three statements are equivalent. Here $Q\left(A_\alpha^{-1}\right)$ is the form domain of A_α^{-1}.

$$f \in \mathcal{D}\left(A_\alpha^{-1/2}\right)$$

$$f \in Q\left(A_\alpha^{-1}\right)$$

$$\lim_{\lambda \to 0^+} \langle f, (A_\alpha + \lambda)^{-1} f\rangle < \infty$$

Using the resolvent identity we see that

$$\begin{aligned} (A+\lambda)^{-1} &= (A_\alpha + \lambda)^{-1} + (A_\alpha + \lambda)^{-1} \alpha f\langle f, \cdot\rangle (A+\lambda)^{-1} \\ \langle f, (A+\lambda)^{-1} f\rangle &= \langle f, (A_\alpha + \lambda)^{-1} f\rangle + \alpha\langle f, (A_\alpha + \lambda)^{-1} f\rangle\langle f, (A+\lambda)^{-1} f\rangle \end{aligned}$$

and

$$\langle f, (A_\alpha + \lambda)^{-1} f\rangle = \frac{1}{\frac{1}{\langle f,(A+\lambda)^{-1} f\rangle} + \alpha} \leq \frac{1}{\alpha}$$

since $A \geq 0$ and thus $(A+\lambda)^{-1} > 0$. □

By the above lemma, $\delta_e - \delta_{-e}$ is in the domain of $R_0^{-1/2}$. From this, it follows that

$f_{\eta,k}$ is in the domain of $R^{-1/2}_{\frac{\sqrt{\eta}k}{2}}$. Indeed,

$$\begin{aligned}\varphi_{\eta,k} &:= R^{-1/2}_{\frac{\sqrt{\eta}k}{2}} f_{\eta,k} \\ &= \left(\frac{-2i\bar{\theta}}{\sqrt{\eta}}\right) \sum_{|e|=1} \sin\left(\frac{\sqrt{\eta}k}{2}\cdot e\right) e^{-i\frac{\sqrt{\eta}k}{2}\cdot X} R_0^{-1/2}(\delta_e - \delta_{-e})\end{aligned}$$

and

$$\begin{aligned}\varphi_{0,k} &:= \lim_{\eta\to 0} R^{-1/2}_{\frac{\sqrt{\eta}k}{2}} f_{\eta,k} \\ &= -i\bar{\theta} \sum_{|e|=1} (k\cdot e)\, R_0^{-1/2}(\delta_e - \delta_{-e}).\end{aligned}$$

Now, it remains to examine the invertibility of $M_{\eta,k}(w)$.

3.4.6 Bounding the Resolvent

Recall that for $w \in \frac{1}{\eta}\Gamma_2$, $Re\, w = -1$ and note that

$$\begin{aligned}Re\, M_{\eta,k} &\geq Re\left(C^{\dagger}_{\sqrt{\eta}k} \frac{1}{F_{\eta,k}} C_{\sqrt{\eta}k}\right) \\ Re\, F_{\eta,k} &\geq \frac{1}{T} \\ D_{\sqrt{\eta}k} &= (B^{-1}C_{\sqrt{\eta}k})^{\dagger}(B^{-1}C_{\sqrt{\eta}k}).\end{aligned}$$

Suppose $f \in \mathcal{D}\left(D_{\sqrt{\eta}k}^{-1/2}\right)$ with $|f| = 1$. It follows that

$$\begin{aligned}
Re\left\langle f,\, C_{\sqrt{\eta}k}^{\dagger}\frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k}f\right\rangle &= \left\langle C_{\sqrt{\eta}k}f,\, Re\left(\frac{1}{F_{\eta,k}}\right)C_{\sqrt{\eta}k}f\right\rangle \\
&= \left\langle C_{\sqrt{\eta}k}f,\, \frac{1}{F_{\eta,k}^{\dagger}}ReF_{\eta,k}\frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k}f\right\rangle \\
&= \left\langle \frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k}f,\, ReF_{\eta,k}\frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k}f\right\rangle \\
&\geq \frac{1}{T}\left\|\frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k}f\right\|^2 \\
&= \frac{1}{T}\left\|\frac{1}{B^{-1}F_{\eta,k}}B^{-1}C_{\sqrt{\eta}k}f\right\|^2 \\
&\geq \frac{1}{T}\left\|B^{-1}F_{\eta,k}\right\|^{-2}\|B^{-1}C_{\sqrt{\eta}k}f\|^2 \\
&= \frac{1}{T}\|B^{-1}F_{\eta,k}\|^{-2}\langle f,\, D_{\sqrt{\eta}k}f\rangle \\
&> c_0\langle f,\, D_{\sqrt{\eta}k}f\rangle
\end{aligned}$$

where we have defined

$$\begin{aligned}
c_0 &= \frac{1}{2T}\lim_{\eta\to 0+}\|B^{-1}F_{\eta,k}\|^{-2} \\
&= \frac{1}{2T}\lim_{\eta\to 0+}\|iB^{-1}P_0^{\perp}\hat{L}_{\sqrt{\eta}k}P_0^{\perp} + P_0^{\perp} - \eta w B^{-1}P_0^{\perp}\|^{-2} \\
&= \frac{1}{2T}\|iB^{-1}P_0^{\perp}\hat{L}_0P_0^{\perp} + P_0^{\perp}\|^{-2}.
\end{aligned}$$

Thus, we have shown

$$
\begin{aligned}
Re\left(C^{\dagger}_{\sqrt{\eta}k}\frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k}\right) \geq c_0 D_{\sqrt{\eta}k} &\geq c_0 R_{\frac{\sqrt{\eta}k}{2}}, \\
Re\left(R^{-1/2}_{\frac{\sqrt{\eta}k}{2}} C^{\dagger}_{\sqrt{\eta}k}\frac{1}{F_{\eta,k}}C_{\sqrt{\eta}k} R^{-1/2}_{\frac{\sqrt{\eta}k}{2}}\right) &\geq c_0,
\end{aligned}
$$

and finally

$$
\left\| R^{1/2}_{\frac{\sqrt{\eta}k}{e}} M^{-1} R^{1/2}_{\frac{\sqrt{\eta}k}{2}} \right\| \leq \frac{1}{c_0}.
$$

With this bound, we may compute the small η limit of the $P_0 \cdots P_0$ term in (3.9).

3.4.7 The Diffusive-Scaling Limit

Recall that $f_{\eta,k} \in \mathcal{D}\left(R^{-1/2}_{\frac{\sqrt{\eta}k}{2}}\right)$ and we have defined $\varphi_{\eta,k} = R^{-1/2}_{\frac{\sqrt{\eta}k}{2}} f_{\eta,k}$. The $P_0 \cdots P_0$ term in the inner product in (3.9) is then

$$
\begin{aligned}
&\left\langle \delta_0 \otimes 1, \left(Q_0 \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0^{\perp}\right) P_0 \frac{1}{iQ_0^{\perp}\hat{L}_{\sqrt{\eta}k}Q_0^{\perp} + BQ_0^{\perp} - \eta w Q_0^{\perp}} P_0 \left(Q_0^{\perp}\frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0\right) \right. \\
&\qquad \left. \delta_0 \otimes 1 \right\rangle \\
&= \left\langle f_{\eta,k}, P_0 \frac{1}{iQ_0^{\perp}\hat{L}_{\sqrt{\eta}k}Q_0^{\perp} + BQ_0^{\perp} - \eta w Q_0^{\perp}} P_0 f_{\eta,k} \right\rangle \\
&= \left\langle R^{1/2}_{\frac{\sqrt{\eta}k}{2}} \varphi_{\eta,k}, M_{\eta,k}(w)^{-1} R^{1/2}_{\frac{\sqrt{\eta}k}{2}} \varphi_{\eta,k} \right\rangle \\
&= \left\langle \varphi_{\eta,k}, R^{1/2}_{\frac{\sqrt{\eta}k}{2}} M_{\eta,k}(w)^{-1} R^{1/2}_{\frac{\sqrt{\eta}k}{2}} \varphi_{\eta,k} \right\rangle
\end{aligned}
$$

which tends to

$$\left\langle \varphi_{0,k},\, R_0^{1/2} \left[(P_0 Q_0^\perp \hat{L}_0 P_0^\perp) \frac{1}{i P_0^\perp \hat{L}_0 P_0^\perp + B P_0^\perp} (P_0^\perp \hat{L}_0 Q_0^\perp P_0) \right]^{-1} R_0^{1/2}\, \varphi_{0,k} \right\rangle$$

in the small η limit. It is now a simple matter to compute the $P_0 \cdots P_0^\perp$, $P_0^\perp \cdots P_0$, and $P_0^\perp \cdots P_0^\perp$ terms of (3.9).

Using the Schur complement formula, the $P_0 \cdots P_0^\perp$ term in the inner product in (3.9) is

$$\begin{aligned} &\left\langle \delta_0 \otimes 1,\, \left(Q_0 \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0^\perp \right) P_0 \frac{1}{i Q_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + B Q_0^\perp - \eta w Q_0^\perp} P_0^\perp \left(Q_0^\perp \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0 \right) \right. \\ &\qquad \left. \delta_0 \otimes 1 \right\rangle \\ = &\left\langle f_{\eta,k},\, P_0 \frac{1}{i Q_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + B Q_0^\perp - \eta w Q_0^\perp} P_0^\perp \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} \delta_0 \otimes 1 \right\rangle \\ = &\left\langle f_{\eta,k},\, -M_{\eta,k}(w)^{-1} (i P_0 Q_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp) \frac{1}{i P_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp + B P_0^\perp - \eta w P_0^\perp} \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} \right. \\ &\qquad \left. \delta_0 \otimes 1 \right\rangle \end{aligned}$$

which tends to

$$\left\langle f_{0,k},\, \left(C_0^\dagger \frac{1}{F_{0,0}} C_0 \right)^{-1} (i P_0 Q_0^\perp \hat{L}_0 P_0^\perp) \frac{1}{i P_0^\perp \hat{L}_0 P_0^\perp + B P_0^\perp} \left(2i \sum_e \theta(0,e,\omega)(k \cdot e) \delta_e \right) \right\rangle$$

since $\delta_0 \otimes 1 \in Ker(\hat{L}_0)$ and

$$\lim_{\eta \to 0+} \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} \delta_0 \otimes 1 = \lim_{\eta \to 0+} \frac{\hat{L}_{\sqrt{\eta}k} - \hat{L}_0}{\sqrt{\eta}} \delta_0 \otimes 1 = -2i \sum_e \theta(0,e,\omega)(k \cdot e) \delta_e.$$

The $P_0^\perp \cdots P_0$ term in the inner product in (3.9) is then

$$\left\langle \delta_0 \otimes 1,\ \left(Q_0 \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0^\perp\right) P_0^\perp \frac{1}{iQ_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + BQ_0^\perp - \eta w Q_0^\perp} P_0 \left(Q_0^\perp \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} Q_0\right) \delta_0 \otimes 1 \right\rangle$$

$$= \left\langle \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} \delta_0 \otimes 1,\ P_0^\perp \frac{1}{iQ_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + BQ_0^\perp - \eta w Q_0^\perp} P_0\, f_{\eta,k} \right\rangle$$

$$= \left\langle \frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}} \delta_0 \otimes 1,\ -\frac{1}{iP_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp + BP_0^\perp - \eta w P_0^\perp} (iP_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp P_0) M_{\eta,k}(w)^{-1} f_{\eta,k} \right\rangle$$

which tends to

$$\left\langle \left(2i \sum_e \theta(0,e,\omega)(k \cdot e)\delta_e\right),\ \frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp} (iP_0^\perp \hat{L}_0 Q_0^\perp P_0) \left(C_0^\dagger \frac{1}{F_{0,0}} C_0\right)^{-1} f_{0,k} \right\rangle.$$

Lastly, we compute the limit of the $P_0^\perp \cdots P_0^\perp$ term.

$$P_0^\perp \frac{1}{iQ_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp + BQ_0^\perp - \eta w Q_0^\perp} P_0^\perp =$$
$$\frac{1}{iP_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp + BP_0^\perp - \eta w P_0^\perp} - \frac{1}{iP_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp + BP_0^\perp - \eta w P_0^\perp} (iP_0^\perp \hat{L}_{\sqrt{\eta}k} Q_0^\perp P_0)$$
$$\cdot M_{\eta,k}(w)^{-1} (iP_0 Q_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp) \frac{1}{iP_0^\perp \hat{L}_{\sqrt{\eta}k} P_0^\perp + BP_0^\perp - \eta w P_0^\perp}$$

and the appropriate matrix element tends to

$$\Bigg\langle \left(2i\sum_e \theta(0,e,\omega)(k\cdot e)\delta_e\right),$$
$$\frac{1}{iP_0^{\perp}\hat{L}_0P_0^{\perp}+BP_0^{\perp}} - \frac{1}{iP_0^{\perp}\hat{L}_0P_0^{\perp}+BP_0^{\perp}}(iP_0^{\perp}\hat{L}_0Q_0^{\perp}P_0)$$
$$\cdot\left(C_0^{\dagger}\frac{1}{F_{0,0}}C_0\right)^{-1}(iP_0Q_0^{\perp}\hat{L}_0P_0^{\perp})\frac{1}{iP_0^{\perp}\hat{L}_0P_0^{\perp}+BP_0^{\perp}}\left(2i\sum_e \theta(0,e,\omega)(k\cdot e)\delta_e\right)\Bigg\rangle.$$

In the above, we have computed

$$J_{\eta,k}(w) :=$$
$$\left\langle \delta_0\otimes 1,\ \left(Q_0\frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}}Q_0^{\perp}\right)\frac{1}{iQ_0^{\perp}\hat{L}_{\sqrt{\eta}k}Q_0^{\perp}+BQ_0^{\perp}-\eta wQ_0^{\perp}}\left(Q_0^{\perp}\frac{\hat{L}_{\sqrt{\eta}k}}{\sqrt{\eta}}Q_0\right)\delta_0\otimes 1\right\rangle$$

and

$$
\begin{aligned}
J_k &:= \lim_{\eta\to 0^+} J_{\eta,k}(w) \qquad (3.15)\\
&= \left\langle \varphi_{0,k}, D_0^{1/2}\left[(P_0Q_0^\perp \hat{L}_0 P_0^\perp)\frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp}(P_0^\perp \hat{L}_0 Q_0^\perp P_0)\right]^{-1} D_0^{1/2}\varphi_{0,k}\right\rangle \\
&\quad +\left\langle f_{0,k}, \left(C_0^\dagger \frac{1}{F_{0,0}} C_0\right)^{-1} (iP_0Q_0^\perp \hat{L}_0 P_0^\perp)\frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp}\right.\\
&\quad \left.\left(2i\sum_e \theta(0,e,\omega)(k\cdot e)\delta_e\right)\right\rangle \\
&\quad +\left\langle \left(2i\sum_e \theta(0,e,\omega)(k\cdot e)\delta_e\right), \frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp}(iP_0^\perp \hat{L}_0 Q_0^\perp P_0)\right.\\
&\quad \left.\left(C_0^\dagger \frac{1}{F_{0,0}} C_0\right)^{-1} f_{0,k}\right\rangle \\
&\quad +\left\langle \left(2i\sum_e \theta(0,e,\omega)(k\cdot e)\delta_e\right), \frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp} - \frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp}\right.\\
&\quad \cdot(iP_0^\perp \hat{L}_0 Q_0^\perp P_0)\left(C_0^\dagger \frac{1}{F_{0,0}} C_0\right)^{-1}(iP_0Q_0^\perp \hat{L}_0 P_0^\perp)\frac{1}{iP_0^\perp \hat{L}_0 P_0^\perp + BP_0^\perp}\\
&\quad \left.\left(2i\sum_e \theta(0,e,\omega)(k\cdot e)\delta_e\right)\right\rangle
\end{aligned}
$$

Although it is not obvious from (3.15) above, J_k is of the form $\langle k, Dk\rangle_{\mathbb{C}^d}$ with D symmetric. To see this, we must compute J_k a different way.

Let $D^{(\eta)}$ be the matrix of time-averaged second moments:

$$
D_{i,j}^{(\eta)} := -\eta^2 \int_0^\infty \sum_{x\in\mathbb{Z}^d} x_i x_j \mathbb{E}\left(|\psi_t(x)|^2\right) e^{-\eta t}\, dt.
$$

This is just a time-averaged second derivative, evaluated at $k=0$, of the left-hand side of the diffusion criterion (3.3). It is clear that this matrix is symmetric. Now by using the

Feynman-Kac-Pillet formula (3.5), we see that

$$D_{i,j}^{(\eta)} = \eta \left\langle \delta_0 \otimes 1, \left(\frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} \frac{1}{i\hat{L}_{\sqrt{\eta}k} + B + \eta} \right) \Bigg|_{k=0} \delta_0 \otimes 1 \right\rangle .$$

But, by computing the derivatives, we see that $\langle k, D^{(\eta)} k \rangle$ is the inner-product on the right hand side of (3.9), which we have already named $J_{\eta,k}$. Thus, J_k is of the form $\langle k, Dk \rangle$ with D symmetric.

All that remains is to compute the limit of the integral in (3.8).

$$\begin{aligned} &-\frac{1}{2\pi i} \int_{\frac{1}{\eta}\Gamma_2} e^{-tw} \frac{1}{-w + J_{\eta,k}} \, dw \\ &= -\frac{1}{2\pi i} \int_{\frac{1}{\eta}\Gamma_2} e^{-tw} \left(\frac{1}{-w + J_{\eta,k}} - \frac{1}{-w + J_k} \right) dw - \frac{1}{2\pi i} \int_{\frac{1}{\eta}\Gamma_2} e^{-tw} \frac{1}{-w + J_k} \, dw \end{aligned}$$

For the first integral, the difference decays like c/w^2 so $\frac{1}{2\pi} \frac{ce^t}{w^2}$ is an integrable upper bound for the integrand. Thus, by the Lebesgue convergence theorem, the first integral goes to zero as $\eta \to 0$.

We will use the residue theorem to compute the final integral. The path

$$\gamma = \left\{ w = -1 + Re^{i\theta} : -\frac{\pi}{2} < \theta < \frac{\pi}{2} \right\}, \quad R = \frac{1 + ||L||}{\eta},$$

together with $\frac{1}{\eta}\Gamma_2$, forms a closed loop. For η sufficiently small, this path encloses J_k. The residue at this pole is e^{-tJ_k}.

On the curve γ,

$$\begin{aligned}\left|\frac{1}{2\pi i}\int_\gamma e^{-tw}\frac{1}{w-J_k}\,dw\right| &= \left|\frac{1}{2\pi i}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-t(-1+Re^{i\theta})}\frac{1}{-1+Re^{i\theta}-J_k}\,iRe^{i\theta}d\theta\right| \\ &\le \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-t(-1+R\cos\theta)}\left|\frac{R}{-1+Re^{i\theta}-J_k}\right|\,d\theta \\ &\le \frac{ce^t}{2\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-tR\cos\theta}\,d\theta,\end{aligned}$$

which goes to zero as $\eta \to 0^+$ by the bounded convergence theorem.

Therefore,

$$\lim_{\eta\to 0^+}\sum_{x\in\mathbb{Z}^d} e^{i\sqrt{\eta}k\cdot x}\mathbb{E}\left(|\psi_{t/\eta}(x)|^2\right) = e^{-tJ_k},$$

J_k is of the form $\sum_{e_1,e_2}(k\cdot e_1)(k\cdot e_2)D_{e_1,e_2}$ as seen above, and the theorem is proven.

Chapter 4

Higher Moments for a Markov-Schrödinger Equation

4.1 Statement of the Problem

The problem we consider here is that of computing moments of the position variable with respect to the probability density function $\mathbb{E}(|\psi_t|^2)$ on $\mathbb{Z}^d$. Here ψ_t is the solution to a Markov-Schrödinger equation on the lattice and the expectation is an average over all realizations of the process. Specifically, $\psi_t \in \ell^2(\mathbb{Z}^d)$ satisfies

$$\begin{cases} i\partial_t \psi_t(x) = \sum_y h_\omega(x, y, t)\psi_t(y), & x \in \mathbb{Z}^d,\ t > 0 \\ \psi_0(x) = \delta_0(x), & x \in \mathbb{Z}^d \end{cases} \tag{4.1}$$

with ω a Markov process and $h_w(\cdot, \cdot, t) \in \ell^2(\mathbb{Z}^d \times \mathbb{Z}^d)$. By way of a gauge transform, this problem is seen to be equivalent to the wave model in [3] and their result is crucial to the one presented here. We begin by giving the necessary details for diffusion in [3] and by showing the equivalence of the two models. A few further assumptions will be made, giving us a ballistic upper bound on solutions thus allowing for the computation of moments.

4.2 Diffusion for a Markov-Schrödinger Wave Equation

Here we will provide the minimum details from [3] to define the original problem and state their main result. For further details, the reader should consult [3].

Suppose $\tilde{h}$ is a function on $\mathbb{Z}^d$ with $\sum_{x\in\mathbb{Z}^d} |x|^2|\tilde{h}(x)| < \infty$ and $\tilde{h}(-x) = \tilde{h}(x)^*$ for all $x \in \mathbb{Z}^d$. Further suppose that for $k \in \mathbb{R}^d$, $\tilde{h}(x) \neq 0$ and $k \cdot x \neq 0$ for some $x \in \mathbb{Z}^d$. We may then define $\tilde{T}\psi(x) = \sum_y \tilde{h}(x,y)\psi(y)$. The assumptions on $\tilde{h}$ imply that T is a bounded, self-adjoint operator from $\ell^2(\mathbb{Z}^d)$ to itself.

Let $\lambda > 0$ be constant, $t \mapsto \omega(t)$ be a Markov process on a probability space (Ω, μ), and for $x \in \mathbb{Z}^d$, suppose $v_x : \Omega \to \mathbb{R}$ is measurable. Given $|\psi_0|_{\ell^2(\mathbb{Z}^d)} = 1$, the problem under consideration is that of finding $\tilde{\psi_t} \in \ell^2(\mathbb{Z}^d)$ for $t > 0$, such that

$$i\partial_t\tilde{\psi}_t(x) = \tilde{T}\tilde{\psi}_t(x) + \lambda v_x(\omega(t))\tilde{\psi}_t(x), \quad x \in \mathbb{Z}^d. \tag{4.2}$$

In the case when $\psi_0 = \delta_0$, their main result is

$$\lim_{\tau\to\infty} \sum_{x\in\mathbb{Z}^d} e^{-i\frac{k}{\sqrt{\tau}}\cdot x}\mathbb{E}(|\psi_{\tau t}(x)|^2) = e^{-t\sum_{i,j} D_{i,j}(\lambda)k_ik_j}, \tag{4.3}$$

for k in the torus $\mathbb{T}^d$ and $D = D(\lambda)$ a positive definite matrix. The result presented here is that we may differentiate (4.3) term-by-term, at $k = 0$, which will allow us to compute higher moments in the diffusive scaling limit. We do this by analytically continuing (4.3) in the variable k to a neighborhood of the origin in $\mathbb{C}^d$. But first, we must draw an equivalence between the models (4.1) and (4.2).

4.3 Equivalence of Models

The result in [3] that is crucial to the result here, is stated in terms of the solution to (4.2). To derive the bounds we need to compute moments, we would prefer to work in terms of (4.1). These two are easily seen to be equivalent. Moreover, the corresponding probability density functions, and hence moments, are equal: $\mathbb{E}(|\psi_t|^2) = \mathbb{E}(|\tilde{\psi}_t|^2)$. To see this, define the following gauge transformation.

$$\begin{aligned} \phi_\omega(x,t) &= \lambda \int_0^t v_x(\omega(s))\, ds \\ h_\omega(x,y,t) &= e^{i\phi_\omega(x,t)} \tilde{h}(x,y) e^{-i\phi_\omega(y,t)} \\ \psi_t(x) &= e^{i\phi_\omega(x,t)} \tilde{\psi}_t(x) \end{aligned} \tag{4.4}$$

Now h_ω in (4.1) is fully defined and h_ω inherits the assumptions placed on $\tilde{h}$ in [3]. We then see that ψ_t satisfies (4.1) if and only if $\tilde{\psi}_t$ is a solution to (4.2). It follows that the probability density functions are equal, as claimed. For the extended result here, we require some additional assumptions on $\tilde{h}$ and $\tilde{\psi}_0$. Namely, those conditions that will guarantee a ballistic upper bound on solutions to (4.2) and equivalently to (4.1). This is the topic of the next section.

4.4 A Ballistic Upper Bound

We assume the following decay conditions on $\tilde{h}$ and the initial condition $\tilde{\psi}_0$. Equivalent assumptions on h_ω and ψ_0 are then inherited and are also stated here.

$$\sum_y e^{\mu|x-y|}|h_\omega(x,y,t)| = \sum_y e^{\mu|x-y|}|\tilde{h}(x,y)| \leq A \tag{4.5}$$
$$c_0 := \sup_x e^{\mu|x|}|\psi_0(x)| = \sup_x e^{\mu|x|}|\tilde{\psi}_0(x)| < \infty$$

To compute a ballistic upper bound, we first integrate equation (4.1) and iterate the result to arrive at

$$\psi_t(x) = \psi_0(x) + \int_0^t H_{r_1}^{(\omega)}\psi_0\,dr_1 + \sum_{n=2}^{\infty}\int_0^t\int_0^{r_1}\cdots\int_0^{r_{n-1}} H_{r_1}^{(\omega)}\ldots H_{r_n}^{(\omega)}\psi_0\,dr_n\cdots dr_1,$$

where $H_t^{(\omega)}\psi(x) = \sum_y h_\omega(x,y,t)\psi_t(y)$. Now we multiply by the exponential

$$\begin{aligned} e^{\mu|x|}\psi_t(x) &= e^{\mu|x|}\psi_0(x) + \int_0^t e^{\mu|x|}H_{r_1}\psi_0\,dr_1 \\ &\quad + \sum_{n=2}^{\infty}\int_0^t\int_0^{r_1}\cdots\int_0^{r_{n-1}} e^{\mu|x|}H_{r_1}\ldots H_{r_n}\psi_0\,dr_n\cdots dr_1 \end{aligned}$$

and notice that if we write

$$e^{\mu|x|} \leq e^{\mu|x-y_1|}e^{\mu|y_1-y_2|}\ldots e^{\mu|y_n|},$$

and understand that H_{r_j} provides a sum over $y_j \in \mathbb{Z}^d$, then the decay conditions (4.5) give us

$$e^{\mu|x|}|\psi_t(x)| \;\leq\; c_0 + \int_0^t c_0 A\, dr_1 + \sum_{n=2}^{\infty} \int_0^t \int_0^{r_1} \cdots \int_0^{r_{n-1}} c_0 A^n\, dr_n \cdots dr_1.$$

But this is just the integral over the simplex $\Gamma_n(t) = \{(r_1, \ldots, r_n) : r_n \leq r_{n-1} \leq \cdots \leq r_1 \leq t\}$ which has $\mathbb{R}^n$-Lebesgue measure $\frac{t^n}{n!}$. This gives us

$$e^{\mu|x|}|\psi_t(x)| \;\leq\; c_0 + c_0 At + \sum_{n=2}^{\infty} c_0 A^n \frac{t^n}{n!} \;=\; c_0 e^{At}$$

and $|\psi_t(x)| \leq c_0 e^{At-\mu|x|}$ is the bound we seek.

4.5 Moments by Analytic Continuation

To show that (4.3) can be analytically continued, we require some notation. For $t > 0$, $\tau \gg 1$, and $z \in \mathbb{C}^d$ with $|z| < \mu$, define

$$\begin{aligned} F_{t,\tau}(z) &= \sum_{x \in \mathbb{Z}^d} e^{\frac{z \cdot x}{\sqrt{\tau}}} \mathbb{E}(|\psi_{\tau t}(x)|^2) \quad \text{and} \\ F_t(z) &= e^{t \sum_{i,j} D_{i,j}(\lambda) z_i z_j}, \end{aligned} \tag{4.6}$$

where ψ_t is a solution to (4.1) and $D_{i,j}(\lambda)$ is given by (4.3). Equation (4.3) is the motivation for these definitions since, in this notation, the main result in [3] is that $\lim_{\tau \to \infty} F_{t,\tau}(-ik) = F_t(-ik)$ for all $k \in \mathbb{T}^d$.

To begin, we wish to show that $\lim_{\tau \to \infty} F_{t,\tau} \equiv F_t$. Since F_t is clearly analytic, this is a result of the identity theorem if we first show that $\lim_{\tau\to\infty} F_{t,\tau}$ is analytic. Moreover, we also wish to show that the derivatives of $F_{t,\tau}$ converge to the corresponding derivatives of F_t. From this, it is a simple matter to compute any moment of the position. One may just differentiate (4.3) with respect to $k \in \mathbb{T}^d$ and substitute $k = 0$.

That these derivatives converge appropriately, is a consequence of the fact that the analytic functions (on regions in $\mathbb{C}$ with the sup norm) form a closed subset of the continuous functions (see [1]). Therefore, it remains only to show that $F_{t,\tau}$ and $\lim_{\tau\to\infty} F_{t,\tau}$ are analytic.

For the remainder of this chapter, when we discuss convergence or analyticity, it is understood that the domain under consideration is $\{z \in \mathbb{C}^d : |z| < \mu_0\}$, for some $\mu_0 \in (0, \mu)$. This extra space between μ_0 and μ will allow us to conclude uniform convergence for the series rather than mere point-wise convergence.

4.6 Convergence and Analyticity

First we show that the series in (4.6) converges uniformly and absolutely. We then show that (4.6) and its limit are analytic. This will complete the argument laid out in section 4.5. Let ω_d be the surface area of the unit ball in $\mathbb{R}^d$.

Lemma 1. *The series in (4.6) is uniformly and absolutely convergent with*

$$\sum_{x\in\mathbb{Z}^d} e^{\frac{|z||x|}{\sqrt{\tau}}} \mathbb{E}(|\psi_{\tau t}(x)|^2) \leq c_0 e^{A\tau t} \frac{\omega_d (d-1)!}{(\mu - \mu_0)^d}.$$

Moreover, $F_{t,\tau}$ defined in (4.6) is analytic.

Proof. The partial sums of the series are analytic and approximate $F_{t,\tau}$. So, to show analyticity, we need only show uniform convergence of the series. Since

$$\left| \sum_{x \in \mathbb{Z}^d} e^{\frac{z \cdot x}{\sqrt{\tau}}} \mathbb{E}(|\psi_{\tau t}(x)|^2) \right| \leq \sum_{x \in \mathbb{Z}^d} e^{\frac{\mu_0 |x|}{\sqrt{\tau}}} \mathbb{E}(|\psi_{\tau t}(x)|^2),$$

it suffices to show $\sum_{x \in \mathbb{Z}^d} e^{\frac{\mu_0 |x|}{\sqrt{\tau}}} \mathbb{E}(|\psi_{\tau t}(x)|^2)$ converges.

For all $x_0 \in \mathbb{Z}^d$, there exists a unique closed unit hypercube $C_{x_0} \subseteq \mathbb{R}^d$ with x_0, the unique point in the hypercube furthest from 0. The union of all such cubes is $\mathbb{R}^d$. Although they are not disjoint, the intersection of any two cubes has Lebesgue measure zero. For $k > 0$, it follows that

$$e^{-k|x_0|} = e^{-k|x_0|} \int_{C_{x_0}} dx \leq \int_{C_{x_0}} e^{-k|x|} \, dx,$$

and we sum over $x_0 \in \mathbb{Z}^d$ to arrive at

$$\sum_{x \in \mathbb{Z}^d} e^{-k|x|} \leq \int_{\mathbb{R}^d} e^{-k|x|} \, dx = \frac{\omega_d (d-1)!}{k^d}.$$

From section 4.4, we have $|\psi_t(x)|^2 \leq c_0 e^{At - \mu|x|}$. Note that $|\psi_t(x)| \leq 1$ since the solution generator is unitary and the initial condition is a unit vector. With this, we may conclude that the series converges absolutely and with constant bound as follows.

$$\begin{aligned}
\sum_{x\in\mathbb{Z}^d} e^{\frac{|z||x|}{\sqrt{\tau}}} |\psi_{\tau t}(x)|^2 &\le \sum_{x\in\mathbb{Z}^d} e^{\mu_0|x|} c_0 e^{A\tau t-\mu|x|} \\
&= c_0 e^{A\tau t} \sum_{x\in\mathbb{Z}^d} e^{-(\mu-\mu_0)|x|} \\
&\le c_0 e^{A\tau t} \frac{\omega_d (d-1)!}{(\mu-\mu_0)^d}
\end{aligned}$$

□

Lemma 2. $\lim_{\tau\to\infty} F_{t,\tau}$ *is analytic.*

Proof. From [3],

$$\sum_{x\in\mathbb{Z}^d} e^{\frac{z\cdot x}{\sqrt{\tau}}} |\psi_{\tau t}(x)|^2 = \left\langle \delta_0 \otimes 1,\, e^{-t\tau \hat{L}_{-iz/\sqrt{\tau}}} \delta_0 \otimes 1 \right\rangle$$

and so it suffices to show

$$\lim_{\tau\to\infty} \left\langle \delta_0 \otimes 1,\, e^{-t\tau \hat{L}_{-iz/\sqrt{\tau}}} \delta_0 \otimes 1 \right\rangle$$

is analytic. As $\hat{L}_{-iz/\sqrt{\tau}}$ is a perturbation of $\hat{L}_0$ on the order of $1/\sqrt{\tau}$, the estimates on the spectral gap in [3] hold. In particular, $E(z)$ is an isolated eigenvalue of $\hat{L}_z$ with $|E(z)| < c/\sqrt{\tau}$. The rest of the numerical range is contained in a sector of the form

$$\Sigma_+ = \left\{ z = x + iy \in \mathbb{C} \,:\, x > \delta_\lambda - \frac{c}{\sqrt{\tau}},\, |y| \le mx \right\}.$$

We may then choose a contour $\Gamma = \Gamma_1 \cup \Gamma_2$, with index 1 around the numerical range.

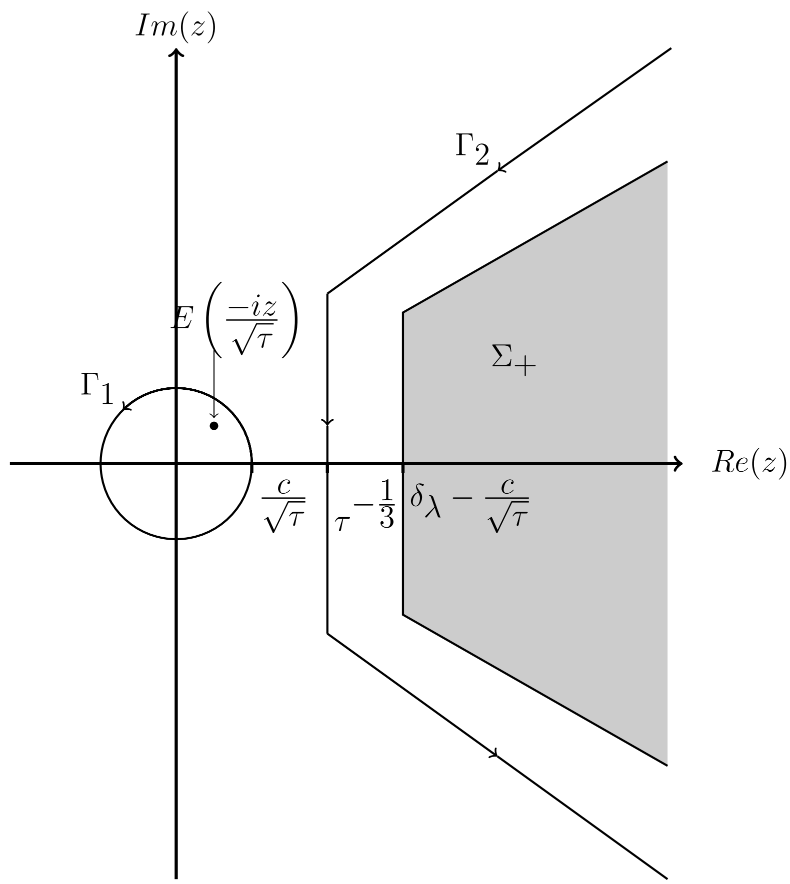

Figure 4.1: The contour Γ and the perturbed numerical range.

Γ_1 is the circle centered at the origin, with radius $c/\sqrt{\tau}$. Then we choose Γ_2 winding once around Σ_+, maintaining a distance at least on the order of $\tau^{-1/3}$ from Σ_+. We will use the fact that

$$dist(\tau\Gamma_2, \tau\Sigma_+) = \mathcal{O}\left(\tau - \tau^{2/3}\right)$$

and so an integral of the resolvent of $\tau\hat{L}_{-iz/\sqrt{\tau}}$ over $\tau\Gamma_2$ is small (see Appendix A). With this contour, we may use the holomorphic functional calculus (see [5]).

$$\left\langle \delta_0 \otimes 1,\, e^{-t\tau\hat{L}_{-iz/\sqrt{\tau}}}\delta_0 \otimes 1 \right\rangle = \frac{1}{2\pi i}\int_{\Gamma} e^{-t\tau w}\left\langle \delta_0 \otimes 1,\, \frac{1}{w - \hat{L}_{-iz/\sqrt{\tau}}}\,\delta_0 \otimes 1 \right\rangle dw$$

To make use of the resolvent estimate above and to avoid an asymptotic integral, we make a linear change of variables to arrive at

$$\frac{1}{2\pi i}\int_{\tau\Gamma} e^{-tw}\left\langle \delta_0 \otimes 1,\, \frac{1}{w - \tau\hat{L}_{-iz/\sqrt{\tau}}}\,\delta_0 \otimes 1 \right\rangle dw$$
$$= \frac{1}{2\pi i}\int_{\tau\Gamma_1} e^{-tw}\left\langle \delta_0 \otimes 1,\, \frac{1}{w - \tau\hat{L}_{-iz/\sqrt{\tau}}}\,\delta_0 \otimes 1 \right\rangle dw + \mathcal{O}\left(\frac{1}{\tau}\right),$$

and the resulting integral over $\tau\Gamma_1$ is an exponential times a Riesz projection. Indeed, if $\Psi(z)$ is a unit vector satisfying $\hat{L}_z\Psi(z) = E(z)\Psi(z)$ then

$$Q_z = \frac{1}{2\pi i}\int_{\Gamma_1} \frac{1}{w - \hat{L}_z}\, dw$$

is the projection onto the span of $\Psi(z)$ and $\hat{L}_z Q_z = E(z) Q_z$. It follows that

$$\sum_{x \in \mathbb{Z}^d} e^{\frac{z \cdot x}{\sqrt{\tau}}} |\psi_{\tau t}(x)|^2 \;=\; e^{-t\tau E(-iz/\sqrt{\tau})} \left\langle \delta_0 \otimes 1,\, Q_{-iz/\sqrt{\tau}}\, \delta_0 \otimes 1 \right\rangle + \mathcal{O}\left(\frac{1}{\tau}\right).$$

It is clear that $\left\langle \delta_0 \otimes 1,\, Q_{-iz/\sqrt{\tau}}\, \delta_0 \otimes 1 \right\rangle$ tends to 1. From [3] we have an expansion for $E(z)$ near zero with $E(0) = 0$ and $\nabla E(0) = 0$ from which we may conclude

$$\lim_{\tau \to \infty} \sum_{x \in \mathbb{Z}^d} e^{\frac{z \cdot x}{\sqrt{\tau}}} |\psi_{\tau t}(x)|^2 \;=\; e^{-th(z)}$$

with $h(z) = \lim_{\tau \to \infty} \tau E(-iz/\sqrt{\tau})$ holomorphic. $\square$

APPENDICES

Appendix A

The Numerical Range of a Linear Operator

Definition 1. *The numerical range [8] of an operator on a Hilbert space is defined by*

$$\mathcal{N}(A) = \{\langle x, Ax\rangle : x \in \mathcal{D}(A), |x| = 1\}.$$

Lemma 2. *Suppose $\mathcal{H}$ is a Hilbert space, $\mathcal{D}(A) \subseteq \mathcal{H}$ is dense, and $A : \mathcal{D}(A) \to \mathcal{H}$. Then the norm of the resolvent is bounded by the inverse of the distance to the numerical range:*

$$\left\| \frac{1}{z - A} \right\| \leq \frac{1}{dist(z, \mathcal{N}(A))}.$$

Proof. Suppose $z \in \mathbb{C}$ such that $dist(z, \mathcal{N}(A)) > 0$ and let $\psi \in \mathcal{H}$ be a unit vector. Define

$c = \left|\frac{1}{z-A}\psi\right|^{-1}$ and $\varphi = c\frac{1}{z-A}\psi$.[1] Then

$$dist(z, \mathcal{N}(A)) \leq |\langle \varphi, (z-A)\varphi \rangle| = c^2 \left| \left\langle \frac{1}{z-A}\psi, \psi \right\rangle \right| \leq c$$

and the result follows by inverting the inequality and taking the supremum over $\{|\psi| = 1\}$. □

As a consequence of this lemma, the spectrum of an operator is contained in the closure of its numerical range. Indeed, if $dist(z, \mathcal{N}(A)) > 0$ then $Ker(z - A) = \{0\}$ and $z \in \rho(A)$. So, if $z \in \sigma(A)$, then $dist(z, \mathcal{N}(A)) = 0$ and $z \in Clo\mathcal{N}(A)$.

[1] At this point, one should verify that φ is well-defined; that the domain of the resolvent is the entire Hilbert space. To do this, it suffices to show that the resolvent is bounded. One approach, and perhaps the simplest, is to define it to be so. In [7] for example, the resolvent set is defined to be those complex numbers such that the resolvent is a bounded operator, defined on the entire space. Alternatively, [4] defines the resolvent set such that the resolvent need only be a bijection on $\mathcal{H}$. Then, the closed graph theorem asserts that the resolvent is bounded.

Appendix B

The Markov Generator

Here we construct the *semigroup* and *generator* corresponding to a *Markov process*. The generator will be an unbounded operator, defined on a subset of L^2-functions on a probability space. This semigroup structure encapsulates the process in the generator, allowing us to reduce the problem of understanding the Markov dynamics (in an averaged sense, see 2.3) to a spectral analysis of the generator. We may focus on the generator itself, and not the process it represents, because of a Feynman-Kac formula due to Pillet [6]. This formula allows us to write the amplitude of a wave-form in terms of a particular matrix element of the overall generator – the generator for the wave model together with the Markov generator. Hence, a detailed study of the Markov process and its underlying probability space is limited to this section, allowing us to concentrate our focus in chapter 3 solely on the generator.

We begin by defining the underlying probability space, a path-space for the Markov process, and the appropriate semigroups. Several assumptions are placed on these spaces so that we indeed have a semigroup, and that this semigroup is a strongly continuous contraction. With this, we may write down its generator and, with a few additional assumptions, derive the key aspects which are required in chapter 3. The development below is nearly identical to [3], except that we construct a *collection* of processes, independent and identically distributed, and indexed by the space through which our wave solution will propagate.

Let $\mathbb{E}^d$ denote the space of *directed edges* between nearest-neighbor pairs in $\mathbb{Z}^d$. That is, $(x, e) \in \mathbb{E}^d$ if $x \in \mathbb{Z}^d$ and e is a unit vector with $x + e \in \mathbb{Z}^d$. We call the points x and $x + e$ in $\mathbb{Z}^d$, nearest neighbors. Each of these directed edges may be thought of as a site at which a Markov process runs.

For each $(x, e) \in \mathbb{E}^d$, we will construct a Markov process as follows. It is assumed that the collection of processes constructed in this way are i.i.d. Let (Ω, μ) be a probability space and suppose we have a collection $\{\mathbb{P}_\alpha : \alpha \in \Omega\}$ of probability measures on the path space $\mathcal{P} = \Omega^{[0,\infty)}$ and that each measure $\mathbb{P}_\alpha$ is supported on those processes which start at α. That is,

$$\mathbb{P}_\alpha(\{\omega(\cdot) \in \mathcal{P} : \omega(0) \neq \alpha\}) = 0.$$

Further, we assume that each path $\omega(\cdot) \in \mathcal{P}$ is right-continuous – $\mathbb{P}_\alpha$-a.s. With these probability measures in mind, we assume that μ is *invariant*:

$$\int_\Omega \mathbb{P}_\alpha(\omega(t) \in A)\, d\mu(\alpha) = \mu(A)$$

for measurable sets $A \subseteq \Omega$.

Let $\mathcal{S}_t$ be the backward shift on $\mathcal{P}$, $\mathcal{S}_t\omega(\cdot) = \omega(\cdot + t)$, so that $\mathcal{S}_t^{-1}(\mathcal{A}) = \{\omega(\cdot) : \omega(\cdot + t) \in$

$\mathcal{A}\}$ for measureable sets $\mathcal{A} \subseteq \mathcal{P}$. Finally, we suppose that the Markov property holds:

$$\int_{\mathcal{P}} \mathbb{P}_{\omega(t)}(\mathcal{A})\, d\mathbb{P}_\alpha(\omega(\cdot)) = \mathbb{P}_\alpha(\mathcal{S}_t^{-1}(\mathcal{A})).$$

We then define

$$S_t f(\alpha) = \mathbb{E}_\alpha(f(\omega(t))), \quad S_t : L^2(\Omega) \to L^2(\Omega),$$

and the above assumptions imply that $\{S_t\}_{t\geq 0}$ is a strongly continuous, contraction semigroup on $L^2(\Omega)$. It follows that the adjoint $S_t^\dagger$ is also a strongly continuous, contraction semigroup given by

$$S_t^\dagger f(\alpha) = \mathbb{E}(f(\omega(0))|\omega(t) = \alpha).$$

Let B denote the generator of $S_t^\dagger$,

$$B\psi = -\lim_{t\to 0^+} \frac{1}{t}\left(S_t^\dagger \psi - \psi\right)$$

so that $e^{-tB} = S_t^\dagger$. The generator B is defined on $\mathcal{D}(B)$ – those $L^2(\Omega)$ functions for which the limit exists. The exponential of an unbounded operator may be interpreted using the holomorphic functional calculus [5]:

$$e^{-tB} = \frac{1}{2\pi i}\int_\Gamma \frac{e^{-tz}}{z - B}\, dz.$$

To ensure convergence of the functional calculus, and to further control the spectrum of the

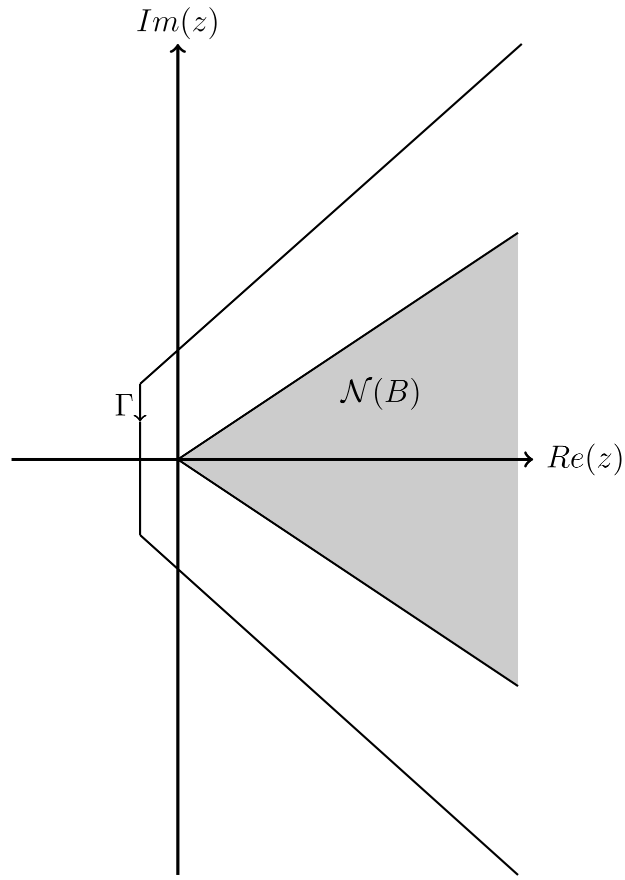

Figure B.1: The contour Γ and the numerical range of the Markov Generator.

overall generator in chapter 3, we assume that the numerical range (see appendix A) of B is *sectoral*. That is, if $z = x + iy \in \mathcal{N}(B)$, then $|y| \leq mx$ for some $m \geq 0$. This condition is easily satisfied if B happens to be self-adjoint.

Appendix C

Another Realization of D_k

The operator D_k plays a special role in showing diffusion for the divergence-form model in chapter 3. Here we derive another useful formulation for D_k.

For $k \in \mathbb{C}^d$, let D_k be the bounded, self-adjoint operator defined in section 3.4.4 by

$$D_k = (B^{-1} P_0^{\perp} \hat{L}_k P_0 Q_0^{\perp})^{\dagger} (B^{-1} P_0^{\perp} \hat{L}_k P_0 Q_0^{\perp}). \tag{C.1}$$

At the present time, we are only concerned with $k \in \mathbb{T}^d$, however the full generality of $k \in \mathbb{C}^d$ will be useful when computing higher moments of position.

Consider $(x, e) \in \mathbb{E}^d$, a directed edge connecting nearest neighbors in $\mathbb{Z}^d$. The opposing direction on the same edge is given by $(x + e, -e)$. Due to translation covariance, θ does not distinguish between these two directions. Indeed, $\theta(x, e, \omega) = \theta(x + e, -e, \omega)$. Moreover, if

(x, e) and (x', e') are distinct edges,

$$\begin{aligned}
&\langle B^{-1}(\theta(x,e,\omega)-\bar{\theta}), B^{-1}(\theta(x',e',\omega)-\bar{\theta})\rangle_{L^2(\Omega)} \\
&\quad = \int_\Omega (B^{-1}(\theta(x,e,\omega)-\bar{\theta}))^* B^{-1}(\theta(x',e',\omega)-\bar{\theta}) d\mu(\omega) \\
&\quad = \int_\Omega (B^{-1}(\theta(x,e,\omega)-\bar{\theta}))^* d\mu(\omega) \int_\Omega B^{-1}(\theta(x',e',\omega)-\bar{\theta}) d\mu(\omega) \\
&\quad = 0
\end{aligned}$$

since the Markov processes on each edge are independent and the set of mean-zero functions are invariant under B. Thus, for any pair of edges (x, e) and (x', e') we may write

$$\langle B^{-1}(\theta(x,e,\omega)-\bar{\theta}), B^{-1}(\theta(x',e',\omega)-\bar{\theta})\rangle_{L^2(\Omega)} \quad = \quad \chi(\delta_x(x')\delta_e(e') + \delta_x(x'+e')\delta_e(-e'))$$

where $\chi = ||B^{-1}(\theta(x,e,\cdot)-\bar{\theta})||^2_{L^2(\Omega)}$. Note that χ is independent of (x, e) since the Markov processes on edges in $\mathbb{E}^d$ are i.i.d. We will use this equality to evaluate matrix elements of D_k. Let $\varphi \in \ell^2(\mathbb{Z}^d)$ with $\varphi = P_0 Q_0^\perp \varphi$. That is, φ is non-random and $\varphi(0) = 0$. Also, define $\tilde{\theta}(x,e,\omega) := P_0^\perp \theta(x,e,\omega) = \theta(x,e,\omega) - \bar{\theta}$. Matrix elements of D_k are evaluated as follows.

$$
\begin{aligned}
&\langle \varphi, D_k \varphi \rangle_{L^2(\mathbb{Z}^d \times \Omega)} = ||B^{-1} P_0^{\perp} \hat{L}_k \varphi||^2_{L^2(\mathbb{Z}^d \times \Omega)} \\
= &\sum_{x \in \mathbb{Z}^d} \int_\Omega (B^{-1} P_0^{\perp} \hat{L}_k \varphi(x,\omega))^* B^{-1} P_0^{\perp} \hat{L}_k \varphi(x,\omega)\, d\mu(\omega) \\
= &\; 4 \sum_{x \in \mathbb{Z}^d} \int_\Omega \\
&\left(B^{-1} P_0^{\perp} \sum_e \left[\theta(x,e,\omega)\,(\varphi(x) - \varphi(x+e)) + \theta(0,e,\omega) \left(e^{-ik\cdot e} \varphi(x-e) - \varphi(x) \right) \right] \right)^* \\
&\left(B^{-1} P_0^{\perp} \sum_{e'} \left[\theta(x,e',\omega) \left(\varphi(x) - \varphi(x+e') \right) + \theta(0,e',\omega) \left(e^{-ik\cdot e'} \varphi(x-e') - \varphi(x) \right) \right] \right) \\
&d\mu(\omega)
\end{aligned}
$$

We now may evaluate the integral by using the definition of χ. That is, by making use of the assumption that the Markov processes at each site are i.i.d.

$$
\begin{aligned}
& \langle \varphi, D_k \varphi \rangle_{L^2(\mathbb{Z}^d \times \Omega)} \\
= \; & 4 \sum_{x,e,e'} \int_\Omega d\mu(\omega) \\
& B^{-1}\tilde{\theta}(x,e,\omega)(\varphi^*(x) - \varphi^*(x+e)) \cdot B^{-1}\tilde{\theta}(x,e',\omega)(\varphi(x) - \varphi(x+e')) \\
& + B^{-1}\tilde{\theta}(x,e,\omega)(\varphi^*(x) - \varphi^*(x+e)) \cdot B^{-1}\tilde{\theta}(0,e',\omega)(e^{-ik\cdot e'}\varphi(x-e') - \varphi(x)) \\
& + B^{-1}\tilde{\theta}(0,e,\omega)(e^{i\bar{k}\cdot e}\varphi^*(x-e) - \varphi^*(x)) \cdot B^{-1}\tilde{\theta}(x,e',\omega)(\varphi(x) - \varphi(x+e')) \\
& + B^{-1}\tilde{\theta}(0,e,\omega)(e^{i\bar{k}\cdot e}\varphi^*(x-e) - \varphi^*(x)) \cdot B^{-1}\tilde{\theta}(0,e',\omega)(e^{-ik\cdot e'}\varphi(x-e') - \varphi(x)) \\
= \; & 4\chi \sum_{x,e,e'} \\
& \qquad (\varphi^*(x) - \varphi^*(x+e))(\varphi(x) - \varphi(x+e'))\delta_e(e') \\
& \quad + \; (\varphi^*(x) - \varphi^*(x+e))(e^{-ik\cdot e'}\varphi(x-e') - \varphi(x))(\delta_0(x)\delta_e(e') + \delta_{e'}(x)\delta_e(-e')) \\
& \quad + \; (e^{i\bar{k}\cdot e}\varphi^*(x-e) - \varphi^*(x))(\varphi(x) - \varphi(x+e'))(\delta_0(x)\delta_e(e') + \delta_e(x)\delta_e(-e')) \\
& \quad + \; (e^{i\bar{k}\cdot e}\varphi^*(x-e) - \varphi^*(x))(e^{-ik\cdot e'}\varphi(x-e') - \varphi(x))\delta_e(e')
\end{aligned}
$$

Evaluating the Kronecker delta functions give us

$$
\begin{aligned}
= \quad & 4\chi \sum_{x,e} (\varphi^*(x) - \varphi^*(x+e))(\varphi(x) - \varphi(x+e)) \\
& -4\chi \sum_{e} e^{-ik\cdot e} \varphi^*(e)\varphi(-e) + \varphi^*(-e)\varphi(-e) \\
& -4\chi \sum_{e} e^{i\bar{k}\cdot e} \varphi^*(-e)\varphi(e) + \varphi^*(e)\varphi(e) \\
& +4\chi \sum_{x,e} (e^{i\bar{k}\cdot e}\varphi^*(x-e) - \varphi^*(x))(e^{-ik\cdot e}\varphi(x-e) - \varphi(x)).
\end{aligned}
$$

In the case when k is real,

$$
\begin{aligned}
\langle \varphi, D_k \varphi \rangle_{L^2(\mathbb{Z}^d \times \Omega)} \quad = \quad & 8\chi \sum_x \varphi^*(x) \sum_e [\varphi(x) - \varphi(x+e)] \\
& +8\chi \sum_x \varphi^*(x) \sum_e \left[\varphi(x) - e^{ik\cdot e}\varphi(x+e)\right] \\
& -8\chi \sum_e \varphi^*(e) \left(e^{-ik\cdot e}\varphi(-e) + \varphi(e)\right)
\end{aligned}
$$

and we will examine each of these three terms separately. The first term is

$$
\begin{aligned}
& 8\chi \sum_{|x|>1} \varphi^*(x) \sum_e [\varphi(x) - \varphi(x+e)] + 8\chi \sum_e \varphi^*(e) \sum_{e' \neq -e} \left[\varphi(e) - \varphi(e+e')\right] \\
& +8\chi \sum_e |\varphi(e)|^2 \\
= \quad & 8\chi \langle \varphi, \triangle_0^N \varphi \rangle + 8\chi \sum_e |\varphi(e)|^2
\end{aligned}
$$

where $\triangle_0^N$ is the "Neumann Laplacian":

$$\triangle_0^N \psi(x) \;=\; (1-\delta_0(x)) \sum_{\substack{y\neq 0 \\ |x-y|=1}} (\psi(x)-\psi(y))$$

This new "Laplacian" is just the traditional discrete Laplacian with Neumann boundary conditions near zero. With the substitution $e = y - x$, the second term is then

$$\begin{aligned}
& 8\chi \sum_{|x|>1} \varphi^*(x) e^{-ik\cdot x} \sum_{\substack{y\in\mathbb{Z}^d \\ |x-y|=1}} \left[e^{ik\cdot x}\varphi(x) - e^{ik\cdot y}\varphi(y)\right] \\
& +8\chi \sum_{e} \varphi^*(e) e^{-ik\cdot e} \sum_{\substack{y\neq 0 \\ |e-y|=1}} \left[e^{ik\cdot e}\varphi(e) - e^{ik\cdot y}\varphi(y)\right] \\
& +8\chi \sum_{e} |\varphi(e)|^2 \\
= \;& 8\chi\langle\varphi, \triangle_k^N \varphi\rangle + 8\chi \sum_{e} |\varphi(e)|^2
\end{aligned}$$

where $\triangle_k^N$ is the Gauge transformation of the Neumann Laplacian,

$$\begin{aligned}
\triangle_k^N &= e^{-ik\cdot X} \triangle_0^N e^{ik\cdot X} \\
\triangle_k^N \psi(x) &= (1-\delta_0(x)) \sum_{\substack{y\neq 0 \\ |x-y|=1}} \left(\psi(x) - e^{ik\cdot(y-x)}\psi(y)\right) \\
&= (1-\delta_0(x)) \sum_{\substack{x+e\neq 0 \\ |e|=1}} \left(\psi(x) - e^{ik\cdot e}\psi(x+e)\right)
\end{aligned}$$

Lastly, we take the third term along with the non-Laplacian terms from above. These may be written as:

$$4\chi\left\langle \varphi, \sum_e \left(\delta_e - e^{ik\cdot e}\delta_{-e}\right)\langle \delta_e - e^{ik\cdot e}\delta_{-e},\,\cdot\rangle\varphi\right\rangle.$$

Combining these three terms, we have our alternate representation of D_k:

$$D_k = 8\chi\triangle_0^N + 8\chi\triangle_k^N + 4\chi\sum_e(\delta_e - e^{ik\cdot e}\delta_{-e})\langle\delta_e - e^{ik\cdot e}\delta_{-e},\cdot\rangle. \tag{C.2}$$

Note that we have only shown the equivalence of *diagonal* matrix elements of the operators in (C.1) and (C.2). However, each of these operators is non-negative. By applying the polarization identity [7] to the operator's square root, one sees that this is sufficient to conclude equality of (C.1) and (C.2). Indeed, if $A \geq 0$ on a Hilbert Space, and $\langle x, Ax\rangle = 0$ for all $x \in \mathcal{D}(A)$, then the polarization identity says

$$\begin{aligned}
\langle x, Ay\rangle &= \langle A^{1/2}x, A^{1/2}y\rangle \\
&= \frac{1}{4}(\|A^{1/2}(x+y)\|^2 - \|A^{1/2}(x-y)\|^2 + i\|A^{1/2}(x-iy)\|^2 - i\|A^{1/2}(x+iy)\|^2) \\
&= \frac{1}{4}(\langle x+y,\, A(x+y)\rangle - \langle x-y,\, A(x-y)\rangle + i\langle x-iy,\, A(x-iy)\rangle \\
&\quad -i\langle x+iy,\, A(x+iy)\rangle) \\
&= 0.
\end{aligned}$$

Appendix D

Inversion of Linear Operators

Lemma 3. *Suppose A is a linear operator on a Hilbert space and $\epsilon = \inf_{z\in\mathcal{N}(A)} |z| > 0$. Then A is boundedly invertible and $\|A^{-1}\| \leq 1/\epsilon$.*

Proof. It is clear that A is invertible, since zero is not in the numerical range, thus not in the spectrum. Suppose $\|A^{-1}\| > 1/\epsilon$. Then there is a unit vector y, in the domain of A^{-1}, such that $|A^{-1}y| > 1/\epsilon$. Let $x = A^{-1}y$ so that $1/|x| < \epsilon$.

$$\left|\left\langle \frac{x}{|x|}, A\frac{x}{|x|}\right\rangle\right| \leq \frac{1}{|x|}\left|\left\langle \frac{x}{|x|}, y\right\rangle\right| < \epsilon$$

This contradicts our assumption on the numerical range of A. □

Indeed, what we have shown is that if an invertible operator fails to be boundedly invertible, then zero is in the closure of the numerical range. Another conclusion we may draw is that, to show an operator is boundedly invertible, it suffices to show that its real (or imaginary) part is bounded away from zero. By the real part of an operator, we mean $\langle x, Re(A)x\rangle = Re\langle x, Ax\rangle$ and we may extend this definition, by way of the polarization identity, to $\langle x, Re(A)y \rangle$. The imaginary part is then $Im(A) = -i(A - Re(A))$ as expected.

Appendix E

The Schur Complement Formula

The *Schur complement* [9] is a generalization of the notion of the determinate of a 2x2 matrix, in the case when the entries do not commute. A formal statement of this fact is given here and the proof is given in section E.1. The formula is particularly useful when used in conjunction with projections that are natural to the operator being inverted, as demonstrated in section E.2.

Lemma 4. *(The Schur Complement Formula) Suppose A, B, C and D are linear operators from a vector space to itself and that D is invertible. Then $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$ is invertible if and only if $(A - BD^{-1}C)$ is invertible. In the affirmative case, we also have*

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{pmatrix}. \tag{E.1}$$

Definition 5. *Equation (E.1) is known as the Schur complement formula whereas* $(A - BD^{-1}C)^{-1}$ *is known as the Schur complement.*

E.1 Proof and a Corollary

Proof. If $(A - BD^{-1}C)^{-1}$ exists, then we may define

$$X = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{pmatrix}$$

and use matrix multiplication to conclude

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} X = X \begin{pmatrix} A & B \\ C & D \end{pmatrix} = I.$$

Conversely, we may factor

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} I & 0 \\ D^{-1}C & I \end{pmatrix}$$

to conclude

$$\begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix}^{-1} \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} I & 0 \\ D^{-1}C & I \end{pmatrix}^{-1},$$

which is clearly invertible. □

Corollary 6. *In the affirmative case, if A is also invertible, then*

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A-BD^{-1}C)^{-1} & -(A-BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A-BD^{-1}C)^{-1} & (D-CA^{-1}B)^{-1} \end{pmatrix}.$$

Proof. Apply the lemma to $\begin{pmatrix} D & C \\ B & A \end{pmatrix}$ and take the (1,1) matrix element. □

E.2 Using the Schur Complement Formula

To see the utility of the Schur complement formula, consider the following. Let $\eta > 0$ and suppose L and B are linear maps from a Hilbert space to itself. Suppose further that L is bounded and self-adjoint and that the numerical range of B satisfies a *gap condition*: $\mathcal{N}(B) \subseteq \{0\} \cup \{Re z \geq c\}$ for some $c > 0$. Let P be the projection onto the kernel of B and suppose that the range of $P^{\perp}$ is invariant under both B and $B^{\dagger}$. When we write $BP^{\perp}$, it is understood that we mean the restriction to the range of B, and thus, $BP^{\perp}$ is invertible. This is exactly the scenario that we encounter in section 3.4.4.

We may now identify the operator $iL + B + \eta$ with its block matrix form:

$$\begin{aligned} (iL+B+\eta)\psi &\sim \begin{pmatrix} P(iL+B+\eta)P & P(iL+B+\eta)P^{\perp} \\ P^{\perp}(iL+B+\eta)P & P^{\perp}(iL+B+\eta)P^{\perp} \end{pmatrix} \begin{pmatrix} P\psi \\ P^{\perp}\psi \end{pmatrix} \\ &= \begin{pmatrix} iPLP+\eta P & iPLP^{\perp} \\ iP^{\perp}LP & P^{\perp}(iL+B+\eta)P^{\perp} \end{pmatrix} \begin{pmatrix} P\psi \\ P^{\perp}\psi \end{pmatrix}. \end{aligned}$$

The Schur complement applies here since

$$Re(P^{\perp}(iL + B + \eta)P^{\perp}) > Re(P^{\perp}BP^{\perp}) \geq c$$

and $P^{\perp}(iL + B + \eta)P^{\perp}$ is invertible. The Schur complement is then:

$$P\frac{1}{iL + B + \eta}P = \left(iPLP + \eta P - iPLP^{\perp}\frac{1}{iP^{\perp}LP^{\perp} + P^{\perp}BP^{\perp} + \eta P^{\perp}}iP^{\perp}LP\right)^{-1}.$$

If another appropriate projection is chosen, we may apply the Schur complement a second time, further reducing the operator in question into its constitute parts. While the resulting equations are more cumbersome, the difficulty in analyzing the original operator is greater than the sum of the difficulties of its parts.

BIBLIOGRAPHY

BIBLIOGRAPHY

[1] John B. Conway. *Functions of One Complex Variable I.* Number 11 in Graduate Texts in Mathematics. Springer, 1978.

[2] Lawrence C. Evans. *Partial Differential Equations*, volume 19 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, Rhode Island, first edition, 1998.

[3] Yang Kang and Jeffrey Schenker. Diffusion of wave packets in a markov random potential. *Journal of Statistical Physics*, 134:1005–1022, 1005.

[4] Peter D. Lax. *Functional Analysis.* Pure and Applied Mathematics. John Wiley & Sons, Inc., eighth edition, 2002.

[5] Klaus-Jochen Engel & Rainer Nagel. *One-Parameter Semigroups for Linear Evolution Equations*, volume 194 of *Graduate Studies in Mathematics*. Springer, 2000.

[6] Claude-Alain Pillet. Some results on the quantum dynamics of a particle in a markovian potential. *Communications in Mathematical Physics*, 102(2):237–254, 1985.

[7] Gerald Teschl. *Mathematical Methods in Quantum Mechanics: With Applications to Schrödinger Operators*, volume 99 of *Graduate Studies in Mathematics*. American Mathematical Society, 2009.

[8] Lloyd Trefethen and David Bau. *Numerical Linear Algebra.* Society for Industrial and Applied Mathematics, 1997.

[9] Fuzhen Zhang. *The Schur Complement and its Applications*, volume 4 of *Numerical Methods and Algorithms*. Springer, 2005.