DIFFUSION IN THE MEAN FOR MARKOV SCHRÖDINGER EQUATIONS

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ABSTRACT

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We consider the evolution of a quantum particle hopping on a cubic lattice in any dimension and subject to a potential consisting of a periodic part and a random part that fluctuates stochastically in time. If the random potential evolves according to a stationary Markov process, we obtain diffusive scaling for moments of the position displacement, with a diffusion constant that grows as the inverse square of the disorder strength at weak coupling. More generally, we show that a central limit theorem holds such that the square amplitude of the wave packet converges, after diffusive rescaling, to a solution of a heat equation. We also consider how the addition of a random, stochastically evolving, potential leads to diffusive propagation in the random dimer and trimmed Anderson models.

ACKNOWLEDGMENTS

The results presented here are based on two papers. The first is a joint work with Jeffrey Schenker and Shiwen Zhang, [34]. The second, which is a joint work with Jeffrey Schenker, is currently being written.

I would like to thank Jeff for his support and guidance.

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CHAPTER 1

INTRODUCTION

Diffusive propagation is expected, and observed, to emerge from wave motion in a random medium in a variety of situations. The general intuition behind this expectation is that repeated scattering due to the random medium leads to a loss of coherence, which in a multi-scattering expansion or path integral formulation suggests a relation with random walks and diffusion. This intuition is notoriously difficult to make precise in the context of a static random environment. Indeed, proving the emergence of diffusion for the Schrödinger wave equation with a weakly disordered potential, in dimension $d \geq 3$, is one of the key outstanding open problems of mathematical physics. For a random environment that fluctuates stochastically in time, the analysis is simpler and diffusive propagation has proved amenable to rigorous methods. Heuristically, this simplification is to be expected because time fluctuations suppress recurrence effects in path expansions.

The present work is a continuation of a project initiated by Schenker and collaborators [23, 18, 27, 33, 17] in which diffusive propagation has been shown to occur for solutions to a tight binding Schrödinger equation with a random potential evolving stochastically in time. In [23, 27], the following stochastic Schrödinger equation on $\ell^2(\mathbb{Z}^d)$ was considered:

$$\mathrm{i}\partial_t \psi_t(x) = H_0 \psi_t(x) + \lambda V(x,t)\psi_t(x), \tag{1.0.1}$$

with H_0 a (non-random) translation invariant Schrödinger operator, $V(x,t)$ a zero-mean random potential with time dependent stochastic fluctuations, and $\lambda \geq 0$ a coupling constant. These models had been considered previously by Tcheremchantsev [36, 37], who obtained diffusive bounds for the p-th position moment,

$$\left\langle X_t^p \right\rangle := \sum_{x \in \mathbb{Z}^d} |x|^p \, \mathbb{E}(|\psi_t(x)|^2), \tag{1.0.2}$$

up to logarithmic corrections:

$$\frac{t^{\frac{p}{2}}}{(\ln t)^{\nu_-}} \lesssim \sum_{x\in\mathbb{Z}^d} |x|^p \, \mathbb{E}(|\psi_t(x)|^2) \lesssim t^{\frac{p}{2}} (\ln t)^{\nu_+}, \qquad t \to \infty. \tag{1.0.3}$$

Given suitable hypotheses on H_0 and V, it was proven in [23] that diffusive scaling (without logarithmic corrections, i.e., $\nu_- = \nu_+ = 0$) holds for $p = 2$, while in [27] diffusive scaling was shown to hold for all moments. Furthermore, it was observed that at weak disorder, $\lambda \to 0$, the corresponding diffusion constant D has the asymptotic form

$$D \sim \frac{C}{\lambda^2}. \tag{1.0.4}$$

The divergence of D as $\lambda \to 0$ seen in Equation (1.0.4) is to be expected, since the translation invariant Schrödinger operator H_0 on its own leads to ballistic transport. In [33], a more subtle situation is considered where the environment is a superposition of two parts:

$$\mathrm{i}\partial_t\psi_t(x) = H_0\psi_t(x) + U(x)\psi_t(x) + \lambda V(x,t)\psi_t(x), \tag{1.0.5}$$

where U is a static random potential that, at $\lambda = 0$, gives rise to Anderson localization (absence of transport). In this particular case, it was observed that diffusion scaling holds and that the diffusion constant has asymptotic form

$$D \sim C\lambda^2. \tag{1.0.6}$$

Taken together, the results in [23, 27, 33] suggest that solutions to (1.0.5) with a general potential U should satisfy diffusion with a diffusion constant whose asymptotic behavior in the small λ limit is governed by the dynamics of the static Schrödinger operator H_0+U. Here we study this idea in the context of models in the form of Equation (1.0.5). In particular, we shall rigorously study the case where U is *periodic*, which in the $\lambda \to 0$ limit, leads to ballistic motion. In addition, we shall numerically study two special cases of the Anderson model: *the random dimer model* and the *trimmed Anderson model*. In the absence of disorder, the former leads to superdiffusive motion, i.e.,

$$\left\langle X_t^2 \right\rangle \sim t^{\rho}, \qquad \rho > 1, \tag{1.0.7}$$

while the latter leads to subdiffusive motion, i.e.,

$$\left\langle X_t^2 \right\rangle \sim t^\rho, \qquad \rho < 1. \tag{1.0.8}$$

In these three cases we show diffusive propagation for the evolution whenever $\lambda \neq 0$. Furthermore, we obtain an asymptotic relationship between the diffusion constant and the coupling constant.

Remark 1.0.1. In the absence of disorder, all three cases that we consider exhibit anomalous diffusion, i.e.,

$$\left\langle X_t^2 \right\rangle \sim t^\rho \tag{1.0.9}$$

for $\rho \neq 1$. However, whenever discussing anomalous diffusion below we exclude the ballistic (U periodic) case from consideration. △

The remainder of this document is organized as follows: In Chapter 2 we describe the types of systems that we are interested in analyzing and state our main results. Chapter 3 discusses related works and their relation to the problems considered here. Equation (1.0.5) with periodic U is the subject of Chapter 4 and Equation (1.0.5) for the anomalous cases is the subject of Chapter 5. Finally in Chapter 6 we conjecture about diffusive propagation for solutions to Equation (1.0.5) with generic U.

CHAPTER 2

MODELS AND STATEMENT OF MAIN RESULTS

2.0.1 Periodic Potentials

First we consider solutions to Equation (1.0.5) with $\{U(x)\}_{x\in\mathbb{Z}^d}$ a real valued $\mathbf{p}$-periodic potential. Recall that given $\mathbf{p} = (p_j)_{j=1}^d \in \mathbb{Z}_{>0}^d$, a function $U : \mathbb{Z}^d \mapsto \mathbb{R}$ is called $\mathbf{p}$-periodic if

$$U(x + p_j e_j) = U(x) \tag{2.0.1}$$

for all $1 \le j \le d$ and $x \in \mathbb{Z}^d$, where e_j denotes the standard basis of $\mathbb{Z}^d$. Without loss of generality, we assume that $p_j \ge 2$ for some j. Otherwise, U is constant and the problem reduces to that studied in [23]. Throughout this paper, we denote by U the multiplication operator, $(U\psi)(x) = U(x)\psi(x)$ for $\psi(x) \in \ell^2(\mathbb{Z}^d)$.

The analysis below will be applicable to a broad class of operators H_0 and $V(x,t)$. To avoid technicalities in this chapter, let us state the main results in terms of hopping H_0 given by the standard discrete Laplacian on $\mathbb{Z}^d$,

$$(-\Delta\psi)(x) = \sum_{y:\|x-y\|=1} \psi(y), \tag{2.0.2}$$

and potential $V(x,t)$ given by the following so-called Markovian "flip process," which is a non-trivial, and somewhat typical, example of a potential satisfying the general requirements. In general, the random potential is given by $V(x,t) = v_x(\omega(t))$, where $\omega(t)$ is an evolving point in an auxiliary state space Ω. For the flip process, we take the state space $\Omega = \{-1,1\}^{\mathbb{Z}^d}$; and $v_x(\omega) = \omega_x$, the x^{th} coordinate of ω. Thus the potential $V(x,t) = v_x(\omega(t))$ takes only the values ± 1. The process $\omega(t)$ is obtained by putting independent, identical Poisson processes at each site x, and allowing each coordinate ω_x to flip sign at the arrival times $t_1(x) \leq t_2(x) \leq \cdots$ of the Poisson process. Now the general equation (1.0.5) becomes:

$$\mathrm{i}\partial_t \psi_t(x) \;=\; \sum_{y:\|y-x\|=1} \psi_t(y) + U(x)\psi_t(x) + \lambda v_x(\omega(t))\psi_t(x). \tag{2.0.3}$$

Remark 2.0.1. The general assumptions we require of the potential are set out in Section 4.1. They allow for a process $v_x(\omega(t))$ which is correlated from site to site and need not take discrete values. A somewhat typical example satisfying our general assumptions is given by $(x,t) \mapsto v_x(\omega(t))$ such that

1. at any fixed time t, the field $x \mapsto v_x(\omega(t))$ is distributed according to the Gibbs state of a translation-invariant, finite-range lattice Hamiltonian $\mathfrak{h}$ at a temperature T for which there is a unique Gibbs state (the high temperature regime); and

2. the evolution $t \mapsto \{v_x(\omega(t)) | x \in \mathbb{Z}^d\}$ is given by a continuous-time Glauber-type dynamics for $\mathfrak{h}$, preserving the Gibbs state at temperature T.

As long as the lattice Hamiltonian $\mathfrak{h}$ includes terms coupling the field at different sites, the resulting dynamics are correlated from site to site. $\triangle$

A sign of diffusive propagation is the existence of a *diffusion constant* for solutions to Equation (2.0.3),

$$D := \lim_{t\to\infty} \frac{1}{t} \sum_x |x|^2 \mathbb{E}(|\psi_t(x)|^2), \tag{2.0.4}$$

characterized by the relationship $x \sim \sqrt{t}$ in the mean amplitude of evolving wave packets. Here, and throughout this introduction, $\mathbb{E}(\cdot)$ denotes averaging with respect to the Poisson flipping times $t_1(x) \leq t_2(x) \leq \cdots$ and the initial values $\{\omega_x(0)\}_{x\in\mathbb{Z}^d}$, taken independent and uniform in $\{-1, 1\}$.

We will show below that the limit in Equation (2.0.4) exists for any $\mathbf{p}$-periodic potential U and any disorder strength $\lambda > 0$, furthermore we show that $D > 0$. To give an unambiguous definition, one may take the initial value $\psi_0(x) = \delta_{\mathbf{0}}(x)$. However, as we will show, the limit remains the same for any other choice of (normalized) ψ_0 with $\sum_x |x|^2 |\psi_0(x)|^2 < \infty$.

We refer to the existence of a finite, positive diffusion constant as in Equation (2.0.4) as *diffusive scaling*. More generally, we have the following

Theorem 2.0.2 (Central limit theorem)**.** *For any periodic potential U and $\lambda > 0$, there is a positive definite $d \times d$ matrix $\mathbf{D} = \mathbf{D}(\lambda, u)$ such that for any bounded continuous function $f : \mathbb{R}^d \to \mathbb{R}$ and any normalized $\psi_0 \in \ell^2(\mathbb{Z}^d)$ we have*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}^d} f\left(\frac{x}{\sqrt{t}}\right) \mathbb{E}\left(|\psi_t(x)|^2\right) \;=\; \int_{\mathbb{R}^d} f(\mathbf{r}) \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \mathrm{e}^{-\frac{1}{2}\left\langle \mathbf{r},\, \mathbf{D}^{-1}\mathbf{r}\right\rangle} \mathrm{d}\mathbf{r}, \tag{2.0.5}$$

where $\psi_t(x)$ is the solution to Equation (2.0.3) *with initial value ψ_0. If furthermore $\sum_x (1 + |x|^2)|\psi_0(x)|^2 < \infty$, then diffusive scaling, Equation* (2.0.4)*, holds with the diffusion constant*

$$D(\lambda) \;=\; \lim_{t\to\infty} \frac{1}{t} \sum_{x\in\mathbb{Z}^d} |x|^2 \mathbb{E}\left(|\psi_t(x)|^2\right) \;=\; \operatorname{tr} \mathbf{D}(\lambda). \tag{2.0.6}$$

Moreover, Equation (2.0.5) *extends to quadratically bounded continuous f with $\sup_x (1 + |x|^2)^{-1}|f(x)| < \infty$.*

It is well known that if $\lambda = 0$ in (2.0.3), then the free periodic Schrödinger equation has Bloch-wave solutions and exhibits ballistic motion by Floquet theory, see [2, 8]:

$$\lim_{t\to\infty} \frac{1}{t^2} \sum_{x\in\mathbb{Z}^d} |x|^2 \left| \left\langle \delta_x,\ \mathrm{e}^{-\mathrm{i}t(\Delta+U)}\delta_0 \right\rangle \right|^2 \in (0, \infty). \tag{2.0.7}$$

Indeed, *strong ballistic motion* was obtained for $\Delta + U$ in [8]. That is, if X is the position operator and $X(t) = e^{\mathrm{i}t(\Delta+U)} X e^{-\mathrm{i}t(\Delta+U)}$ its Heisenberg evolution, then there exists a bounded, self-adjoint operator Q, with $\ker(Q) = \{0\}$, such that for any ψ in the domain of X,

$$\lim_{t\to\infty} \frac{1}{t} X(t)\psi = Q\psi.$$

If we extend the definition of $D(\lambda)$ in (2.0.6) to $\lambda = 0$, then $D(0) = \infty$. We are primarily interested here in the regime $\lambda \sim 0$, although we will demonstrate diffusion for all $\lambda > 0$. However, for small λ the diffusion constant will be large and has the following asymptotic behavior as $\lambda \to 0$:

Theorem 2.0.3. *Under the hypotheses of Theorem 2.0.2, there is a positive definite $d \times d$ matrix $\mathbf{D}^0$ such that*

$$\mathbf{D}(\lambda) = \frac{1}{\lambda^2}\left(\mathbf{D}^0 + o(1)\right) \quad \text{and} \quad D(\lambda) = \operatorname{tr}\mathbf{D}(\lambda) \;=\; \frac{1}{\lambda^2}\left(\operatorname{tr}\mathbf{D}^0 + o(1)\right) \quad \text{as } \lambda \to 0. \tag{2.0.8}$$

The conclusions of Theorems 2.0.2 and 2.0.3 are true for Equation (1.0.5) under much more general assumptions on the hopping H_0 and the time dependent stochastic potential $V(x,t)$. We will state the general assumptions and results in Section 4.1.

2.0.2 Anomalous Diffusion

Recall that the Anderson model on $\ell^2(\mathbb{Z})$ is given by a Hamiltonian of the form

$$H_\alpha = -\Delta + gU_\alpha, \tag{2.0.9}$$

where $\alpha = \big(\alpha(x)\big)_{x\in\mathbb{Z}} \subset [-1,1]^{\mathbb{Z}}$ is a collection of i.i.d. random variables, $U_\alpha(x) = \alpha(x)$, and $g > 0$. It is known that for *almost every* choice of U and any nonzero value of g the eigenfuctions of (2.0.9) are localized; in particular,

$$\sup_{t\geq 0} \sum_{x\in\mathbb{Z}} |x|^2 |\langle \delta_x, \mathrm{e}^{-\mathrm{i}tH_\alpha}\delta_0\rangle|^2 < \infty. \tag{2.0.10}$$

It follows immediately from (2.0.10) that, over large time scales, any solution to (2.0.9) will have a diffusion constant equal to zero. As mentioned in the introduction, we will be interested in two special cases of (2.0.9): the *random dimer model* and the *trimmed Anderson model*. Both of these cases, which occur with probability zero, exhibit transport properties different than the almost sure case.

The random dimer model is obtained from (2.0.9) by selecting a realization of the random variables $\big(\alpha(x)\big)_{x\in\mathbb{Z}}$ from the set $\{-\varepsilon_a, \varepsilon_b\}^{\mathbb{Z}} \subset [-1,1]^{\mathbb{Z}}$ with the additional requirement that

$$\alpha(2x) = \alpha(2x+1), \tag{2.0.11}$$

for every integer x, see figure 2.1. To simplify notation we will absorb g into the site energies $\varepsilon_a, \varepsilon_b$ and thus allow them to take any real value. Assuming $\psi_0 = \delta_0(x)$, the magnitude of $|\varepsilon_a - \varepsilon_b|$ determines the transport properties of the random dimer model (see figure 2.2):

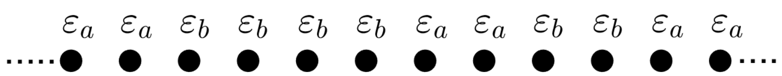

Figure 2.1: A graphical representation of the dimer model potential

1. When $|\varepsilon_a - \varepsilon_b| = 0$, the transport is ballistic.
2. When $0 < |\varepsilon_a - \varepsilon_b| < 2$, the transport is superdiffusive. Specifically,

$$\left\langle X_t^2 \right\rangle \sim t^{3/2}. \tag{2.0.12}$$

3. When $|\varepsilon_a - \varepsilon_b| = 2$, the transport is diffusive.
4. When $|\varepsilon_a - \varepsilon_b| > 2$, the transport is localized.

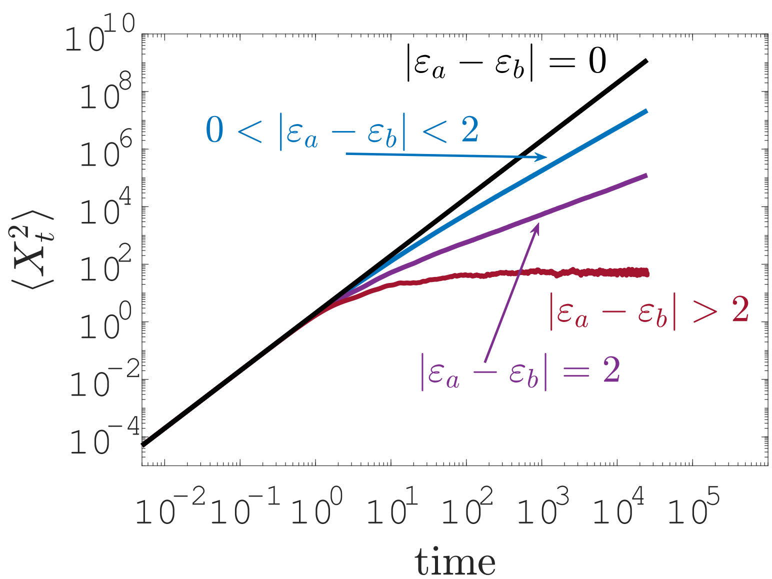

Figure 2.2: The different transport regimes of the random dimer model. The system exhibits ballistic motion when $\Delta\varepsilon = 0$ (black), superdiffusive motion when $0 < \Delta\varepsilon < 2$ (blue), diffusive motion when $\Delta\varepsilon = 2$ (purple), and localization when $\Delta\varepsilon > 2$ (red).

The trimmed Anderson model can be characterized as the Anderson model without a covering condition. Specifically, this means that the potential is only defined on a subset

$\Gamma \subsetneq \mathbb{Z}$,

$$U_\alpha(n) = \begin{cases} \alpha(n), & n \in \Gamma \\ 0, & n \in \Gamma^c \end{cases}. \tag{2.0.13}$$

The transport properties of this model depend on Γ as well as the strength of the coupling g. For example, if

$$\Gamma^c = \bigcup_{j \in J} B_j, \tag{2.0.14}$$

where each B_j is connected, has finite length, and $\text{dist}(B_i, B_j) \geq 3$ for $i \neq j$, then no non-trivial solution can be supported on Γ^c and localization occurs, see [13] and figure 2.3. Presently, we will be interested in the case $\Gamma = 2\mathbb{Z}$. Using the numerical methods outlined in Chapter 5, we find that the solutions to (2.0.9) exhibit subdiffusive propagation, see figure 2.3.

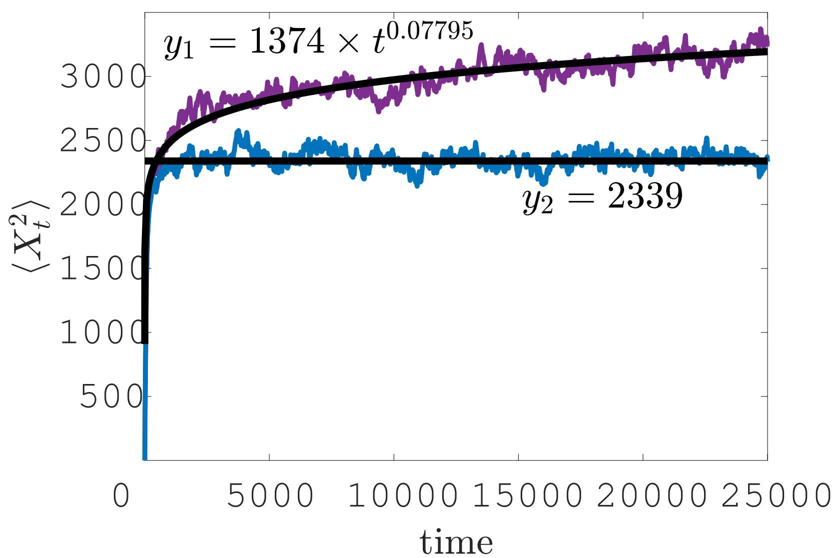

Figure 2.3: Subdiffusive and localized transport in the trimmed Anderson model. The purple line, which corresponds to subdiffusive propagation, is obtained by taking $\Gamma = 2\mathbb{Z}$. The blue line, which corresponds to localization, is obtained by letting $\Gamma = \bigcup_{j \in \mathbb{Z}} B_j$ with $B_j = \{8j, 1 + 8j, 2 + 8j, 3 + 8j\}$.

In Chapter 5, we consider

$$\mathrm{i}\partial_t \psi_t(x) = H_\alpha \psi_t(x) + \lambda v_x(\omega(t))\psi_t(x) \tag{2.0.15}$$

where H_α is given by either the random dimer model or the trimmed Anderson model, and $v_x(\omega(t))$ is the "flip process". We will show numerically that for $\lambda > 0$ these models exhibit diffusive scaling. In particular, we will see that in the small λ limit the diffusion constant scales as

$$D \sim \lambda^{-1}, \tag{2.0.16}$$

for the random dimer model, and as

$$D \sim \lambda^{1.186}, \tag{2.0.17}$$

for the trimmed Anderson model.

CHAPTER 3

HISTORY

3.1 Periodic

A brief history of related studies is as follows: In 1974, Ovchinnikov and Erikman obtained diffusion for a Gaussian Markov ("white noise") potential [29]. This result was generalized by Madhukar and Post [26] to include models with site diagonal and nearest-neighbor off-diagonal disorder. In the 80s, Pillet obtained results on transience of the wave in related models and derived a Feynman-Kac representation [30] which we employ here. Using Pillet's Feynman-Kac formula, Tchermentchansev [36, 37] showed that position moments exhibit diffusive scaling, up to logarithmic corrections for any bounded potential $U(x)$ in (1.0.5):

$$t^{\frac{s}{2}} \frac{1}{(\ln t)^{\nu_-}} \lesssim \sum_x |x|^s \mathbb{E}\left(|\psi_t(x)|^2\right) \lesssim t^{\frac{s}{2}} (\ln t)^{\nu_+}, \quad t \to \infty. \tag{3.1.1}$$

The case $U(x) \equiv 0$ (or equivalently, $\mathbf{p} = (1, \cdots, 1)$) was considered by Schenker in [23], where (3.1.1) was shown to hold for $s = 2$ with $\nu_- = \nu_+ = 0$. Moreover, the central limit theorem (2.0.5) and the asymptotic behavior (2.0.8) were also obtained in [23]. The proof in [23] was revisited by Musselman and Schenker in [27] to obtain diffusive scaling for all position moments of the mean wave amplitude. The models studied in [23] are special cases of those considered here.

For a certain class of random potentials $U(x)$, including the case of an i.i.d. potential, diffusive scaling and the central limit theorem were proven by Schenker in [33]. Moreover, if $H_0 + U$ exhibits Anderson localization, then $O(\lambda^2)$ asymptotics (1.0.6) were proved for the diffusion constant. The arguments in [33] do not require strict independence of the static potential at different sites. However, the *Equivalence of Twisted Shifts* assumption taken in [33] excludes $\mathbf{p}$-periodic background potentials, as well as almost-periodic background potentials. The periodic case falls in an intermediate regime between the period-free case and the i.i.d. case. This is a motivation to revisit the proofs in [23] and [33] and develop the current approach to the $\mathbf{p}$-periodic case, for both diffusive scaling and limiting behavior.

In [17], Fröhlich and Schenker used the techniques of [33] to study diffusion for a lattice particle governed by a Lindblad equation describing jumps in momentum driven by interaction with a heat bath. In some sense, this is the quantum analogue of the classical dynamics of a disordered oscillator system perturbed by noise in the form of a momentum jump process, considered in [3, 4] and reviewed in [5]. A key feature of the noise in [3, 4] is that energy is conserved in the system with noise; this is necessary so that one can speak about heat flux. By contrast, in the present work, and in [23, 27, 33, 17], energy conservation is broken by the noise. Indeed the *only* conserved quantity for the evolution we consider is quantum probability; and it is this quantity which is subject to diffusive transport. (In comparing the present work with results on Markovian limit master equations as in [3, 4, 17], it is useful to note that in the formal derivation of quantum or classical master equations one obtains the square of the coupling to the heat bath multiplying the Lindbladian or stochastic term. Thus it is the square of the coupling λ^2 which should be compared with the coupling constants in [3, 4, 17]. The scaling $\mathbf{D}(\lambda) \sim \mathbf{D}_0\lambda^{-2}$ seen here is consistent with the inverse linear scaling seen in those works.)

That *diffusive* transport emerges from (1.0.5) depends on the fact that it is a lattice, or *tight-binding*, equation. A time-dependent potential coupled with the unbounded kinetic energy present in continuum models can lead to stochastic acceleration resulting in super-diffusive, or even super-ballistic, transport. Stochastic acceleration has been well studied in the context of classical systems, see for example [1, 32, 35]. For quantum systems in the continuum, transport has been studied in the context of Gaussian white-noise potentials [15, 16, 20, 19], for which the super-ballistic transport $\langle x^2 \rangle \sim t^3$ has been proved.

There are also parallel works on diffusion for the continuum Schrödinger equation with Markovian forcing and periodic boundary conditions in space, e.g., [14]. One physical interpretation of this continuous model is as a rigid rotator coupled to a classical heat bath. In

[14], the H^s norm of the wave function is shown to behave as $t^{s/4}$. It is interesting to point out that, as in the present work, the existence of a spectral gap for the Markov generator is essential both for their analysis and the results. In many models with Markovian forcing, the potential $V(x, t)$ is quite rough. However, Bourgain studied the case where $V(x, t)$ is analytic/smooth in x and quasi-periodic/smooth in t. In [6], he showed that energy may grow logarithmically. We refer readers to, e.g., [10, 28, 38], for more work on Sobolev norm growth and controllability of Schrödinger equations with time-dependent potentials.

The proof we present here is a generalization of that in [23]. Some of the arguments are essentially standard fare and parallel the work of [23] closely. However, there are three places in the proof where some substantially new arguments were needed. First, the Fourier analysis (see Section 4.2.2) in our work is more subtle and requires careful consideration due to the periodic potential. The extension developed here is of independent interest and may benefit the future study of the limit-periodic and quasi-periodic cases. Secondly, the spectral gap Lemma 4.3.8 and the proof of the main results in Section 4.4 are technically more involved in the current work. The interaction between the periodic part and the hopping terms complicates the block decomposition on the augmented space. Finally, in the present proof, the analysis of the asymptotic behavior of the diffusion constant is quite a bit more involved. In [23], (1.0.4) essentially follows from a formula derived for the diffusion constant in the midst of the proof of diffusion. Unfortunately, Theorem 2.0.3 in the $\mathbf{p}$-period case does not have such a simple proof and is obtained by a new approach. The proof is based on an interesting observation linking the ballistic motion of the unperturbed part to the diffusive scaling. This observation is part of the motivation behind our conjecture below on the more general situations, linking the transport exponent to the limiting behavior of the diffusion constant.

3.2 Anomalous Diffusion

3.2.1 Dimer Model

The random dimer model was first considered by Dunlap, Phillips, and Wu in [9]. They argue that whenever the two site energies $\varepsilon_a, \varepsilon_b$, satisfy the inequality

$$-1 < \varepsilon_a - \varepsilon_b < 1, \tag{3.2.1}$$

there will be $\sqrt{N}$ eigenstates with localization length of order N. These extended states contribute to transport and have diffusion constant which scales like $t^{1/2}$. This, in turn, implies superdiffusive scaling with $\left\langle X_t^2 \right\rangle \sim t^{3/2}$. Numerical confirmation of this result is provided in the same paper. Bovier [7] confirms this result with the use of invariant measures and perturbation theory. Rigorous confirmation of superdiffusive scaling is given by a lower bound on transport proven by Jitomirskaya, Schulz-Baldes, and Stolz [22], and an upper bound proven by Jitomirskaya and Schulz-Baldes [21].

3.2.2 Trimmed Anderson Model

Three particularly relevant articles on the trimmed Anderson model are [12, 13, 31]. In [31], Rojas-Molina provides Wegner estimates for the trimmed Anderson model and proves dynamical localization at the bottom of the spectrum for strong disorder. Elgart and Klein prove similar results in [12] for the trimmed Anderson model plus an arbitrary bounded background potential. Finally, Elgart and Sodin [13] examine how the strength of the disorder g and the density of the sub-lattice Γ influence transport away from the bottom of the spectrum. Furthermore, [13] explores the possibility of delocalization, in dimension $d \geq 3$, for strong disorder.

CHAPTER 4

RIGOROUS ANALYSIS OF DIFFUSION FOR PERIODIC POTENTIALS

In this chapter we consider the case when U is periodic. In Section 4.1, a more general class of operators is introduced and the main result, Theorem 4.1.11, which generalizes Theorems 2.0.2 and 2.0.3, is formulated. In Section 4.2 the basic analytic tools of "augmented space analysis," developed previously in [23, 33], are reviewed. In Section 4.3, we present the heart of our argument: a block decomposition to study the spectral gap of the induced operator on the augmented space. Section 4.4 is devoted to a proof of the main result. Certain technical results used below are collected in Appendix A.

4.1 General assumptions and statement of the main result

We study a more general class of equations with hopping terms other than nearest neighbor and a perturbing potential V that is not necessarily the "flip process." More precisely, we shall consider equation (1.0.5) in the form

$$\mathrm{i}\partial_t\psi_t(x) = H_0\psi_t(x) + U(x)\psi_t(x) + \lambda V_x(\omega(t))\psi_t(x) \tag{4.1.1}$$

Here U is the real-valued, $\mathbf{p}$-periodic potential as in (2.0.1) for some $\mathbf{p} \in \mathbb{Z}^d_{>0}$; H_0 is a self-adjoint, short-ranged, translation invariant hopping operator with non-zero hopping along a set of vectors that generate $\mathbb{Z}^d$; $V_x(\omega(t))$ is a time-dependent random potential that fluctuates according to a stationary Markov process $\omega(t)$; and $\lambda \geq 0$ is a coupling constant used to set the strength of the disorder. These assumptions will be made precise in the section that follows.

4.1.1 Assumptions

Assumption 4.1.1 (Probability space)**.** Throughout, let (Ω, μ) be a probability space, on which the additive group $\mathbb{Z}^d$ acts through a collection of μ-measure preserving maps. That is, for each $x \in \mathbb{Z}^d$ there is a μ-measure preserving map, $\tau_x : \Omega \to \Omega$, where τ_0 is the identity map and $\tau_x \circ \tau_y = \tau_{x+y}$ for each $x, y \in \mathbb{Z}^d$. We refer to the maps τ_x, $x \in \mathbb{Z}^d$ as "disorder translations."

Assumption 4.1.2 (Markov dynamics)**.** The space Ω is a compact Hausdorff space, μ is a Borel measure and for each $\alpha \in \Omega$ there is a probability measure $\mathbb{P}_\alpha$ on the σ-algebra generated by Borel-cylinder subsets of the path space $\mathcal{P}(\Omega) = \Omega^{[0,\infty)}$. Furthermore, the collection of these measures has the following properties

1. *Right continuity of paths*: For each $\alpha \in \Omega$, with $\mathbb{P}_\alpha$ probability one, every path $t \mapsto \omega(t)$ is right continuous and has initial value $\omega(0) = \alpha$.

2. *Shift invariance in distribution*: For each $\alpha \in \Omega$ and $x \in \mathbb{Z}^d$, $\mathbb{P}_{\tau_x \alpha} = \mathbb{P}_\alpha \circ \mathcal{S}_x^{-1}$, where $\mathcal{S}_x(\{\omega(t)\}_{t \geq 0}) = \{\tau_x \omega(t)\}_{t \geq 0}$ is the shift τ_x lifted to path space $\mathcal{P}(\Omega)$.

3. *Stationary Markov property*: There is a filtration $\{\mathcal{F}_t\}_{t \geq 0}$ on the Borel σ-algebra of $\mathcal{P}(\Omega)$ such that $\omega(t)$ is $\mathcal{F}_t$ measurable and

$$\mathbb{P}_\alpha \left(\{\omega(t+s)\}_{t \geq 0} \in \mathcal{E} \middle| \mathcal{F}_s \right) = \mathbb{P}_{\omega(s)}(\mathcal{E})$$

for any measurable $\mathcal{E} \subset \mathcal{P}(\Omega)$ and any $s > 0$.

4. *Invariance of μ*: For any Borel measurable $E \subset \Omega$ and each $t > 0$,

$$\int_\Omega \mathbb{P}_\alpha(\omega(t) \in E) \, \mu(\mathrm{d}\alpha) \;=\; \mu(E).$$

We use $\mathbb{E}_\alpha(\cdot)$ to denote averaging with respect to $\mathbb{P}_\alpha$ and $\mathbb{E}(\cdot)$ to denote the combined average $\int_\Omega \mathbb{E}_\alpha(\cdot) \, \mu(\mathrm{d}\alpha)$ over the Markov paths and the initial value of the process. Invariance of μ under the dynamics is equivalent to the identity $\mathbb{E}(f(\omega(t))) = \mathbb{E}(f(\omega(0)))$ for $f \in L^1(\Omega)$. An important tool for studying Markov processes is conditioning on the value of a process at a given time. The proper definition can be found in, e.g. [33]. Conditioning on the value of the processes at $t = 0$ determines the initial value: $\mathbb{E}(\cdot | \omega(0) = \alpha) = \mathbb{E}_\alpha(\cdot)$. To the process $\{\omega(t)\}_{t\geq 0}$, there is associated a Markov semigroup, obtained by averaging over the initial value conditioned on the value of the process at later times:

$$S_t f(\alpha) \ := \ \mathbb{E}\left(f(\omega(0))|\omega(t)=\alpha\right).$$

As is well known, S_t is a strongly continuous contraction semi-group on $L^p(\Omega)$ for $1 \leq p < \infty$. The semigroup S_t has a generator

$$Bf \ := \ \lim_{t\downarrow 0} \frac{1}{t}\left(f - S_t f\right), \tag{4.1.2}$$

defined on the domain $\mathcal{D}(B)$ where the right hand side exists in the L^2-norm.[1] By the Lumer-Phillips theorem, B is a *maximally accretive operator.* Note that $S_t\mathbb{1} = \mathbb{1}$ by definition, where $\mathbb{1}(\alpha) = 1$ for all $\alpha \in \Omega$. The invariance of μ under the process $\{\omega(t)\}_{t\geq 0}$ implies further that $S_t^\dagger \mathbb{1} = \mathbb{1}$. It follows that

$$L^2_0(\Omega) \ := \ \left\{ f \in L^2(\Omega) \ \middle| \ \int_\Omega f(\alpha)\mu(\mathrm{d}\alpha) \ = \ 0 \right\}$$

is invariant under the semi-group S_t and its adjoint $S_t^\dagger$. We assume that B is sectorial and strictly dissipative on $L^2_0(\Omega)$.

Assumption 4.1.3 (*Sectoriality of B*)**.** There are $b, \gamma \geq 0$ such that

$$|\mathrm{Im}\,\langle f,\ Bf\rangle| \ \leq \ \gamma\,\mathrm{Re}\,\langle f,\ Bf\rangle + b\|f\|^2 \tag{4.1.3}$$

for all $f \in \mathcal{D}(B)$. Here $\langle f,\ g\rangle = \int \overline{f} g \mathrm{d}\mu$ denotes the inner product on $L^2(\Omega)$.

Assumption 4.1.4 (*Gap condition for B*)**.** There is $T > 0$ such that

$$\mathrm{Re}\,\langle f,\ Bf\rangle \ \geq \ \frac{1}{T}\left\| f - \int_\Omega f \mathrm{d}\mu \right\|^2_{L^2(\Omega)} \tag{4.1.4}$$

for all $f \in \mathcal{D}(B)$.

[1] Note Equation (4.1.2) defines a generator with positive real part; while, it is common in probability theory to define a generator with negative real part.

Remark 4.1.5. 1) Given the generator B we formally write the semigroup S_t as e^{-tB}. 2) The *resolvent* of the semigroup e^{-tB} is the operator valued analytic function $R(z) := (B-z)^{-1} = \int_0^\infty \mathrm{e}^{tz}\mathrm{e}^{-tB}\mathrm{d}t$, which is defined and satisfies $\|R(z)\| \le \frac{1}{|\mathrm{Re}\, z|}$ when $\mathrm{Re}\, z < 0$. Sectoriality is equivalent to the existence of a analytic continuation of $R(z)$ to $z \in \mathbb{C} \setminus K_{b,\gamma}$ with the bound $\|R(z)\| \le \mathrm{dist}^{-1}(z, K_{b,\gamma})$ where $K_{b,\gamma}$ is the sector $\{\mathrm{Re}\, z \ge 0\} \cap \{|\mathrm{Im}\, z| \le b + \gamma|\mathrm{Re}\, z|\}$ (see [24, Theorem V.3.2]). In particular Assumption 4.1.3 holds (with $b = 0$ and $\gamma = 0$) if the Markov dynamics is reversible, in which case B is self-adjoint. 3) The gap assumption implies that the restriction of B to $L^2_0(\Omega)$ is strictly accretive, and thus that $\left\| S_t|_{L^2_0(\Omega)} \right\| \le \mathrm{e}^{-\frac{t}{T}}$. △

Assumption 4.1.6 (Translation covariance, boundedness and non-degeneracy of the potential)**.** The potentials $V_x(\omega)$ appearing in the Schrödinger equation (4.1.1) are given by $V_x(\omega) = v(\tau_x\omega)$ where $v \in L^\infty(\Omega)$. We assume that $\|v\|_\infty = 1$, $\int_\Omega v(\omega)\mu(\mathrm{d}\omega) = 0$, and v is non-degenerate in the sense that there is $\chi > 0$ such that

$$\left\| B^{-1}(v(\tau_x \cdot) - v(\tau_y \cdot)) \right\|_{L^2(\Omega)} \ge \chi \tag{4.1.5}$$

for all $x, y \in \mathbb{Z}^d$, $x \ne y$.

Remark 4.1.7. Since the Markov process is translation invariant, B commutes with the translations $T_x f(\alpha) = f(\tau_x\alpha)$ of $L^2(\Omega)$. Thus (4.1.5) is equivalent to

$$\left\| B^{-1}(v(\tau_x \cdot) - v(\cdot)) \right\|_{L^2(\Omega)} \ge \chi. \tag{4.1.6}$$

for all $x \in \mathbb{Z}^d$, $x \ne \mathbf{0}$. The non-degeneracy essentially amounts to requiring that $B^{-1}(v\tau_x)$ are uniformly non-parallel to $B^{-1}(v)$ for $x \ne 0$. In particular, the condition is trivially satisfied if for example if the processes $v(\tau_x\omega(t))$ and $v(\omega(t))$ are independent for $x \ne 0$, as in the "flip process". △

Assumption 4.1.8 (Translation invariance and non-degeneracy of the hopping terms)**.** The hopping operator, H_0, on $\ell^2(\mathbb{Z}^d)$ is defined by

$$H_0\psi(x) = \sum_{\xi \ne x} h(x - \xi)\psi(\xi). \tag{4.1.7}$$

Additionally, the hopping kernel $h : \mathbb{Z}^d \setminus \{\mathbf{0}\} \to \mathbb{C}$ is

1. Self-adjoint:
$$h(-\xi) = \overline{h(\xi)};$$

2. Short range:
$$\sum_{\xi \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} |\xi|^2 |h(\xi)| < \infty; \tag{4.1.8}$$

3. Non-degenerate:
$$\operatorname{span}_{\mathbb{Z}} (\operatorname{supp} h) = \mathbb{Z}^d, \tag{4.1.9}$$

   where $\operatorname{supp} h = \left\{ \xi \in \mathbb{Z}^d : \ h(\xi) \neq 0 \right\}$.

Remark 4.1.9. 1) It follows from (1) and (2) that $\widehat{h}(\mathbf{k}) = \sum_x \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot x} h(x)$ is a real-valued C^2 function on the torus $[0, 2\pi)^d$. In particular, H_0 is a bounded self-adjoint operator with $\|H_0\|_{\ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{Z}^d)} = \max_{\mathbf{k}} |\widehat{h}(\mathbf{k})|$ and

$$\|\widehat{h}\|_\infty, \|\widehat{h}'\|_\infty, \|\widehat{h}''\|_\infty \leq \sum_{\xi \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} (1 + |\xi|^2) |h(\xi)| < \infty. \tag{4.1.10}$$

2) It is natural to assume that $\operatorname{supp} h$ can generate the entire $\mathbb{Z}^d$ lattice, otherwise the system can always be reduced a direct sum of systems over several sub-lattices. △

Below we will need the following simple consequence of the non-degeneracy of h:

Proposition 4.1.10. *For each non-zero* $\mathbf{k} \in \mathbb{R}^d$,

$$\sum_{\xi \in \mathbb{Z}^d} |\mathbf{k} \cdot \xi|^2 |h(\xi)|^2 > 0. \tag{4.1.11}$$

Proof. Suppose on the contrary that $\sum_{\xi \in \mathbb{Z}^d} |\mathbf{k} \cdot \xi|^2 |h(\xi)|^2 = 0$ for some $\mathbf{k} \neq \mathbf{0}$. It follows that $\mathbf{k} \cdot \xi = 0$ for all $\xi \in \operatorname{supp} h$, violating the non-degeneracy of h. □

4.1.2 General result

The main result is the following

Theorem 4.1.11 (Central limit theorem)**.** *For any periodic potential U and $\lambda > 0$, there is a positive definite $d \times d$ matrix $\mathbf{D} = \mathbf{D}(\lambda, U)$ such that for any bounded continuous function $f : \mathbb{R}^d \to \mathbb{R}$ and any normalized $\psi_0 \in \ell^2(\mathbb{Z}^d)$ we have*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}^d} f\left(\frac{x}{\sqrt{t}}\right) \mathbb{E}\left(|\psi_t(x)|^2\right) \;=\; \int_{\mathbb{R}^d} f(\mathbf{r}) \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \mathrm{e}^{-\frac{1}{2}\left\langle \mathbf{r},\, \mathbf{D}^{-1}\mathbf{r}\right\rangle} \mathrm{d}\mathbf{r}, \tag{4.1.12}$$

where $\psi_t(x)$ is the solution to Equation (4.1.1)*. If furthermore $\sum_x (1 + |x|^2)|\psi_0(x)|^2 < \infty$, then diffusive scaling Equation* (2.0.4) *holds with the diffusion constant*

$$D(\lambda) \;=\; \lim_{t\to\infty} \frac{1}{t} \sum_{x\in\mathbb{Z}^d} |x|^2 \mathbb{E}\left(|\psi_t(x)|^2\right) \;=\; \operatorname{tr} \mathbf{D}(\lambda). \tag{4.1.13}$$

Moreover, Equation (4.1.12) *extends to quadratically bounded continuous f with* $\sup_x (1 + |x|^2)^{-1}|f(x)| < \infty$.

Assume further that

$$\lim_{T\to\infty} \frac{2}{T^3} \int_0^\infty \mathrm{e}^{-\frac{2t}{T}} \sum_{x\in\mathbb{Z}^d} x_j^2 \left|\left\langle \delta_x,\ \mathrm{e}^{-\mathrm{i}t(H_0+U)}\delta_0 \right\rangle\right|^2 \mathrm{d}t > 0, \quad j = 1\cdots, d, \tag{4.1.14}$$

then there is a positive definite $d \times d$ matrix $\mathbf{D}^0$ such that

$$\mathbf{D}(\lambda) = \frac{1}{\lambda^2}\left(\mathbf{D}^0 + o(1)\right) \quad \text{and} \quad D(\lambda) = \operatorname{tr} \mathbf{D}(\lambda) \;=\; \frac{1}{\lambda^2}\left(\operatorname{tr} \mathbf{D}^0 + o(1)\right) \quad \textit{as } \lambda \to 0. \tag{4.1.15}$$

Remark 4.1.12. 1) In the case with the short range hopping H_0 and periodic U, the strong limit of all the j-th velocity operators $\lim_t t^{-1} X_j(\psi_t)$ always exist, which implies the existence of the limit in (4.1.14). We say $H_0 + U$ has ballistic motion if the limit in (4.1.14) is positive. 2) $\delta_{\mathbf{0}}$ in (4.1.14) can be replaced by any ψ_0 with compact support. 3) There always exists a *semi*-positive definite $d \times d$ matrix $\mathbf{D}^0$ such that (4.1.15) holds regardless of (4.1.14). If (4.1.14) is true for $j \in S$ with $S \subset \{1, 2, \cdots, d\}$, then the restriction of $\mathbf{D}^0$ on $S \times S$ is positive definite, and we still have $D(\lambda) \sim \lambda^{-2}$ since $\operatorname{tr} \mathbf{D}^0 > 0$. △

4.2 Augmented space analysis

4.2.1 The Markov semigroup on augmented spaces and the Pillet-Feynman-Kac formula

As in the works [23, 33], our analysis of the Schrödinger equation, Equation (4.1.1), is based on a formula of Pillet [30] for $\mathbb{E}(\rho_t)$, where $\rho_t(x, y) = \psi_t(x)\overline{\psi_t(y)}$ is the density matrix corresponding to a solution ψ_t to Equation (4.1.1). Pillet's formula relates $\mathbb{E}(\rho_t)$ to matrix elements of a contraction semi-group on the "augmented space"

$$\mathcal{H} := L^2(\Omega; \mathcal{H}S(\mathbb{Z}^d)), \tag{4.2.1}$$

where $\mathcal{H}S(\mathbb{Z}^d)$ denotes the Hilbert-Schmidt ideal in the bounded operators on $\ell^2(\mathbb{Z}^d)$.

The term "augmented space" refers to a space of functions obtained by "augmenting" functions defined on $X = \mathbb{Z}^d$ or $X = \mathbb{Z}^d \times \mathbb{Z}^d$ by allowing dependence on the disorder $\omega \in \Omega$. More specifically, it refers to spaces of the form

Definition 4.2.1 (Definition 3.1 of [33])**.** Let $(\mathcal{B}(X), \|\cdot\|_{\mathcal{B}(X)})$ be a Banach space of functions on X whose norm satisfies

1. If $g \in \mathcal{B}(X)$ and $0 \le |f(x)| \le |g(x)|$ for every $x \in X$, then $f \in \mathcal{B}(X)$ and $\|f\|_{\mathcal{B}(X)} \le \|g\|_{\mathcal{B}(X)}$.

2. For every $x \in X$, the evaluation $x \mapsto f(x)$ is a continuous linear functional on $\mathcal{B}(X)$.

For $p \ge 1$, the **augmented space** $\mathcal{B}^p(X \times \Omega)$ is the set of maps $F : X \times \Omega \to \mathbb{C}$ such that $x \to \|F(x, \cdot)\|_{L^p(\Omega)} \in \mathcal{B}(X)$.

A general theory of such spaces is developed in [33]. In particular, it is shown there that $\mathcal{B}^p(X \times \Omega)$ is a Banach space under the norm

$$\|F\|_{\mathcal{B}^p(X\times\Omega)} := \left\| \left(\int_\Omega |F(x, \omega)|^p \, \mu(d\omega) \right)^{\frac{1}{p}} \right\|_{\mathcal{B}(X)},$$

with $\|F\|_{\mathcal{B}^p(X\times\Omega)} \le \left(\int_\Omega \|F(\cdot,\omega)\|^p \mu(\mathrm{d}x)\right)^{\frac{1}{p}}$ [33, Prop. 3.1]. It follows that $L^p(\Omega;\mathcal{B}) \subset \mathcal{B}^p(X\times\Omega)$, although in general equality may not hold. For $\mathcal{B}(X) = \ell^p(X)$ and $1 \le q \le \infty$, we denote $\mathcal{B}^q(X)$ by $\ell^{p;q}(X)$. Then, for $1 \le p < \infty$,

$$\ell^{p;p}(X\times\Omega) = L^p(\Omega;\ell^p(X)) = L^p(X\times\Omega),$$

where we take the product measure Counting Measure $\times\ \mu$ on $X\times\Omega$ [33, Prop 3.2]. In particular, $\ell^{2;2}(X\times\Omega)$ is a Hilbert space with inner product

$$\langle F,\ G\rangle \;=\; \sum_{x\in X}\int_\Omega \overline{F(x,\omega)}G(x,\omega)\mu(\mathrm{d}\omega).$$

Another space that will play an important role below is $\ell^{\infty;1}(X\times\Omega)$ which is the space of maps with

$$\|F\|_{\ell^{\infty;1}} \;:=\; \sup_{x\in X}\int_\Omega |F(x,\omega)|\mu(\mathrm{d}\omega) \;<\; \infty.$$

Returning now to $\mathcal{H} = L^2(\Omega;\mathcal{HS}(\mathbb{Z}^d))$, we note that we may think of an element $F\in\mathcal{H}$ as a $\mathbb{C}$-valued map on

$$M \;:=\; \mathbb{Z}^d\times\mathbb{Z}^d\times\Omega, \tag{4.2.2}$$

via the identification

$$F(x,y,\omega) \;:=\; \langle\delta_x, F(\omega)\delta_y\rangle. \tag{4.2.3}$$

It follows from [33, Prop. 3.2] that

$$\mathcal{H} \;=\; \ell^{2;2}(\mathbb{Z}^d\times\mathbb{Z}^d\times\Omega) \;=\; L^2(M),$$

provided M is given the product measure $m = \Big(\text{counting measure on } \mathbb{Z}^d\times\mathbb{Z}^d\Big)\times\mu$.

We define operators $\mathcal{K}$, $\mathcal{U}$ and $\mathcal{V}$ that lift the commutators with H_0, U and V_ω to $\mathcal{H}$:

$$\mathcal{K}F(\omega) \;:=\; [H_0, F(\omega)]\,,\quad \mathcal{U}F(\omega) \;:=\; [U, F(\omega)]\,,$$
$$\text{and}\quad \mathcal{V}F(\omega) \;:=\; [V_\omega, F(\omega)]\,. \tag{4.2.4}$$

The following proposition follows immediately from Equation (4.2.4).

Proposition 4.2.2. *The operators $\mathcal{K}$, $\mathcal{U}$ and $\mathcal{V}$ are self-adjoint, bounded and are given by the following explicit expressions*

$$\mathcal{K}F(x,y,\omega) \;=\; \sum_{\xi\neq\mathbf{0}} h(\xi)\left[F(x-\xi,y,\omega)-F(x,y-\xi,\omega)\right], \tag{4.2.5}$$

$$\mathcal{U}F(x,y,\omega) \;=\; \left[U(x)-U(y)\right]F(x,y,\omega) \tag{4.2.6}$$

and

$$\mathcal{V}F(x,y,\omega) \;=\; \left[v(\tau_x\omega)-v(\tau_y\omega)\right]F(x,y,\omega), \tag{4.2.7}$$

for any $F \in L^2(M)$.

The final ingredient for Pillet's formula is the lift of the Markov generator B to $L^2(M)$. Throughout, we will use e^{-tB} to denote the Markov semigroup lifted to the augmented space $\mathcal{B}^p(X\times\Omega)$, with B the corresponding generator. This semigroup is defined by

$$\mathrm{e}^{-tB}F(x,\alpha) \;:=\; \mathbb{E}_\Omega\left(F(x,\omega(0))\,|\,\omega(t)=\alpha\right). \tag{4.2.8}$$

In particular, given $\phi\in\mathcal{B}(X)$ and $f\in L^p(\Omega)$ we have

$$\mathrm{e}^{-tB}(\phi\otimes f) \;=\; \phi\otimes\mathrm{e}^{-tB}f,$$

where $\phi\otimes f$ denotes the function

$$(\phi\otimes f)(x,\omega) := \phi(x)f(\omega).$$

Proposition 4.2.3 (Prop. 3.3 of [33]). *The semigroup e^{-tB} is contractive and positivity preserving on $\mathcal{B}^p(X\times\Omega)$ and B is sectorial on $L^2(X\times\Omega)$, with the same constants b and γ as appear in Assumption 4.1.3.*

Pillet's formula expresses the average of the time dependent dynamics (2.0.3) in terms of the semi-group on $L^2(M)$ generated by $\mathcal{L} = \mathrm{i}\mathcal{K}+\mathrm{i}\mathcal{U}+\mathrm{i}\lambda\mathcal{V}+B$.

Lemma 4.2.4 (Pillet's formula [30]). *Let*

$$\mathcal{L} \;:=\; \mathrm{i}\mathcal{K}+\mathrm{i}\mathcal{U}+\mathrm{i}\lambda\mathcal{V}+B \tag{4.2.9}$$

on the domain $\mathcal{D}(B) \subset L^2(M)$. Then $\mathcal{L}$ is maximally accretive and sectorial and if $\rho_t = \psi_t \langle \psi_t, \cdot \rangle$ is the density matrix corresponding to a solution ψ_t to Equation (4.1.1) *with $\psi_0 \in \ell^2(\mathbb{Z}^d)$, then*

$$\mathbb{E}\left(\rho_t | \omega(t) = \alpha\right) = [\mathrm{e}^{-t\mathcal{L}}(\rho_0 \otimes \mathbb{1})](\alpha), \tag{4.2.10}$$

where $\mathbb{1}(\alpha) = 1$ for all α. Consequently, we have

$$\mathbb{E}\left(\rho_t\right) = \int_\Omega \left[\mathrm{e}^{-t\mathcal{L}}(\rho_0 \times \mathbb{1})\right](\omega)\mu(\mathrm{d}\omega). \tag{4.2.11}$$

Furthermore, for a solution ψ_t to Equation (4.1.1)*, we have*

$$\mathbb{E}\left(\psi_t(x)\overline{\psi_t(y)}\right) = \left\langle \delta_x \otimes \delta_y \otimes \mathbb{1},\ \mathrm{e}^{-t\mathcal{L}}\left(\psi_0 \otimes \overline{\psi_0} \otimes \mathbb{1}\right)\right\rangle_{L^2(M)}. \tag{4.2.12}$$

In particular, we have

$$\mathbb{E}\left(\rho_t(x,x)\right) = \left\langle \delta_x \otimes \delta_x \otimes \mathbb{1}, \mathrm{e}^{-t\mathcal{L}}\rho_0 \otimes \mathbb{1} \middle| \delta_x \otimes \delta_x \otimes \mathbb{1}, \mathrm{e}^{-t\mathcal{L}}\rho_0 \otimes \mathbb{1}\right\rangle_{\mathcal{H}}. \tag{4.2.13}$$

Remark 4.2.5. Here and below we will use tensor product notation for elements of $\ell^2(\mathbb{Z}^d \times \mathbb{Z}^d)$,

$$[\phi \otimes \psi](x,y) = \phi(x)\psi(y).$$

Thus a rank one operator $\psi \langle \phi, \cdot \rangle \in \mathcal{HS}(\mathbb{Z}^d)$ corresponds to $\psi \otimes \overline{\phi}$. △

For the derivation of this result, we refer the reader to [33, Lemmas. 3.5 and 3.6]. In [33], the term $\mathcal{U}$ is different, stemming as it does there from the background static random potential. However, an essentially identical proof works in the present context.

4.2.2 Vector valued Fourier Analysis

For each $\xi \in \mathbb{Z}^d$, we define the (simultaneous position and disorder) shift operator

$$S_\xi \Psi(x,y,\omega) := \Psi(x - \xi, y - \xi, \tau_\xi \omega) \tag{4.2.14}$$

for any function Ψ defined on $\mathbb{Z}^d \times \mathbb{Z}^d \times \Omega$.

Proposition 4.2.6. *The map $\xi \mapsto S_\xi$ is a unitary representation of the additive group $\mathbb{Z}^d$ on the Hilbert space $\mathcal{H}$, and for every $\xi \in \mathbb{Z}^d$*

$$\left[S_\xi, \mathcal{K}\right] \;=\; \left[S_\xi, \mathcal{V}\right] \;=\; \left[S_\xi, B\right] \;=\; 0.$$

The potential term $\mathcal{U}$ only commutes with a subgroup of translations S_ξ, corresponding to translation over a period of the potential. For $\xi \in \mathbb{Z}^d$ let

$$\mathbf{p} \circ \xi \;:=\; (p_1\xi_1, \ldots, p_d\xi_d) \tag{4.2.15}$$

and

$$\mathbf{p}\mathbb{Z}^d = \{\mathbf{p} \circ \xi : \; \xi \in \mathbb{Z}^d\}. \tag{4.2.16}$$

Then

Proposition 4.2.7. *For every $\xi \in \mathbb{Z}^d$, $\left[S_{\mathbf{p}\circ\xi}, \mathcal{U}\right] = 0$.*

Because of Props. 4.2.6, 4.2.7, a suitable Floquet transform will give a fibre decomposition of the various operators $\mathcal{K}$, $\mathcal{U}$, $\mathcal{V}$ and B. Let $\mathbb{T}^d = [0, 2\pi)^d$ denote the torus,

$$\widehat{M} \;:=\; \mathbb{Z}^d \times \Omega,$$

and let $\mathbb{Z}_{\mathbf{p}} = \mathbb{Z}_{p_1} \times \cdots \times \mathbb{Z}_{p_d}$ denote the fundamental cell of the periodicity group on $\mathbb{Z}^d$. Note that $\ell^2(\mathbb{Z}_{\mathbf{p}}) \cong \mathbb{C}^{\otimes\mathbf{p}} := \mathbb{C}^{p_1} \otimes \cdots \otimes \mathbb{C}^{p_d}$. Using this identification, let $\pi_\sigma : \mathbb{C}^{\otimes\mathbf{p}} \to \mathbb{C}$ be the coordinate evaluation map associated to a point $\sigma = (\sigma_1, \cdots, \sigma_d) \in \mathbb{Z}_{\mathbf{p}}$. For $f, g \in L^2(\widehat{M}; \mathbb{C}^{\otimes\mathbf{p}})$, we use the natural inner product on $L^2(\widehat{M}; \mathbb{C}^{\otimes\mathbf{p}})$

$$\langle f, \; g\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} = \sum_{\sigma\in\mathbb{Z}_{\mathbf{p}}} \langle \pi_\sigma f, \; \pi_\sigma g\rangle_{L^2(\widehat{M};\mathbb{C})} \,. \tag{4.2.17}$$

Given $\Psi \in L^2(M)$ and $\mathbf{k} \in \mathbb{T}^d$, the *Floquet transform of* $\Psi \in L^2(M)$ *at* $\mathbf{k}$ is defined to be a map $\widehat{\Psi}_{\mathbf{k}} : \widehat{M} \to \mathbb{C}^{\otimes\mathbf{p}}$ as follows:

$$\begin{aligned} \pi_\sigma \widehat{\Psi}_{\mathbf{k}}(x, \omega) &:= \sum_{\xi\in\mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}\,\mathbf{k}\cdot(\mathbf{p}\circ\xi+\sigma)}\, S_{\mathbf{p}\circ\xi+\sigma}\Psi(x, 0, \omega) \\ &= \sum_{n\in\mathbf{p}\mathbb{Z}^d+\sigma} \mathrm{e}^{-\mathrm{i}\,\mathbf{k}\cdot n}\, \Psi(x - n, -n, \tau_n\omega), \end{aligned} \tag{4.2.18}$$

for each $\sigma \in \mathbb{Z}_{\mathbf{p}}$. Initially we define this Floquet transform on the augmented space

$$\mathcal{W}^1(M) \ := \ \left\{ F : M \to \mathbb{C} \ \middle| \ \sup_x \sum_y \int |F(x+y, y, \omega)| \mu(\mathrm{d}\omega) < \infty \right\}. \tag{4.2.19}$$

The basic results of Fourier analysis are naturally extended to this Floquet transform. In particular, if $F \in \mathcal{W}^1(M)$, then $\widehat{F}_{\mathbf{k}} \in \ell^{\infty;1}(\widehat{M})$ for each $\mathbf{k}$ and $\mathbf{k} \mapsto \widehat{F}_{\mathbf{k}}$ is continuous. Furthermore, Plancherel's Theorem,

$$\|F\|^2_{L^2(M)} \ = \ \int_{\mathbb{T}^d} \|\widehat{F}_{\mathbf{k}}\|^2_{L^2(\widehat{M})} \nu(\mathrm{d}\mathbf{k}),$$

holds for $F \in \mathcal{W}^1(M) \bigcap L^2(M)$, where ν denotes normalized Lebesgue measure on the torus $\mathbb{T}^d$. Thus, the Floquet transform extends naturally to $L^2(M)$. Throughout the rest of the paper, we assume that the Floquet transform is properly defined on $L^2(M)$. For more details of this extension in a similar context, we refer readers to Section 3 in [33].

One may easily compute

$$\begin{aligned}
\pi_\sigma \left(\widehat{\mathcal{K}\Psi}\right)_{\mathbf{k}}(x, \omega) &= \sum_{\xi \neq \mathbf{0}} h(\xi) \left[\pi_\sigma \widehat{\Psi}_{\mathbf{k}}(x - \xi, \omega) - \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\xi} \pi_{\sigma-\xi} \widehat{\Psi}_{\mathbf{k}}(x - \xi, \tau_\xi \omega) \right]; \\
\pi_\sigma \left(\widehat{\mathcal{U}\Psi}\right)_{\mathbf{k}}(x, \omega) &= \left(u(x - \sigma) - u(-\sigma)\right) \pi_\sigma \, \widehat{\Psi}_{\mathbf{k}}(x, \omega); \\
\pi_\sigma \left(\widehat{\mathcal{V}\Psi}\right)_{\mathbf{k}}(x, \omega) &= \left(v(\tau_x \omega) - v(\omega)\right) \pi_\sigma \, \widehat{\Psi}_{\mathbf{k}}(x, \omega); \\
\pi_\sigma \left(\widehat{B\Psi}\right)_{\mathbf{k}}(x, \omega) &= B \, \pi_\sigma \, \widehat{\Psi}_{\mathbf{k}}(x, \omega),
\end{aligned}$$

where on the right hand side, B acts on $\pi_\sigma \widehat{\Psi}_{\mathbf{k}}$ as in Equation (4.2.8). With the above computations in mind, let $\widehat{\mathcal{K}}_{\mathbf{k}}$, $\widehat{\mathcal{U}}$, and $\widehat{\mathcal{V}}$ denote the following operators on functions $\phi : \widehat{M} \to \mathbb{C}^{\otimes \mathbf{p}}$:

$$\pi_\sigma(\widehat{\mathcal{K}}_{\mathbf{k}} \, \phi) \, (x, \omega) = \sum_{\xi \neq \mathbf{0}} h(\xi) \left[\pi_\sigma \phi(x - \xi, \omega) - \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\xi} \pi_{\sigma-\xi} \phi(x - \xi, \tau_\xi \omega) \right]; \tag{4.2.20}$$

$$\pi_\sigma \, (\widehat{\mathcal{U}} \, \phi)(x, \omega) = \left(u(x - \sigma) - u(-\sigma)\right) \pi_\sigma \phi(x, \omega); \tag{4.2.21}$$

and

$$(\widehat{\mathcal{V}} \phi)(x, \omega) = \left(v(\tau_x \omega) - v(\omega)\right) \ \phi(x, \omega). \tag{4.2.22}$$

We now present three lemmas (Lemmas 4.2.8-4.2.12), which describe the basic properties of the operators $\widehat{\mathcal{K}}_{\mathbf{k}}$, $\widehat{\mathcal{U}}$, and $\widehat{\mathcal{V}}$. These results are the adaptation to the present context of Lemmas 3.13-3.15 of [33], with the main difference being that here we consider the vector valued space $L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$ instead of $L^2(\widehat{M};\mathbb{C})$. We omit the details of the proofs here.

Lemma 4.2.8. *Let $\widehat{M}=\mathbb{Z}^d\times\Omega, \widehat{\mathcal{K}}_{\mathbf{k}}$, $\widehat{\mathcal{U}}$ and $\widehat{\mathcal{V}}$ be given as above, then*

1. *$\widehat{\mathcal{K}}_{\mathbf{k}}$, $\widehat{\mathcal{U}}$ and $\widehat{\mathcal{V}}$ are bounded on $\ell^{\infty;1}(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$.*

2. *$\widehat{\mathcal{K}}_{\mathbf{k}}$, $\widehat{\mathcal{U}}$ and $\widehat{\mathcal{V}}$ are bounded and self-adjoint on $L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$ with the following bounds:*

$$\left\|\widehat{\mathcal{K}}_{\mathbf{k}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})}\leq 2\|\widehat{h}\|_\infty,\quad \left\|\widehat{\mathcal{U}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})}\leq 2\|u\|_\infty,\quad \left\|\widehat{\mathcal{V}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})}\leq 2$$

3. *If $\Psi\in L^2(M;\mathbb{C})$ and let $\widehat{\Psi}_{\mathbf{k}}$ be given as in (4.2.18), then*

$$\widehat{(\mathcal{K}\Psi)}_{\mathbf{k}} \;=\; \widehat{\mathcal{K}}_{\mathbf{k}}\widehat{\Psi}_{\mathbf{k}},\quad \widehat{(\mathcal{U}\Psi)}_{\mathbf{k}} \;=\; \widehat{\mathcal{U}}\,\widehat{\Psi}_{\mathbf{k}}\quad \textit{and}\quad \widehat{(\mathcal{V}\Psi)}_{\mathbf{k}} \;=\; \widehat{\mathcal{V}}\,\widehat{\Psi}_{\mathbf{k}}$$

   for ν-almost every $\mathbf{k}\in\mathbb{T}^d$.

Because the Markov process has a distribution invariant under the shifts, the Markov semigroup commutes with Floquet transform:

Lemma 4.2.9 (Lemma 3.14,[33])**.** *Let the Markov semigroup e^{-tB} be defined as in Equation* (4.2.8)*. Then,*

$$\left[\widehat{\mathrm{e}^{-tB}\Psi}\right]_{\mathbf{k}} \;=\; \mathrm{e}^{-tB}\widehat{\Psi}_{\mathbf{k}}$$

for $\Psi\in L^2(M)$ and ν-almost every $\mathbf{k}\in\mathbb{T}^d$.

Lemma 4.2.10. *Let $\widehat{\mathcal{K}}_{\mathbf{k}}$ be given as in* (4.2.20) *with h that satisfies* (4.1.8)*. Then the map $\mathbf{k}\mapsto\widehat{\mathcal{K}}_{\mathbf{k}}$ is C^2 on $\mathbb{T}^d$, considered either as a map into the bounded operators on $\ell^{\infty;1}(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$ or as a map into the bounded operators on $L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$.*

Moreover, we have the explicit expression for the derivatives for any $\phi(x,\omega)\in L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$, $\mathbf{k}\in\mathbb{T}^d$ and $1\leq i,j\leq d$:

$$\pi_\sigma\partial_{k_j}\widehat{\mathcal{K}}_{\mathbf{k}}\phi(x,\omega)=\mathrm{i}\sum_{\xi\neq\mathbf{0}}\xi_j\,h(\xi)\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\xi}\pi_{\sigma-\xi}\phi(x-\xi,\tau_\xi\omega), \tag{4.2.23}$$

$$\pi_\sigma \partial_{k_i}\partial_{k_j}\widehat{\mathcal{K}}_{\mathbf{k}}\phi(x,\omega) = \sum_{\xi\neq\mathbf{0}} \xi_i\,\xi_j\,h(\xi)\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\xi}\pi_{\sigma-\xi}\phi(x-\xi,\tau_\xi\omega). \tag{4.2.24}$$

with bounds

$$\left\|\partial_{k_j}\widehat{\mathcal{K}}_{\mathbf{k}}\right\| \leq \|\widehat{h}'\|_\infty, \quad \left\|\partial_{k_i}\partial_{k_j}\widehat{\mathcal{K}}_{\mathbf{k}}\right\| \leq \|\widehat{h}''\|_\infty, \tag{4.2.25}$$

where $\|\widehat{h}'\|_\infty, \|\widehat{h}''\|_\infty$ *are bounded in* (4.1.10).

In particular, let $\overrightarrow{1} \in \mathbb{C}^{\otimes\mathbf{p}}$ *be the vector with* $\pi_\sigma\overrightarrow{1} = 1$ *for all* $\sigma \in \mathbb{Z}_{\mathbf{p}}$*. Then*

$$\partial_{k_j}\widehat{\mathcal{K}}_{\mathbf{0}}\,\delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1} = \mathrm{i}\sum_{\xi\neq\mathbf{0}} \xi_j\,h(\xi)\,\delta_\xi \otimes \overrightarrow{1} \otimes \mathbb{1}, \tag{4.2.26}$$

$$\partial_{k_i}\partial_{k_j}\widehat{\mathcal{K}}_{\mathbf{0}}\,\delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1} = \sum_{\xi\neq\mathbf{0}} \xi_i\,\xi_j\,h(\xi)\,\delta_\xi \otimes \overrightarrow{1} \otimes \mathbb{1}. \tag{4.2.27}$$

Remark 4.2.11. Throughout the rest of the paper, we will frequently use the notation $\overrightarrow{1}_q \in \mathbb{C}^q$ for any $q \in \mathbb{Z}_{>0}$ to indicate the constant vector in $\mathbb{C}^q$ with all entries 1 and write $\overrightarrow{1} = \overrightarrow{1}_{\otimes\mathbf{p}}$ for simplicity. △

Putting these results together we obtain

Lemma 4.2.12. *For each* $\mathbf{k} \in \mathbb{T}^d$*, let*

$$\widehat{\mathcal{L}}_{\mathbf{k}} := \mathrm{i}\,\widehat{\mathcal{K}}_{\mathbf{k}} + \mathrm{i}\widehat{\mathcal{U}} + \mathrm{i}\lambda\widehat{\mathcal{V}} + B \tag{4.2.28}$$

on the domain $\mathcal{D}(B) \subset L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$*. Then* $\widehat{\mathcal{L}}_{\mathbf{k}}$ *is maximally accretive on* $L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$*. Furthermore*

1. *For* $t > 0$*,* $\mathbf{k} \mapsto \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}$ *is*

   a) a C^2 *map from* $\mathbb{T}^d$ *into the contractions on* $L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$*; and*

   b) a C^2 *map from* $\mathbb{T}^d$ *into the bounded operators on* $\ell^{\infty;1}(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$*.*

2. *The operators* $\{\widehat{\mathcal{L}}_{\mathbf{k}}\}_{\mathbf{k}\in\mathbb{T}^d}$ *are uniformly sectorial; that is for every* $\mathbf{k} \in \mathbb{T}^d$ *and every* $f \in L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})$

$$\left|\operatorname{Im}\left\langle f,\ \widehat{\mathcal{L}}_{\mathbf{k}}f\right\rangle\right| \ \leq\ \gamma\operatorname{Re}\left\langle f,\ \widehat{\mathcal{L}}_{\mathbf{k}}f\right\rangle + b'\|f\|_{L^2}^2 \tag{4.2.29}$$

   where γ, b *are given as in* (4.1.3) *and* $b' = 2b + 2\|\widehat{h}\|_\infty + 2\|u\|_\infty + 2\lambda$*.*

3. If $\Psi \in \mathcal{W}^1(M)$, then

$$\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\widehat{\Psi}_{\mathbf{k}} \;:=\; \left[\widehat{\mathrm{e}^{-t\mathcal{L}}\Psi}\right]_{\mathbf{k}} \tag{4.2.30}$$

for every $\mathbf{k} \in \mathbb{T}^d$. For $\Psi \in L^2(M)$, Equation (4.2.30) holds for ν-almost every $\mathbf{k}$.

Combining (4.2.30) with Pillet's formula (Lemma 4.2.4), we obtain the following Floquet transformed Pillet formula in vector form:

Lemma 4.2.13 (Floquet transformed Pillet formula)**.** *Let $\psi_0 \in \ell^2(\mathbb{Z}^d)$ and define $\widehat{\rho}_{0;\mathbf{k}}(x) \in \mathbb{C}^{\otimes \mathbf{p}}$ for $x \in \mathbb{Z}^d, \mathbf{k} \in \mathbb{T}^d$ as*

$$\pi_\sigma \widehat{\rho}_{0;\mathbf{k}}(x) \;:=\; \sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot n} \psi_0(x-n)\overline{\psi_0(-n)},\ \sigma \in \mathbb{Z}_{\mathbf{p}}. \tag{4.2.31}$$

Then

$$\sum_{y \in \mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot y} \mathbb{E}\left(\psi_t(x-y)\overline{\psi_t(-y)}\right)$$

$$= \left\langle \delta_x \otimes \overrightarrow{1} \otimes \mathbb{1},\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\left(\widehat{\rho}_{0;\mathbf{k}} \otimes \mathbb{1}\right)\right\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})}, \tag{4.2.32}$$

where ψ_t is the solution to Equation (4.1.1) with initial condition ψ_0. Here $\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}(\widehat{\rho}_{0;\mathbf{k}} \otimes \mathbb{1}) \in \ell^{\infty;1}(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})$ for each $\mathbf{k}$ and is in $L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})$ for ν-almost every $\mathbf{k}$.

In particular, for every $\mathbf{k} \in \mathbb{T}^d$,

$$\sum_{x \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot x} \mathbb{E}\left(|\psi_t(x)|^2\right) \;=\; \left\langle \delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1},\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\left(\widehat{\rho}_{0;\mathbf{k}} \otimes \mathbb{1}\right)\right\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})}. \tag{4.2.33}$$

Proof. Let $\Psi(x,y,\omega) = \left(\mathrm{e}^{-t\mathcal{L}}(\rho_0 \otimes \mathbb{1})\right)(x,y,\omega) = \left\langle \delta_x \otimes \delta_y,\ \mathrm{e}^{-t\mathcal{L}}(\rho_0 \otimes \mathbb{1}(\omega))\right\rangle_{L^2(\mathbb{Z}^d \times \mathbb{Z}^d)}$. Pillet's formula (4.2.12) can be rewritten as

$$\begin{aligned}\mathbb{E}\left(\Psi(x,y,\cdot)\right) &= \int_\Omega \left(\mathrm{e}^{-t\mathcal{L}}(\rho_0 \otimes \mathbb{1})\right)(x,y,\omega)\,\mu(\mathrm{d}\omega) \\ &= \left\langle \delta_x \otimes \delta_y \otimes \mathbb{1},\ \mathrm{e}^{-t\mathcal{L}}(\rho_0 \otimes \mathbb{1})\right\rangle_{L^2(\mathbb{Z}^d \times \mathbb{Z}^d \times \Omega)} = \mathbb{E}\left(\psi_t(x)\overline{\psi_t(y)}\right).\end{aligned}$$

We note that $\rho_0 \otimes \mathbb{1} \in \mathcal{W}^1(M)$ and that $\mathrm{e}^{-t\mathcal{L}}$ is a bounded operator on $\mathcal{W}^1(M)$ (see [33, Lemma 3.9]). Thus $\Psi \in \mathcal{W}^1(M)$ and its Floquet transform

$$\pi_\sigma \widehat{\Psi}_{\mathbf{k}}(x,\omega) = \sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} \mathrm{e}^{-\mathrm{i}\,\mathbf{k}\cdot n}\, \Psi(x-n,-n,\tau_n\omega).$$

is continuous in $\mathbf{k}$. Direct computation shows that

$$\int_{\mathbb{T}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot y}\, \pi_\sigma \widehat{\Psi}_{\mathbf{k}}(x,\omega)\, \nu(\mathrm{d}\mathbf{k}) \;=\; \Psi(x-y,-y,\tau_y\omega)\delta_{\mathbf{p}\mathbb{Z}+\sigma}(y).$$

Thus, by the Fourier-inversion formula,

$$\sum_{y \in \mathbf{p}\mathbb{Z}^d + \sigma} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot y} \Psi(x-y,-y,\tau_y\omega) \;=\; \pi_\sigma \widehat{\Psi}_{\mathbf{k}}(x,\omega),$$

and

$$\sum_{y \in \mathbf{p}\mathbb{Z}^d + \sigma} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot y} \mathbb{E}\left(\Psi(x-y,-y,\cdot)\right) \;=\; \pi_\sigma \mathbb{E}\left(\widehat{\Psi}_{\mathbf{k}}(x,\cdot)\right) \;=\; \left\langle \delta_x \otimes \mathbb{1},\ \pi_\sigma \widehat{\Psi}_{\mathbf{k}} \right\rangle_{L^2(\widehat{M};\mathbb{C})}$$

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

On the other hand, by (4.2.30), for $\Phi = \rho_0 \otimes \mathbb{1}$, we have

$$\widehat{\Psi}_{\mathbf{k}} = (\widehat{\mathrm{e}^{-t\mathcal{L}}\Phi})_{\mathbf{k}} \;=\; \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\, \widehat{\Phi}_{\mathbf{k}},$$

where

$$\pi_\sigma \widehat{\Phi}_{\mathbf{k}} \;=\; \pi_\sigma (\widehat{\rho_0 \otimes \mathbb{1}})_{\mathbf{k}}(x,\omega) \;=\; \sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} \mathrm{e}^{-\mathrm{i}\,\mathbf{k}\cdot n}\, \psi_0(x-n)\overline{\psi_0(-n)} \otimes \mathbb{1}.$$

Clearly, $\widehat{\Phi}_{\mathbf{k}} = \widehat{\rho}_{0;\mathbf{k}} \otimes \mathbb{1}$, by the definition (4.2.31) of $\widehat{\rho}_{0;\mathbf{k}}$. Putting everything together, we have

$$\sum_{y \in \mathbf{p}\mathbb{Z}^d + \sigma} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot y} \mathbb{E}\left(\psi_t(x-y)\overline{\psi_t(-y)}\right) \;=\; \left\langle \delta_x \otimes \mathbb{1},\ \pi_\sigma\, \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\, \widehat{\rho}_{0;\mathbf{k}} \otimes \mathbb{1} \right\rangle_{L^2(\widehat{M};\mathbb{C})}.$$

Finally, summing over σ in the periodicity cell $\mathbb{Z}_{\mathbf{p}}$, we find that

$$\sum_{y \in \mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot y} \mathbb{E}\left(\psi_t(x-y)\overline{\psi_t(-y)}\right) \;=\; \left\langle \delta_x \otimes \overrightarrow{1} \otimes \mathbb{1},\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\, \widehat{\rho}_{0;\mathbf{k}} \otimes \mathbb{1} \right\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})}. \qquad \square$$

4.3 Spectral analysis on the augmented space

4.3.1 Spectral analysis of $\widehat{\mathcal{K}}_{\mathbf{0}}$

The spectral analysis of $\widehat{\mathcal{L}}_{\mathbf{k}}$ plays an important role in studying the diffusive scaling of this model. We begin by showing that 0 is an eigenvalue of $\widehat{\mathcal{K}}_0$. This observation allows us to write down a block decomposition and to find a spectral gap for $\widehat{\mathcal{L}}_{\mathbf{0}}$ in the two sections that follow.

The key observation regarding $\widehat{\mathcal{K}}_0$ is the following:

Lemma 4.3.1. *Let $x \in \mathbb{Z}^d$ and $\overrightarrow{w} \in \mathbb{C}^{\otimes \mathbf{p}}$. Then*

$$\widehat{\mathcal{K}}_{\mathbf{0}}\, \delta_x \otimes \overrightarrow{w} \otimes \mathbb{1} \;=\; \sum_{\xi \neq \mathbf{0}} h(\xi)\, \delta_{x-\xi} \otimes (\mathrm{I} - \mathcal{A}_{\mathbf{p}}^{-\xi})\overrightarrow{w} \otimes \mathbb{1}, \tag{4.3.1}$$

where $\mathcal{A}_{\mathbf{p}}^{\xi} = \bigotimes_{j=1}^{d} (A_{p_j})^{\xi_j}$ with A_p the $p \times p$ right shift matrix,

$$A_p := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}. \tag{4.3.2}$$

Proof. This follows from direct computation:

$$\begin{aligned} \pi_\sigma \widehat{\mathcal{K}}_{\mathbf{0}}(\delta_x \otimes \overrightarrow{w} \otimes \mathbb{1}) &= \sum_{\xi \neq 0} h(\xi)[\pi_\sigma \delta_{x-\xi} \otimes \overrightarrow{w} \otimes \mathbb{1} - \pi_{\sigma-\xi}\delta_{x-\xi} \otimes \overrightarrow{w} \otimes \mathbb{1}] \\ &= \sum_{\xi \neq 0} h(\xi)\delta_{x-\xi} \otimes [\pi_\sigma - \pi_{\sigma-\xi}]\overrightarrow{w} \otimes \mathbb{1} \\ &= \sum_{\xi \neq 0} h(\xi)\, \delta_{x-\xi} \otimes \pi_\sigma (I - \mathcal{A}_{\mathbf{p}}^{-\xi})\overrightarrow{w} \otimes \mathbb{1}. \end{aligned}$$ □

To proceed we need to consider the matrices $\mathcal{A}_{\mathbf{p}}^{\xi}$. We begin with A_p, the $p \times p$ right shift.

Lemma 4.3.2. *Let $m \in \mathbb{Z}$, $p \in \mathbb{Z}_{>0}$. The matrix $A_p^m = (A_p)^m$ has $\frac{p}{\gcd(m,p)}$ distinct eigenvalues,*

$$\mathrm{e}^{2\pi\mathrm{i}\frac{\ell m}{p}}, \quad \ell = 0, 1, \cdots, \frac{p}{\gcd(m,p)} - 1, \tag{4.3.3}$$

each of multiplicity $\gcd(m,p)$.

Proof. Since $A_p^p = \mathbb{1}$, it suffices to restrict our attention to $0 < m < p$. The eigenvalues of A_p are all p-th roots of unity

$$\lambda_\ell = \mathrm{e}^{2\pi\mathrm{i}\frac{\ell}{p}}, \quad \ell = 0, 1, \cdots, p-1,$$

and each eigenvalue has multiplicity one. The corresponding eigenvectors are the elements of the discrete Fourier basis. For $1 < m < p$, it follows from the spectral mapping theorem that A_p^m has eigenvalues λ_ℓ^m for $\ell = 0, 1, \cdots, p-1$. From here, it is easy to verify that $\lambda_\ell^m = \lambda_{\ell'}^m$ whenever $|\ell - \ell'| = \frac{np}{\gcd(m,p)}$ for some integer n. Finally, since $|\ell - \ell'| < p$, it follows that there are $\frac{p}{\gcd(m,p)}$ distinct eigenvalues each of multiplicity $\gcd(m,p)$. $\square$

This result has an immediate extension to $\mathcal{A}_{\mathbf{p}}$, the tensor product of right shift operators.

Corollary 4.3.3. *If $\mathbf{p} = (p_1, \cdots, p_d) \in \mathbb{Z}_{>0}^d$ and $\mathbf{m} = (m_1, \cdots m_d) \in \mathbb{Z}^d$, then $\mathcal{A}_{\mathbf{p}}^{\mathbf{m}} := \bigotimes_{j=1}^d A_{p_j}^{m_j}$ has eigenvalues*

$$\prod_{j=1}^d \mathrm{e}^{2\pi\mathrm{i}\frac{\ell_j m_j}{p_j}}; \quad \ell_j = 0, 1, \cdots, \frac{p_j}{\gcd(m_j, p_j)} - 1. \tag{4.3.4}$$

In particular, if $(\mathbf{e}_j)_{j=1}^d$ is the standard basis on $\mathbb{Z}^d$, then

$$\mathrm{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{e}_j}) = \mathbb{C}^{p_1} \otimes \cdots \otimes \{\overrightarrow{1}_{p_j}\} \otimes \cdots \otimes \mathbb{C}^{p_d}. \tag{4.3.5}$$

Note that, by Equation (4.3.5),

$$\bigcap_{j=1}^d \mathrm{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{e}_j}) \ = \ \mathrm{span}\{\overrightarrow{1}\}.$$

The following lemma extends this result to a collection $\mathcal{A}_{\mathbf{p}}^{\mathbf{m}_j}$, $j = 1, \ldots, k$, where the vectors $\mathbf{m}_1, \ldots, \mathbf{m}_k$ generate $\mathbb{Z}^d$.

Lemma 4.3.4. *Let $\mathbf{m}_1, \cdots, \mathbf{m}_k \in \mathbb{Z}^d$, $n_1, \cdots, n_k \in \mathbb{Z}$, and $\mathbf{M} = n_1\mathbf{m}_1 + \cdots + n_k\mathbf{m}_k$ for some $k \geq 1$. Then, we have*

$$\bigcap_{j=1}^{k} \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{m}_j}) \subset \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{M}}). \tag{4.3.6}$$

In particular, if $\mathbf{m}_1, \cdots, \mathbf{m}_k$ generate $\mathbb{Z}^d$, then

$$\bigcap_{j=1}^{k} \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{m}_j}) = \bigcap_{j=1}^{d} \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{e}_j}) = \operatorname{span}\{\overrightarrow{1}\}. \tag{4.3.7}$$

Proof. Suppose $w \in \bigcap_{j=1}^{k} \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{m}_j})$, then for each $j = 1, 2, \cdots, k$,

$$w = \mathcal{A}_{\mathbf{p}}^{\mathbf{m}_j} w = \left(\mathcal{A}_{\mathbf{p}}^{\mathbf{m}_j}\right)^{n_j} w = \mathcal{A}_{\mathbf{p}}^{n_j\mathbf{m}_j} w. \tag{4.3.8}$$

Repeated application of (4.3.8) yields

$$w = \mathcal{A}_{\mathbf{p}}^{n_1\mathbf{m}_1} = \mathcal{A}_{\mathbf{p}}^{n_k\mathbf{m}_k} w = \mathcal{A}_{\mathbf{p}}^{\mathbf{M}} w.$$

Thus, $w \in \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{M}})$.

If $\mathbf{m}_1, \cdots, \mathbf{m}_k$ generate $\mathbb{Z}^d$, then (4.3.6) implies the first equality in (4.3.7). The second equality follows from Corollary 4.3.3 since

$$\bigcap_{j=1}^{d} \operatorname{Ker}(I - \mathcal{A}_{\mathbf{p}}^{\mathbf{e}_j}) = \bigcap_{j=1}^{d} \left(\mathbb{C}^{p_1} \otimes \cdots \otimes \overrightarrow{1}_{p_j} \otimes \cdots \otimes \mathbb{C}^{p_d}\right) = \operatorname{span}\{\overrightarrow{1}\}. \qquad \square$$

We return now to consideration of $\widehat{\mathcal{K}}_0$. The non-degenerate support condition (4.1.9) guarantees that the hopping kernel, h, is non-zero on a spanning set, $\{\xi_j\}_{j \in J}$, of $\mathbb{Z}^d$. Combining this fact with Lemma 4.3.4, we can see that $(I - \mathcal{A}_{\mathbf{p}}^{-\xi})\overrightarrow{w} = 0$ for all ξ with $h(\xi) \neq 0$ if and only if $\overrightarrow{w} \parallel \overrightarrow{1}$. In particular, Lemma 4.3.1 leads to the following

Corollary 4.3.5. *Let $x \in \mathbb{Z}^d$ and $\overrightarrow{w} \in \mathbb{C}^{\otimes \mathbf{p}}$. Then $\widehat{\mathcal{K}}_0(\delta_x \otimes \overrightarrow{w} \otimes \mathbb{1}) = 0$ if and only if $\overrightarrow{w} \parallel \overrightarrow{1}$. Moreover, there is $c_0 > 0$ such that for $\overrightarrow{w} \perp \overrightarrow{1}$,*

$$\left\|\widehat{\mathcal{K}}_{\mathbf{0}}(\delta_x \otimes \overrightarrow{w} \otimes \mathbb{1})\right\|^2 \;\geq\; c_0 \|\overrightarrow{w}\|^2. \tag{4.3.9}$$

Proof. By Lemma 4.3.1, we have

$$\left\|\widehat{\mathcal{K}}_{\mathbf{0}}(\delta_x \otimes \overrightarrow{w} \otimes \mathbb{1})\right\|^2 \;=\; \sum_{\xi} |h(\xi)|^2 \left\|(I - A_{\mathbf{p}}^{-\xi})\overrightarrow{w}\right\|^2.$$

The right hand side is a quadratic form $Q(w)$ on the finite dimensional space $\mathbb{C}^{\otimes \mathbf{p}}$. Furthermore, by Lemma 4.3.1, $Q(w)$ vanishes only if $\mathbf{w} \parallel \overrightarrow{1}$. The lower bound (4.3.9) follows. In fact, by Lemma 4.3.2 the smallest eigenvalue of $Q(w)$ on $\{\overrightarrow{1}\}^{\perp}$ is

$$c_0 \;=\; \min_{\ell \in \mathbb{Z}_{\mathbf{p}} \setminus 0} \sum_{\xi} |h(\xi)|^2 \left| 1 - \exp\left(-2\pi \mathrm{i} \sum_{j=1}^{d} \frac{\ell_j \xi_j}{p_j}\right)\right|^2.$$

Thus $c_0 \neq 0$ and Equation (4.3.9) holds. □

4.3.2 Block decomposition of $\widehat{\mathcal{L}}_{\mathbf{0}}$

In the previous section, we showed that $\delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1}$ is an eigenvector of $\widehat{\mathcal{K}}_{\mathbf{0}}$ corresponding to the eigenvalue 0. Using (4.2.21) and (4.2.22), it is easy to check that this claim also holds for $\widehat{\mathcal{U}}$ and $\widehat{\mathcal{V}}$. Finally, the Markov generator satisfies $B\mathbb{1} = B^{\dagger}\mathbb{1} = 0$. Therefore,

$$\widehat{\mathcal{L}}_{\mathbf{0}}\, \delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1} = \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\, \delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1} \;=\; 0. \tag{4.3.10}$$

To further analyze the spectrum of $\widehat{\mathcal{L}}_{\mathbf{k}}$ we will use a block decomposition associated to the following direct sum decomposition of $L^2(\widehat{M}; \mathbb{C}^{\otimes \mathbf{p}}) \;\cong\; \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^{\otimes \mathbf{p}} \otimes L^2(\Omega)$:

$$\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^{\otimes \mathbf{p}} \otimes L^2(\Omega) \;=\; \widehat{\mathcal{H}}_0 \oplus \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 \oplus \widehat{\mathcal{H}}_3, \tag{4.3.11}$$

where

$$\widehat{\mathcal{H}}_0 \;:= \mathrm{span}\{\delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1}\},$$

$$\widehat{\mathcal{H}}_1 \;:=\; \delta_{\mathbf{0}} \otimes \{\overrightarrow{1}\}^{\perp} \otimes \mathbb{1},$$

$$\widehat{\mathcal{H}}_2 \;:=\; \{\delta_{\mathbf{0}}\}^{\perp} \otimes \mathbb{C}^{\otimes \mathbf{p}} \otimes \mathbb{1} \;=\; \ell^2(\mathbb{Z}^d \backslash \{\mathbf{0}\}) \otimes \mathbb{C}^{\otimes \mathbf{p}} \otimes \mathbb{1},$$

and

$$\widehat{\mathcal{H}}_3 \;:=\; \left(\widehat{\mathcal{H}}_0 \oplus \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2\right)^{\perp} \;=\; \left\{\Psi(x,\omega) \;:\; \int_{\Omega} \Psi(x,\omega)\mathrm{d}\mu(\omega) = 0\right\}.$$

Note that $\dim \widehat{\mathcal{H}}_0 = 1$, $\dim \widehat{\mathcal{H}}_1 = p_1 \cdots p_d - 1$, and $\dim \widehat{\mathcal{H}}_2 = \dim \widehat{\mathcal{H}}_3 = \infty$.

We will write operators on $L^2(\widehat{M}; \mathbb{C}^{\otimes \mathbf{p}})$ as 4×4 matrices of operators acting between the various spaces $\widehat{\mathcal{H}}_j, j = 0,1,2,3$. Throughout we will use the notation:

1. $P_j \;=$ the orthogonal projection onto $\widehat{\mathcal{H}}_j$,
2. $P_j^{\perp} \;=\; 1 - P_j$.

In particular, $P = P_3^{\perp} = P_0 + P_1 + P_2$ is the orthogonal projection of $L^2(\widehat{M}; \mathbb{C}^{\otimes \mathbf{p}})$ onto the space $\widehat{\mathcal{H}}_0 \oplus \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^{\otimes \mathbf{p}} \otimes \mathbb{1}$ of "non-random" functions:

$$P\Psi(x) \;=\; \int_{\Omega} \Psi(x,\omega)\mathrm{d}\mu(\omega).$$

Then $P_3 = P^{\perp} = 1 - P$ is the projection onto the space of mean zero functions $\widehat{\mathcal{H}}_3$.

Lemma 4.3.6. *On $\widehat{\mathcal{H}}_0 \oplus \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 \oplus \widehat{\mathcal{H}}_3$ the operators $\widehat{\mathcal{K}}_{\mathbf{0}}, \widehat{\mathcal{U}}, \widehat{\mathcal{V}}$, and B have following block decomposition*

$$\widehat{\mathcal{K}}_{\mathbf{0}} \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2 & 0 \\ 0 & P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1 & P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_2 & 0 \\ 0 & 0 & 0 & P_3\widehat{\mathcal{K}}_{\mathbf{0}}P_3 \end{pmatrix}, \qquad \widehat{\mathcal{U}} \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & P_2\widehat{\mathcal{U}}P_2 & 0 \\ 0 & 0 & 0 & P_3\widehat{\mathcal{U}}P_3 \end{pmatrix},$$

$$\widehat{\mathcal{V}} \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & P_2\widehat{\mathcal{V}}P_3 \\ 0 & 0 & P_3\widehat{\mathcal{V}}P_2 & P_3\widehat{\mathcal{V}}P_3 \end{pmatrix}, \quad \textit{and} \quad B \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & P_3BP_3 \end{pmatrix}.$$

Proof. The eigenvalue equation (4.3.10) gives

$$P_0\mathcal{T} = \mathcal{T}P_0 = 0$$

for $\mathcal{T} = \widehat{\mathcal{K}}_{\mathbf{0}}, \widehat{\mathcal{U}}, \widehat{\mathcal{V}}, B, \widehat{\mathcal{L}}_{\mathbf{0}}$. From the definition (4.2.20) of $\widehat{\mathcal{K}}_{\mathbf{0}}$ we see that this operator is "off-diagonal" with respect to position, in the sense that $\left\langle \delta_x \otimes F,\ \widehat{\mathcal{K}}_{\mathbf{0}} \delta_x \otimes G \right\rangle = 0$ for any x and any $F, G \in L^2(\Omega; \mathbb{C}^{\mathbf{p}})$. Thus $P_1 \widehat{\mathcal{K}}_0 P_1 = 0$. The definitions (4.2.21), (4.2.22) of $\widehat{\mathcal{U}}$, $\widehat{\mathcal{V}}$ imply that they vanish on $\delta_{\mathbf{0}} \otimes F$, so

$$P_1 \widehat{\mathcal{U}} = P_1 \widehat{\mathcal{V}} = 0, \quad \widehat{\mathcal{U}} P_1 = \widehat{\mathcal{V}} P_1 = 0.$$

Since $\widehat{\mathcal{K}}_{\mathbf{0}}, \widehat{\mathcal{U}}$ are "non-random", we have for $j = 0, 1, 2$,

$$P_j \widehat{\mathcal{K}}_{\mathbf{0}} P_3 = 0, \ P_3 \widehat{\mathcal{K}}_{\mathbf{0}} P_j = 0, \quad P_j \widehat{\mathcal{U}} P_3 = 0, \ P_3 \widehat{\mathcal{U}} P_j = 0.$$

Since $\widehat{\mathcal{V}}$ is mean zero on $L^2(\Omega)$ and $B\mathbb{1} = B^\dagger \mathbb{1} = 0$, we have

$$P_3^\perp \widehat{\mathcal{V}} P_3^\perp = 0, \quad P_3^\perp B = B P_3^\perp = 0. \qquad \square$$

Corollary 4.3.7. *On $\widehat{\mathcal{H}}$ the operator $\widehat{\mathcal{L}}_{\mathbf{0}} = \mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}} + \mathrm{i}\lambda \widehat{\mathcal{V}} + B$ has block decomposition*

$$\widehat{\mathcal{L}}_{\mathbf{0}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \mathrm{i}P_1 \widehat{\mathcal{K}}_{\mathbf{0}} P_2 & 0 \\ 0 & \mathrm{i}P_2 \widehat{\mathcal{K}}_{\mathbf{0}} P_1 & P_2(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}}) P_2 & \mathrm{i}\lambda P_2 \widehat{\mathcal{V}} P_3 \\ 0 & 0 & \mathrm{i}\lambda P_3 \widehat{\mathcal{V}} P_2 & P_3 \widehat{\mathcal{L}}_{\mathbf{0}} P_3 \end{pmatrix}. \tag{4.3.12}$$

4.3.3 Spectral gap

With the block decomposition (4.3.12), we are now in a position to prove that $\widehat{\mathcal{L}}_{\mathbf{0}}$ has a spectral gap.

Lemma 4.3.8. *If $\lambda > 0$, then 0 is a non-degenerate eigenvalue of $\widehat{\mathcal{L}}_{\mathbf{0}}$ and there is $g > 0$ such that*

$$\sigma(\widehat{\mathcal{L}}_{\mathbf{0}}) \ = \ \{0\} \cup \Sigma_+$$

with $\Sigma_+ \subset \{z \ : \ \mathrm{Re}\, z > g\}$. For λ small, there is $c = c(\mathbf{p}, \|\widehat{h}\|_\infty, \|u\|_\infty, \gamma, T, b) > 0$ such that $g \geq c\lambda^2$.

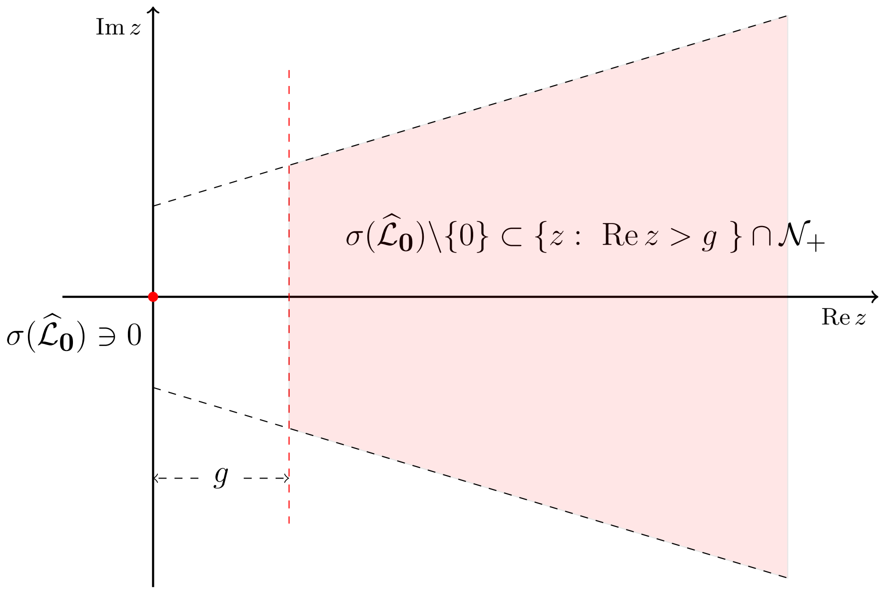

Figure 4.1: Spectral gap of $\widehat{\mathcal{L}}_{\mathbf{0}}$

Before proceeding to the proof of the lemma, we note that the sectoriality of B places further restrictions on Σ_+. Indeed, $\operatorname{Re}\widehat{\mathcal{L}}_{\mathbf{0}} = \operatorname{Re} B \geq 0$ in the sense of quadratic forms. Thus, by the sectoriality of B,

$$\left|\operatorname{Im}\left\{\langle\Phi, \widehat{\mathcal{L}}_{\mathbf{0}}\Phi\rangle\right\}\right| \;\leq\; \left\|\widehat{\mathcal{K}}_0 + \widehat{\mathcal{U}} + \lambda\widehat{\mathcal{V}}\right\| + |\operatorname{Im}\{\langle\Phi, B\Phi\rangle\}|$$
$$\leq\; 2\|\widehat{h}\|_\infty + 2\|u\|_\infty + 2\lambda + \gamma \operatorname{Re}\langle\Phi, \widehat{\mathcal{L}}_{\mathbf{0}}\Phi\rangle,$$

if $\|\Phi\| = 1$. It follows that the numerical range $\operatorname{Num}(\widehat{\mathcal{L}}_{\mathbf{0}}) = \left\{\left\langle\Phi,\ \widehat{\mathcal{L}}_{\mathbf{0}}\Phi\right\rangle \,\middle|\, \|\Phi\| = 1\right\}$ is contained in

$$\mathcal{N}_+ \;:=\; \{z \;:\; \operatorname{Re} z \geq 0 \text{ and } |\operatorname{Im} z| \leq 2\|\widehat{h}\|_\infty + 2\|u\|_\infty + 2\lambda + \gamma \operatorname{Re} z\}. \tag{4.3.13}$$

Since $\sigma(\widehat{\mathcal{L}}_{\mathbf{0}}) \subset \operatorname{Num}(\widehat{\mathcal{L}}_{\mathbf{0}})$, we find that $\Sigma_+ \subset \{\operatorname{Re} z > g\} \cap \mathcal{N}_+$ —see Figure 4.1.

To prove Lemma 4.3.8, it suffices to show that the restriction of $\widehat{\mathcal{L}}_{\mathbf{0}}$ to $\widehat{\mathcal{H}}_0^\perp = \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 \oplus \widehat{\mathcal{H}}_3$,

$$\mathcal{J} \;=\; \begin{pmatrix} 0 & \mathrm{i}P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2 & 0 \\ \mathrm{i}P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1 & P_2(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}})P_2 & \mathrm{i}\lambda P_2\widehat{\mathcal{V}}P_3 \\ 0 & \mathrm{i}\lambda P_3\widehat{\mathcal{V}}P_2 & P_3\widehat{\mathcal{L}}_{\mathbf{0}}P_3 \end{pmatrix}, \tag{4.3.14}$$

has spectrum contained in $\{\operatorname{Re} z > g\}$.

Lemma 4.3.9. *There is $g > 0$, such that whenever* $\operatorname{Re} z < g$,

1. $\Gamma_3 - z$ *is boundedly invertible on* $\widehat{\mathcal{H}}_3$, *where* $\Gamma_3 = P_3 \widehat{\mathcal{L}}_{\mathbf{0}} P_3$,

2. $\Gamma_2(z) - z$ *is boundedly invertible on* $\widehat{\mathcal{H}}_2$, *where*

$$\Gamma_2(z) \;=\; P_2 \left(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}} + \lambda^2 \widehat{\mathcal{V}} \left(\Gamma_3 - z\right)^{-1} \widehat{\mathcal{V}} \right) P_2, \tag{4.3.15}$$

3. $\mathcal{J} - z$ *is boundedly invertible on* $\widehat{\mathcal{H}}_0^{\perp}$.

In particular, $\mathcal{J}$ *is boundedly invertible. Let* Π_2 *be the projection onto* $\operatorname{Ker}(P_1 \widehat{\mathcal{K}}_0) \subsetneq \widehat{\mathcal{H}}_2$. *If* $\Pi_2 \widetilde{\phi} \neq 0$ *for some* $\widetilde{\phi} \in \widehat{\mathcal{H}}_2$, *then* $P_2 \mathcal{J}^{-1} \widetilde{\phi} \neq 0$ *and*

$$\operatorname{Re} \left\langle \widetilde{\phi},\ P_2 \mathcal{J}^{-1} \widetilde{\phi} \right\rangle \geq g \| P_2 \mathcal{J}^{-1} \widetilde{\phi} \|^2 > 0. \tag{4.3.16}$$

Proof. We obtain this result by repeated applications of the Schur complement formula. As observed above, we may restrict attention to the sectorial domain $z \in \mathcal{N}_+$. Fix $z \in \mathcal{N}_+$ and consider the equation

$$(\mathcal{J} - z) \begin{pmatrix} \zeta \\ \phi \\ \Phi \end{pmatrix} \;=\; \begin{pmatrix} -z & \mathrm{i} P_1 \widehat{\mathcal{K}}_{\mathbf{0}} P_2 & 0 \\ \mathrm{i} P_2 \widehat{\mathcal{K}}_{\mathbf{0}} P_1 & P_2(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}}) P_2 - z & \mathrm{i}\lambda P_2 \widehat{\mathcal{V}} P_3 \\ 0 & \mathrm{i}\lambda P_3 \widehat{\mathcal{V}} P_2 & P_3 \widehat{\mathcal{L}}_{\mathbf{0}} P_3 - z \end{pmatrix} \begin{pmatrix} \zeta \\ \phi \\ \Phi \end{pmatrix} \;=\; \begin{pmatrix} \widetilde{\zeta} \\ \widetilde{\phi} \\ \widetilde{\Phi} \end{pmatrix}, \tag{4.3.17}$$

for $(\zeta, \phi, \Phi) \in \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 \oplus \widehat{\mathcal{H}}_3$ given $(\widetilde{\zeta}, \widetilde{\phi}, \widetilde{\Phi}) \in \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 \oplus \widehat{\mathcal{H}}_3$. By the gap condition (4.1.4) on B,

$$\operatorname{Re} P_3 \widehat{\mathcal{L}}_{\mathbf{0}} P_3 \;=\; \operatorname{Re} P_3 (\mathrm{i}\widehat{\mathcal{K}}_0 + \mathrm{i}\widehat{\mathcal{U}} + B + \mathrm{i}\lambda \widehat{\mathcal{V}}) P_3 \;\geq\; \frac{1}{T} P_3.$$

Therefore, $\Gamma_3 - z = P_3 \widehat{\mathcal{L}}_{\mathbf{0}} P_3 - z$ is boundedly invertible on $\widehat{\mathcal{H}}_3$ provided $\operatorname{Re} z < \frac{1}{T}$. For such z, we may solve the third equation of (4.3.17) to obtain

$$\Phi \;=\; (\Gamma_3 - z)^{-1} \widetilde{\Phi} - (\Gamma_3 - z)^{-1}\, \mathrm{i}\lambda \widehat{\mathcal{V}} \phi. \tag{4.3.18}$$

Using the solution (4.3.18), we reduce the second equation of (4.3.17) to

$$[\Gamma_2(z) - z]\ \phi \;=\; \widetilde{\phi} - \mathrm{i} P_2 \widehat{\mathcal{K}}_{\mathbf{0}} \zeta - \mathrm{i}\lambda P_2 \widehat{\mathcal{V}} \left(\Gamma_3 - z\right)^{-1} \widetilde{\Phi} \tag{4.3.19}$$

with $\Gamma_2(z)$ as in (4.3.15). For $\varphi\otimes\mathbb{1}\in\widehat{\mathcal{H}}_2=L^2(\mathbb{Z}^d\backslash\{\mathbf{0}\};\mathbb{C}^{\otimes\mathbf{P}})$, notice that $\varphi\otimes\mathbb{1}=P_2\varphi\otimes\mathbb{1}$ and $\Gamma_2=P_2\Gamma_2$, we have

$$
\begin{aligned}
&\operatorname{Re}\langle\varphi\otimes\mathbb{1},\ \Gamma_2(z)\,\varphi\otimes\mathbb{1}\rangle_{\widehat{\mathcal{H}}_2}\\
&\qquad=\operatorname{Re}\langle\varphi\otimes\mathbb{1},\ \Gamma_2(z)\,\varphi\otimes\mathbb{1}\rangle_{\widehat{\mathcal{H}}}\\
&\qquad=\left\langle\varphi\otimes\mathbb{1},\ \frac{1}{2}(\Gamma_2(z)+\Gamma_2^{\dagger}(z))\,\varphi\otimes\mathbb{1}\right\rangle_{\widehat{\mathcal{H}}}\\
&\qquad=\lambda^2\left\langle P_3(\Gamma_3-z)^{-1}\widehat{\mathcal{V}}\,\varphi\otimes\mathbb{1},\ (\operatorname{Re}B-\operatorname{Re}z)\,P_3(\Gamma_3-z)^{-1}\widehat{\mathcal{V}}\,\varphi\otimes\mathbb{1}\right\rangle_{\widehat{\mathcal{H}}}\\
&\qquad\geq\lambda^2\left(\frac{1}{T}-\operatorname{Re}z\right)\left\|P_3(\Gamma_3-z)^{-1}\widehat{\mathcal{V}}\,\varphi\otimes\mathbb{1}\right\|^2_{\widehat{\mathcal{H}}}\\
&\qquad=\lambda^2\left(\frac{1}{T}-\operatorname{Re}z\right)\left\|(\Gamma_3-z)^{-1}\widehat{\mathcal{V}}\,\varphi\otimes\mathbb{1}\right\|^2_{\widehat{\mathcal{H}}_3}\\
&\qquad=\lambda^2\left(\frac{1}{T}-\operatorname{Re}z\right)\left\|\Big(B^{-1}(\Gamma_3-z)\Big)^{-1}B^{-1}\widehat{\mathcal{V}}\,\varphi\otimes\mathbb{1}\right\|^2_{\widehat{\mathcal{H}}_3}
\end{aligned}
\tag{4.3.20}
$$

where the inverse of B is well defined since $\widehat{\mathcal{V}}\varphi\otimes\mathbb{1}\in\widehat{\mathcal{H}}_3=\operatorname{Ran}P_3$. Furthermore, B^{-1} is bounded on $\widehat{\mathcal{H}}_3$, with $\|B^{-1}P_3\|\leq T$. Thus $B^{-1}(\Gamma_3-z)$ is bounded for $z\in\mathcal{N}_+\cap\{\operatorname{Re}z<\frac{1}{T}\}$ by,

$$
\begin{aligned}
\left\|B^{-1}P_3(\Gamma_3-z)P_3\right\|_{\widehat{\mathcal{H}}}&\leq 1+\left\|B^{-1}P_3(\widehat{\mathcal{K}}_{\mathbf{0}}+\widehat{\mathcal{U}}+\lambda\widehat{\mathcal{V}})\right\|+|z|\left\|B^{-1}P_3\right\|\\
&\leq 1+T(2\|\widehat{h}\|_\infty+2\|u\|_\infty+2\lambda+|z|)\\
&\leq 2+\gamma+4T(\|\widehat{h}\|_\infty+\|u\|_\infty+\lambda).
\end{aligned}
\tag{4.3.21}
$$

Putting (4.3.20), (4.3.21) and (4.1.6) together, we obtain

$$
\begin{aligned}
\operatorname{Re}\langle\varphi\otimes\mathbb{1},\ \Gamma_2(z)\,\varphi\otimes\mathbb{1}\rangle_{\widehat{\mathcal{H}}_2}&\geq\lambda^2\left(\frac{1}{T}-\operatorname{Re}z\right)\frac{\left\|B^{-1}\widehat{\mathcal{V}}\,\varphi\otimes\mathbb{1}\right\|^2_{\widehat{\mathcal{H}}}}{\|B^{-1}(\Gamma_3-z)\|^2_{\widehat{\mathcal{H}}}}\\
&\geq\lambda^2\left(\frac{1}{T}-\operatorname{Re}z\right)\frac{\sum\limits_{\sigma\in\mathbb{Z}_{\mathbf{P}}}\sum\limits_{x\neq\mathbf{0}}\chi^2|\pi_\sigma\varphi(x)|^2}{\Big(2+\gamma+4T(\|\widehat{h}\|_\infty+\|u\|_\infty+\lambda)\Big)^2}\\
&=\frac{\lambda^2\chi^2(1-T\operatorname{Re}z)}{T\Big(2+\gamma+4T(\|\widehat{h}\|_\infty+\|u\|_\infty+\lambda)\Big)^2}\,\|\varphi\otimes\mathbb{1}\|^2_{\widehat{\mathcal{H}}_2}.
\end{aligned}
$$

Let

$$c_1 \;=\; \frac{\lambda^2\chi^2}{T\left(\lambda^2\chi^2 + 2\left(2+\gamma+4T(\|\widehat{h}\|_\infty + \|u\|_\infty + \lambda)\right)^2\right)}, \tag{4.3.22}$$

so that $\dfrac{\lambda^2\chi^2}{T\left(2+\gamma+4T(\|\widehat{h}\|_\infty+\|u\|_\infty+\lambda)\right)^2}(1-Tc_1) = 2c_1$. Then for $z \in \mathcal{N}_+ \cap \{\operatorname{Re} z \le c_1\}$, we have

$$\operatorname{Re}\Gamma_2(z) - \operatorname{Re} z \ge 2c_1 - \operatorname{Re} z \ge c_1, \tag{4.3.23}$$

implying that $\Gamma_2(z)-z$ is boundedly invertible. Thus, (4.3.19) can be solved on $\widehat{\mathcal{H}}_2$ to obtain

$$\begin{aligned}\phi \;=\; & (\Gamma_2(z)-z)^{-1}\widetilde{\phi} - (\Gamma_2(z)-z)^{-1}\mathrm{i}P_2\widehat{\mathcal{K}}_{\mathbf{0}}\zeta \\ & - (\Gamma_2(z)-z)^{-1}\mathrm{i}\lambda P_2\widehat{\mathcal{V}}\,(\Gamma_3-z)^{-1}\widetilde{\Phi}.\end{aligned} \tag{4.3.24}$$

Now, the first equation of (4.3.17) reduces to the following

$$\begin{aligned}[\Gamma_1(z)-z]\zeta \;=\; & \widetilde{\zeta} - \mathrm{i}P_1\widehat{\mathcal{K}}_{\mathbf{0}}\,(\Gamma_2(z)-z)^{-1}\widetilde{\phi} \\ & - \lambda P_1\widehat{\mathcal{K}}_{\mathbf{0}}(\Gamma_2(z)-z)^{-1}P_2\widehat{\mathcal{V}}\,(\Gamma_3-z)^{-1}\widetilde{\Phi},\end{aligned} \tag{4.3.25}$$

where $\Gamma_1(z) = P_1\widehat{\mathcal{K}}_{\mathbf{0}}(\Gamma_2(z)-z)^{-1}P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1$. We will use the same strategy to show that $\Gamma_1(z)-z$ is invertible. Take $\zeta = \delta_{\mathbf{0}} \otimes \overrightarrow{w} \otimes \mathbb{1} \in \widehat{\mathcal{H}}_1$. Recall, by definition of $\widehat{\mathcal{H}}_1$, that $\overrightarrow{w} \perp \overrightarrow{1}$. Thus, by (4.3.23) and Corollary 4.3.5,

$$\begin{aligned}&\operatorname{Re}\langle\zeta,\ \Gamma_1(z)\zeta\rangle_{\widehat{\mathcal{H}}_1} \\ &\quad = \left\langle(\Gamma_2(z)-z)^{-1}\widehat{\mathcal{K}}_{\mathbf{0}}\zeta,\ (\operatorname{Re}\Gamma_2(z)-\operatorname{Re} z)\,(\Gamma_2(z)-z)^{-1}\,\widehat{\mathcal{K}}_{\mathbf{0}}\zeta\right\rangle_{\widehat{\mathcal{H}}} \\ &\quad \ge \frac{c_1c_0}{\|\Gamma_2(z)-z\|^2_{\widehat{\mathcal{H}}}}\|\zeta\|^2_{\widehat{\mathcal{H}}}.\end{aligned} \tag{4.3.26}$$

For $z \in \mathcal{N}_+ \cap \{\operatorname{Re} z < \frac{1}{2T}\}$,

$$\begin{aligned}\|\Gamma_2(z)-z\|_{\widehat{\mathcal{H}}} \;\le\; & 2\|\widehat{h}\|_\infty + 2\|u\|_\infty + 4\lambda^2\left\|(P_3\widehat{\mathcal{L}}_{\mathbf{0}}P_3 - z)^{-1}\right\|_{\widehat{\mathcal{H}}_3} + |z| \\ \le\; & 4\|\widehat{h}\|_\infty + 4\|u\|_\infty + 4\lambda^2\left(\frac{1}{T}-\frac{1}{2T}\right)^{-1} + 2\lambda + (\gamma+1)\operatorname{Re} z \\ =\; & 4\|\widehat{h}\|_\infty + 4\|u\|_\infty + 8T\lambda^2 + 2\lambda + (\gamma+1)(2T)^{-1},\end{aligned} \tag{4.3.27}$$

by (4.3.15) and (4.1.4). Putting (4.3.26) and (4.3.27) together, we obtain

$$\begin{aligned}&\operatorname{Re}\langle\zeta,\ \Gamma_1(z)\zeta\rangle_{\widehat{\mathcal{H}}_1}\\ &\qquad\geq \frac{c_1c_0}{\left(4\|\widehat{h}\|_\infty+4\|u\|_\infty+8T\lambda^2+2\lambda+(\gamma+1)(2T)^{-1}\right)^2}\|\zeta\|^2_{\widehat{\mathcal{H}}} \ =: \ c_2\|\zeta\|^2_{\widehat{\mathcal{H}}}.\end{aligned}$$

Therefore, $\operatorname{Re}\Gamma_1(z) > \operatorname{Re} z$ on $\widehat{\mathcal{H}}_1$ provided $z \in \mathcal{N}_+$ and $\operatorname{Re} z < \min\{c_1, \frac{1}{2T}, c_2\} =: g$. For such z it follows that $\Gamma_1(z) - z$ is boundedly invertible and (4.3.25) can be solved on $\widehat{\mathcal{H}}_1$. Therefore, (4.3.17) is explicitly solvable on $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2 \oplus \widehat{\mathcal{H}}_3$ and $\mathcal{J} - z$ is boundedly invertible for all $z \in \{z : |\operatorname{Re} z| < g\} \bigcap \mathcal{N}_+$.

To prove the second part of Lemma 4.3.9, it is enough to solve $\mathcal{J}\Psi = \widetilde{\Psi}$ for $\Psi = (\zeta, \phi, \Phi)$ given $\widetilde{\Psi} = (0, \widetilde{\phi}, 0)$. The three equations are reduced to

$$\begin{aligned}\mathrm{i}P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2\ \phi &= 0\\ \mathrm{i}P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1\ \zeta + P_2(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}})P_2\ \phi + \mathrm{i}\lambda P_2\widehat{\mathcal{V}}P_3\ \Phi &= \widetilde{\phi}\\ \mathrm{i}\lambda P_3\widehat{\mathcal{V}}P_2\ \phi + P_3\widehat{\mathcal{L}}_{\mathbf{0}}P_3\ \Phi &= 0\end{aligned}$$

The first equation implies $\phi \in \operatorname{Ker}(P_1\widehat{\mathcal{K}}_0)$. Therefore, $\phi = \Pi_2\phi$, where Π_2 is the projection onto the kernel of $P_1\widehat{\mathcal{K}}_0$. As derived in the general case, the second and the third equations imply that

$$\mathrm{i}P_2\widehat{\mathcal{K}}_{\mathbf{0}}\,P_1\zeta + \Gamma_2\phi = \widetilde{\phi}. \tag{4.3.28}$$

If ξ satisfies $P_1\widehat{\mathcal{K}}_{\mathbf{0}}\xi = 0$, then $\left\langle\xi,\ \widehat{\mathcal{K}}_{\mathbf{0}}\,P_1\zeta\right\rangle = \left\langle P_1\widehat{\mathcal{K}}_{\mathbf{0}}\xi,\ \ P_1\zeta\right\rangle = 0$. Therefore, $\Pi_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1\zeta = 0$. Applying Π_2 to (4.3.28), we have

$$\Pi_2\Gamma_2\Pi_2\,\phi = \Pi_2\widetilde{\phi}.$$

Clearly, if $\Pi_2\widetilde{\phi} \neq 0$, then $\phi = P_2\Psi = P_2\mathcal{J}^{-1}\widetilde{\phi} \neq 0$. Notice that $\left\langle\widehat{\mathcal{K}}_{\mathbf{0}}\,P_1\zeta,\ \phi\right\rangle = \left\langle\widehat{\mathcal{K}}_{\mathbf{0}}\,P_1\zeta,\ \Pi_2\phi\right\rangle = \left\langle\Pi_2\widehat{\mathcal{K}}_{\mathbf{0}}\,P_1\zeta,\ \Pi_2\phi\right\rangle = 0$. Equation (4.3.28) also implies that

$$\operatorname{Re}\left\langle\widetilde{\phi},\ \phi\right\rangle = \operatorname{Re}\left\langle\mathrm{i}P_2\widehat{\mathcal{K}}_{\mathbf{0}}\,P_1\zeta + \Gamma_2\phi,\ \phi\right\rangle = \operatorname{Re}\langle\Gamma_2\phi,\ \phi\rangle \geq 2c_1\,\|\phi\|^2 \geq g\,\|\phi\|^2 > 0,$$

which completes the proof of (4.3.16). ∎

The spectral gap g of $\widehat{\mathcal{L}}_{\mathbf{0}}$ has consequences for the dynamics of the semi-group.

Lemma 4.3.10. *Let $Q_{\mathbf{0}}$ = orthogonal projection onto $\widehat{\mathcal{H}}_0 = \operatorname{span} \delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes 1$ in $L^2(\widehat{M}; \mathbb{C}^{\otimes \mathbf{p}})$. Then $\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}(1-Q_{\mathbf{0}})$ is a contraction semi-group on $\operatorname{ran}(1-Q_{\mathbf{0}})$, and for all sufficiently small $\epsilon > 0$ there is $C_\epsilon > 0$ such that*

$$\left\| \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}(1 - Q_{\mathbf{0}}) \right\|_{L^2(\widehat{M}; \mathbb{C}^{\otimes \mathbf{p}})} \ \leq \ C_\epsilon \mathrm{e}^{-t(g-\epsilon)} \tag{4.3.29}$$

Lemma 4.3.11. *There is $c_0 > 0$ such that*

$$\left\| \widehat{\mathcal{L}}_{\mathbf{k}} - \widehat{\mathcal{L}}_{\mathbf{0}} \right\|_{L^2(\widehat{M}; \mathbb{C}^{\otimes \mathbf{p}})} \ \leq \ c_0 |\mathbf{k}|.$$

If $|\mathbf{k}|$ is sufficiently small, the spectrum of $\widehat{\mathcal{L}}_{\mathbf{k}}$ consists of:

1. *A non-degenerate eigenvalue $E(\mathbf{k})$ contained in $S_0 = \{z \,:\, |z| < c_0|\mathbf{k}|\}$.*
2. *The rest of the spectrum is contained in the half plane $S_1 = \{z : \operatorname{Re} z > g - c_0|\mathbf{k}|\}$ such that $S_0 \cap S_1 = \emptyset$.*

Furthermore, $E(\mathbf{k})$ is C^2 in a neighborhood of $\mathbf{0}$,

$$E(\mathbf{0}) = 0, \quad \boldsymbol{\nabla} E(\mathbf{0}) = 0. \tag{4.3.30}$$

Denote $\partial_j = \partial_{k_j}$ and $\varphi_{\mathbf{0}} = \frac{1}{\sqrt{\otimes \mathbf{p}}} \delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1}$ for simplicity where $\otimes \mathbf{p} = p_1 \cdot p_2 \cdots p_d$, then

$$\partial_i \partial_j E(0) \ = \left\langle \partial_j \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}},\ P_2 \mathcal{J}^{-1} \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\rangle + \left\langle \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}},\ P_2 \mathcal{J}^{-1} \partial_j \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\rangle \tag{4.3.31}$$

where $P_2, \mathcal{J}$ and $\mathcal{J}^{-1}$ are given in (4.3.14) and Lemma 4.3.9.

Remark 4.3.12. Let $\mathbf{D} := \left(\mathbf{D}_{i,j}\right)_{d\times d} = \left(\partial_i \partial_j E(\mathbf{0})\right)_{d \times d}$. It is clear from (4.3.31) that $\mathbf{D}$ is symmetric. Furthermore, for any $\mathbf{k} \in \mathbb{T}^d$, in view of the expression of $\partial_i \widehat{\mathcal{K}}_{\mathbf{0}}$ in (4.2.26), $0 \neq \sum_i k_i \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \in \ell^2(\mathbb{Z}^d) \otimes \overrightarrow{1} \otimes \mathbb{1}$. It is non-zero due the non-degeneracy of h. Therfore, by (4.3.16) in Lemma 4.3.9,

$$\operatorname{Re} \langle \mathbf{k},\ \mathbf{D}\mathbf{k} \rangle \ = \ 2 \operatorname{Re} \left\langle \sum_i k_i \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}},\ P_2 \mathcal{J}^{-1} \sum_i k_i \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\rangle \ > \ 2g \left\| P_2 \mathcal{J}^{-1} \sum_i k_i \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\|^2 > 0.$$

In the next section, we will relate the matrix element of $\mathbf{D}$ with limits of diffusively scaled moments. From the real valued moments, we will see that $\partial_i\partial_j E(\mathbf{0}) \in \mathbb{R}$ and then $\mathbf{D}$ is positive definite. $\triangle$

Similar to Lemma 4.3.10, dynamical information about the semi-group $\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}$ follows from the spectral gap of $\widehat{\mathcal{L}}_{\mathbf{k}}$ in Lemma 4.3.11:

Lemma 4.3.13. *If ϵ is sufficiently small, then there is $C_\epsilon < \infty$ such that*

$$\left\| \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}(1 - Q_{\mathbf{k}}) \right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} \le C_\epsilon \mathrm{e}^{-t(g-\epsilon-c_0|\mathbf{k}|)}$$

for all sufficiently small $\mathbf{k}$.

Notice that $\otimes\mathbf{p} = p_1 \cdot p_2 \cdots p_d$. The case where $d = 1$ and $\otimes\mathbf{p} = p_1 = 1$ is equivalent to the free case considered in [23], where the above lemmas were proved. The proof follows from the standard perturbation theory of analytic semi-groups—see for instance [11, 24]. There are no essential differences in the proof when $\otimes\mathbf{p} > 1$. We omit the proofs for Lemma 4.3.10-Lemma 4.3.13 here. We only sketch the proofs for (4.3.30) and (4.3.31), which plays the most important role for the explicit expression of the diffusion constant in the next section.

Proof of (4.3.30) *and* (4.3.31). Write $\partial_j = \partial_{k_j}$ for short. Let $E(\mathbf{k})$ be the non-degenerate eigenvalue of $\widehat{\mathcal{L}}_{\mathbf{k}}$, and the associated normalized eigenvector $\varphi_{\mathbf{k}}$. Let $Q_{\mathbf{k}}$ be the orthogonal projection onto $\varphi_{\mathbf{k}}$. Clearly $E(\mathbf{0}) = 0$, $\varphi_{\mathbf{0}} = \frac{1}{\sqrt{\otimes\mathbf{p}}}\delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1}$ and $\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}} = \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\varphi_{\mathbf{0}} = 0$. Since

$$\widehat{\mathcal{L}}_{\mathbf{k}}\varphi_{\mathbf{k}} \;=\; E(\mathbf{k})\varphi_{\mathbf{k}}, \tag{4.3.32}$$

direct computation shows

$$\partial_j\widehat{\mathcal{L}}_{\mathbf{k}}\,\varphi_{\mathbf{k}} + \widehat{\mathcal{L}}_{\mathbf{k}}\partial_j\varphi_{\mathbf{k}} \;=\; \partial_j E(\mathbf{k})\varphi_{\mathbf{k}} + E(\mathbf{k})\partial_j\varphi_{\mathbf{k}} \tag{4.3.33}$$

$$\Longrightarrow \partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}} + \widehat{\mathcal{L}}_0\partial_j\varphi_{\mathbf{0}} \;=\; \partial_j E(\mathbf{0})\varphi_{\mathbf{0}}. \tag{4.3.34}$$

Notice that $\partial_j\widehat{\mathcal{L}}_{\mathbf{0}} = \mathrm{i}\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}$ maps $\widehat{\mathcal{H}}_0 = \mathrm{ran}Q_{\mathbf{0}}$ to $\widehat{\mathcal{H}}_2$, therefore, $Q_{\mathbf{0}}\partial_j\widehat{\mathcal{L}}_{\mathbf{0}} = 0$ and

$$\partial_j E(\mathbf{0}) = \left\langle \varphi_{\mathbf{0}},\ \partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}} \right\rangle + \left\langle \varphi_{\mathbf{0}},\ \widehat{\mathcal{L}}_{\mathbf{0}}\partial_j\varphi_{\mathbf{0}} \right\rangle = \left\langle Q_{\mathbf{0}}\varphi_{\mathbf{0}},\ \partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}} \right\rangle + \left\langle \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\varphi_{\mathbf{0}},\ \partial_j\varphi_{\mathbf{0}} \right\rangle = 0.$$

Differentiating (4.3.33) again, we have

$$
\begin{aligned}
&\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{k}}\varphi_{\mathbf{k}}+\partial_j\widehat{\mathcal{L}}_{\mathbf{k}}\partial_i\varphi_{\mathbf{k}}+\partial_i\widehat{\mathcal{L}}_{\mathbf{k}}\partial_j\varphi_{\mathbf{k}}+\widehat{\mathcal{L}}_{\mathbf{k}}\partial_i\partial_j\varphi_{\mathbf{k}}\\
=&\partial_i\partial_j E(\mathbf{k})\varphi_{\mathbf{k}}+\partial_j E(\mathbf{k})\partial_i\varphi_{\mathbf{k}}+\partial_i E(\mathbf{k})\partial_j\varphi_{\mathbf{k}}+E(\mathbf{k})\partial_i\partial_j\varphi_{\mathbf{k}}.
\end{aligned}
\tag{4.3.35}
$$

Evaluating (4.3.35) at $k=\mathbf{0}$ and using $\boldsymbol{\nabla}E(\mathbf{0})=0$, we have that

$$
\partial_i\partial_j\widehat{\mathcal{L}}_0\varphi_{\mathbf{0}}+\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\partial_i\varphi_{\mathbf{0}}+\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\partial_j\varphi_{\mathbf{0}}+\widehat{\mathcal{L}}_0\partial_i\partial_j\varphi_{\mathbf{0}}=\partial_i\partial_j E(\mathbf{0})\varphi_{\mathbf{0}}.
$$

We also have $Q_{\mathbf{0}}\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}=0$ for the same reason as for $Q_0\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}$. Notice that $\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}=\mathrm{i}\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}=-\partial_j\widehat{\mathcal{L}}_0^{\dagger}$ and $\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}}\in\ell^2(\mathbb{Z}^d\backslash\{\mathbf{0}\})\otimes\overrightarrow{1}\otimes\mathbb{1}$ because of (4.2.26). Corollary 4.3.5 implies $\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}}\in\mathrm{Ker}(P_1\widehat{\mathcal{K}}_{\mathbf{0}})=\mathrm{ran}(\Pi_2)\subsetneq\widehat{\mathcal{H}}_2$. Therefore,

$$
\begin{aligned}
\partial_j\partial_j E(\mathbf{0})=&\left\langle\varphi_{\mathbf{0}},\ \partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\partial_i\varphi_{\mathbf{0}}\right\rangle+\left\langle\varphi_{\mathbf{0}},\ \partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\partial_j\varphi_{\mathbf{0}}\right\rangle\\
=&\mathrm{i}\left\langle\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ \partial_i\varphi_{\mathbf{0}}\right\rangle+\mathrm{i}\left\langle\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ \partial_j\varphi_{\mathbf{0}}\right\rangle\\
=&\mathrm{i}\left\langle P_2\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ P_2\partial_i\varphi_{\mathbf{0}}\right\rangle+\mathrm{i}\left\langle P_2\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ P_2\partial_j\varphi_{\mathbf{0}}\right\rangle.
\end{aligned}
$$

It remains to solve

$$
\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\varphi_{\mathbf{0}}+\widehat{\mathcal{L}}_0\partial_j\varphi_{\mathbf{0}}\ =0
$$

i.e.,

$$
\mathrm{i}\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}+\widehat{\mathcal{L}}_0\partial_j\varphi_{\mathbf{0}}\ =0 \tag{4.3.36}
$$

for $P_2\partial_i\varphi_{\mathbf{0}}$. Recall the block form of $\widehat{\mathcal{L}}_{\mathbf{0}}$ in (4.3.12) and $\mathcal{J}$ in (4.3.14). The key fact $\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}=\Pi_2\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\in\widehat{\mathcal{H}}_2$ reduces Equation (4.3.36) to what we have considered in the second part of Lemma 4.3.9:

$$
\begin{pmatrix}
0 & 0 & 0 & 0\\
0 & 0 & \mathrm{i}P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2 & 0\\
0 & \mathrm{i}P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1 & P_2(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}}+\mathrm{i}\widehat{\mathcal{U}})P_2 & \mathrm{i}\lambda P_2\widehat{\mathcal{V}}P_3\\
0 & 0 & \mathrm{i}\lambda P_3\widehat{\mathcal{V}}P_2 & P_3\widehat{\mathcal{L}}_{\mathbf{0}}P_3
\end{pmatrix}
\begin{pmatrix}
*\\ *\\ P_2\partial_j\varphi_{\mathbf{0}}\\ *
\end{pmatrix}
=
\begin{pmatrix}
0\\ 0\\ -\mathrm{i}\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\\ 0
\end{pmatrix}.
$$

As derived in Lemma 4.3.9:

$$
P_2\partial_j\varphi_{\mathbf{0}}=-\mathrm{i}P_2\mathcal{J}^{-1}\,\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}},
$$

where P_2 is the projection onto $\widehat{\mathcal{H}}_2$. Therefore,

$$\begin{aligned}\partial_j\partial_j E(\mathbf{0}) =& \mathrm{i}\left\langle \partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ -\mathrm{i}P_2\mathcal{J}^{-1}\,\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\right\rangle + \mathrm{i}\left\langle \partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ -\mathrm{i}P_2\mathcal{J}^{-1}\,\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\right\rangle \\ =& \left\langle \partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ P_2\mathcal{J}^{-1}\,\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\right\rangle + \left\langle \partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}},\ P_2\mathcal{J}^{-1}\,\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\right\rangle,\end{aligned}$$

which gives (4.3.31). □

4.4 Proof of the main results

4.4.1 Central limit theorem

We first prove (4.1.12) for bounded continuous f and normalized $\psi_0 \in \ell^2(\mathbb{Z}^d)$. The extension to quadratically bounded f follows from some standard arguments combining (4.1.12) for bounded continuous f and diffusive scaling for second moments, Lemma 4.4.1. We refer readers to Section 4.5 in [33] for more details about this extension. We omit the proof of the extension here.

To prove (4.1.12) for bounded continuous f, it suffices, by Levy's Continuity Theorem and a limiting argument, to prove

$$\lim_{t\to\infty}\sum_{x\in\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\frac{x}{\sqrt{t}}}\mathbb{E}\left(|\psi_t(x)|^2\right) \;=\; \mathrm{e}^{-\frac{1}{2}\langle\mathbf{k},\,\mathbf{D}\mathbf{k}\rangle}, \tag{4.4.1}$$

where $\psi_t(x) \in \ell^2(\mathbb{Z}^d)$ is the solution to Equation (4.1.1) with initial condition $\psi_0 \in \ell^2(\mathbb{Z}^d)$. As pointed out in Section 4.2, [33], it is enough to establish Equation (4.4.1) for $\psi_0 \in \ell^1(\mathbb{Z}^d)$; it then extends to all of $\psi_0 \in \ell^2(\mathbb{Z}^d)$ by a limiting argument. So throughout this section, we assume that

$$\|\psi_0\|_{\ell^2} = 1, \quad \text{and} \quad \|\psi_0\|_{\ell^1} := \sum_{x\in\mathbb{Z}^d}|\psi_0(x)| < \infty. \tag{4.4.2}$$

We also denote for simplicity

$$\varphi_{\mathbf{0}} := \varphi_{\mathbf{0}}(x,\omega) = \frac{1}{\sqrt{\otimes\mathbf{p}}}\delta_{\mathbf{0}}\otimes\overrightarrow{1}\otimes\mathbb{1},\ \ \Phi_{\mathbf{k}} := \Phi_{\mathbf{k}}(x,\omega) = \sqrt{\otimes\mathbf{p}}\cdot\widehat{\rho}_{0;\mathbf{k}}(x)\otimes\mathbb{1}, \tag{4.4.3}$$

where $\overrightarrow{1}, \widehat{\rho}_{0;\mathbf{k}}(x) \in \mathbb{C}^{\otimes \mathbf{p}}$ are defined in (4.2.31). Recall that for any $\sigma \in \mathbb{Z}_{\mathbf{p}}$

$$\pi_\sigma \overrightarrow{1} = 1, \qquad \pi_\sigma \widehat{\rho}_{0;\mathbf{0}}(x) = \sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} \psi_0(x-n)\overline{\psi_0(-n)}.$$

By (4.2.33), we have

$$\sum_{x \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\frac{\mathbf{k}}{\sqrt{t}}x} \mathbb{E}\left(|\psi_t(x)|^2\right) = \left\langle \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}/\sqrt{t}}} \Phi_{\frac{\mathbf{k}}{\sqrt{t}}} \right\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})}.$$

Letting $Q_{\mathbf{k}}$ denote the Riesz projection onto the eigenvector of $\widehat{\mathcal{L}}_{\mathbf{k}}$ near zero, we have

$$\begin{aligned}\sum_{x \in \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\frac{\mathbf{k}}{\sqrt{t}}x} \mathbb{E}\left(|\psi_t(x)|^2\right) =& \left\langle \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}/\sqrt{t}}} Q_{\frac{\mathbf{k}}{\sqrt{t}}} \Phi_{\frac{\mathbf{k}}{\sqrt{t}}} \right\rangle + \left\langle \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}/\sqrt{t}}} \left(1 - Q_{\frac{\mathbf{k}}{\sqrt{t}}}\right) \Phi_{\frac{\mathbf{k}}{\sqrt{t}}} \right\rangle \\ =& \mathrm{e}^{-tE(\frac{\mathbf{k}}{\sqrt{t}})} \left\langle \varphi_{\mathbf{0}} \ , \ Q_{\frac{\mathbf{k}}{\sqrt{t}}} \Phi_{\frac{\mathbf{k}}{\sqrt{t}}} \right\rangle + \left\langle \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}/\sqrt{t}}} \left(1 - Q_{\frac{\mathbf{k}}{\sqrt{t}}}\right) \Phi_{\frac{\mathbf{k}}{\sqrt{t}}} \right\rangle.\end{aligned} \tag{4.4.4}$$

By Lemma 4.3.13, the second term in (4.4.4) is exponentially small in the large t limit,

$$\begin{aligned}\left|\left\langle \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}/\sqrt{t}}} \left(1 - Q_{\frac{\mathbf{k}}{\sqrt{t}}}\right) \Phi_{\frac{\mathbf{k}}{\sqrt{t}}} \right\rangle\right| &\le \left\|(1 - Q_{\frac{\mathbf{k}}{\sqrt{t}}})\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}/\sqrt{t}}}\right\| \cdot \|\varphi_{\mathbf{0}}\| \cdot \left\|\Phi_{\frac{\mathbf{k}}{\sqrt{t}}}\right\| \\ &\le C_\epsilon \mathrm{e}^{-t(g-\epsilon-c\frac{|\mathbf{k}|}{\sqrt{t}})} \cdot \|\varphi_{\mathbf{0}}\| \cdot \left\|\Phi_{\frac{\mathbf{k}}{\sqrt{t}}}\right\|.\end{aligned} \tag{4.4.5}$$

Direct computation shows that

$$\begin{aligned}\lim_{t\to\infty} \left\|\Phi_{\frac{\mathbf{k}}{\sqrt{t}}}\right\|^2_{L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{p}})} =& (\otimes \mathbf{p}) \left\|\widehat{\rho}_{0;\mathbf{0}}\right\|^2_{\ell^2(\mathbb{Z}^d;\mathbb{C}^{\otimes \mathbf{p}})} \\ \le& (\otimes \mathbf{p}) \sum_{\sigma \in \mathbb{Z}_{\mathbf{p}}} \sum_{x \in \mathbb{Z}^d} \left| \sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} \psi_0(x-n)\overline{\psi_0(-n)} \right|^2 \\ \le& (\otimes \mathbf{p}) \|\psi_0\|^2_{\ell^2} \sum_{\sigma \in \mathbb{Z}_{\mathbf{p}}} \left(\sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} |\psi_0(-n)| \right)^2 \\ \le& (\otimes \mathbf{p}) \|\psi_0\|^2_{\ell^2} \cdot \|\psi_0\|^2_{\ell^1} < \infty.\end{aligned}$$

Therefore, in (4.4.5), $\left|\left\langle \varphi_{\mathbf{0}}\ ,\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\frac{\mathbf{k}}{\sqrt{t}}}}\left(1-Q_{\frac{\mathbf{k}}{\sqrt{t}}}\right)\Phi_{\frac{\mathbf{k}}{\sqrt{t}}}\right\rangle\right| \longrightarrow 0$ as $t\to\infty$.

Regarding the first term in (4.4.4), we have by Taylor's formula,

$$E\left(\frac{\mathbf{k}}{\sqrt{t}}\right) \ = \ \frac{1}{2}\sum_{i,j}\partial_j\partial_j E(\mathbf{0})\frac{k_i}{\sqrt{t}}\frac{k_j}{\sqrt{t}} \ + \ o(\frac{1}{t}) = \ \frac{1}{2t}\sum_{i,j}\partial_j\partial_j E(\mathbf{0})k_ik_j \ + \ o(\frac{1}{t}),$$

since $E(\mathbf{0}) = \boldsymbol{\nabla} E(\mathbf{0}) = 0$. Thus,

$$\mathrm{e}^{-tE(\mathbf{k}/\sqrt{t})} \ = \ \mathrm{e}^{-t\,\frac{1}{2t}\sum_{i,j}\partial_j\partial_j E(\mathbf{0})k_ik_j} + o(1) = \mathrm{e}^{-\frac{1}{2}\sum_{i,j}\partial_j\partial_j E(\mathbf{0})k_ik_j} + o(1). \qquad (4.4.6)$$

Direct computation shows that

$$\begin{aligned}\langle\varphi_{\mathbf{0}},\ \Phi_{\mathbf{0}}\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} &= \left\langle \delta_{\mathbf{0}}\otimes\overrightarrow{1}\otimes\mathbb{1}\ ,\ \widehat{\rho}_{0;\mathbf{0}}\otimes\mathbb{1}\right\rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} \\ &= \sum_{\sigma\in\mathbb{Z}_{\mathbf{p}}}\ \sum_{n\in\mathbf{p}\mathbb{Z}^d+\sigma}\psi_0(-n)\overline{\psi_0(-n)} = \|\psi_0\|^2_{\ell^2(\mathbb{Z}^d;\mathbb{C})} = 1.\end{aligned}$$

Thus,

$$Q_{\mathbf{0}}\Phi_{\mathbf{0}} = \mathrm{Proj}_{\varphi_{\mathbf{0}}}\Phi_{\mathbf{0}} = \langle\varphi_{\mathbf{0}},\ \Phi_{\mathbf{0}}\rangle\cdot\frac{\varphi_{\mathbf{0}}}{\|\varphi_{\mathbf{0}}\|^2} = \varphi_{\mathbf{0}}. \qquad (4.4.7)$$

Putting together everything, we have

$$\begin{aligned}\lim_{t\to\infty}\sum_{x\in\mathbb{Z}^d}\mathrm{e}^{\mathrm{i}\frac{\mathbf{k}}{\sqrt{t}}x}\,\mathbb{E}\left(|\psi_t(x)|^2\right) &= \lim_{t\to\infty}\mathrm{e}^{-tE\left(\frac{\mathbf{k}}{\sqrt{t}}\right)}\left\langle\varphi_{\mathbf{0}}\ ,\ Q_{\frac{\mathbf{k}}{\sqrt{t}}}\Phi_{\frac{\mathbf{k}}{\sqrt{t}}}\right\rangle \\ &= \mathrm{e}^{-\frac{1}{2}\sum_{i,j}\partial_j\partial_j E(\mathbf{0})k_ik_j}\langle\varphi_{\mathbf{0}}\ ,\ Q_{\mathbf{0}}\Phi_{\mathbf{0}}\rangle = \mathrm{e}^{-\frac{1}{2}\sum_{i,j}\partial_j\partial_j E(\mathbf{0})k_ik_j}.\end{aligned}$$

Therefore, (4.4.1) holds true with $\mathbf{D}_{i,j} = \partial_j\partial_j E(\mathbf{0})$ for any normalized $\psi_0\in\ell^2(\mathbb{Z}^d)$. □

4.4.2 Diffusive scaling and reality of the diffusion matrix

We proceed to prove the diffusive scaling (4.1.13) under the assumption that

$$\sum_x|\psi_0(x)|^2 = 1,\ \ \sum_x|x|^2|\psi_0(x)|^2 < \infty. \qquad (4.4.8)$$

Similar to (4.4.2), it is enough to establish the results for $x\psi_0 \in \ell^1(\mathbb{Z}^d)$; it then extends to all of $x\psi_0 \in \ell^2(\mathbb{Z}^d)$ by a limiting argument. We assume that

$$\sum_x |x||\psi_0(x)| < \infty. \tag{4.4.9}$$

We continue to use the notation in (4.4.3). Also, $\langle \cdot,\ \cdot \rangle$ will stand for $\langle \cdot,\ \cdot \rangle_{L^2(\widehat{M};\mathbb{C}^{\otimes \mathbf{P}})}$ unless otherwise specified. We also denote $\partial_i = \partial_{k_i}, i = 1, \cdots, d$ for short.

As pointed out in Section 4.4 in [33], $\sum_x (1 + |x|^2)|\psi_t(x)|^2 \leq \mathrm{e}^{Ct}$ for each $t > 0$. Thus the second moments of the position

$$M_{i,j}(t) \ := \ \sum_{x \in \mathbb{Z}^d} x_i x_j \mathbb{E}\left(|\psi_t(x)|^2\right) \tag{4.4.10}$$

are well defined and finite. The main task of this section is to show that $M_{i,j}(t) \sim \mathbf{D}_{i,j} t$, where $\mathbf{D}_{i,j} = \partial_i \partial_j E(\mathbf{0})$ are given in (4.3.31). More precisely,

Lemma 4.4.1. *Let $P_2 \mathcal{J}^{-1}$ be as in Lemma 4.3.9 . Suppose the initial value ψ_0 satisfies* (4.4.8)*, then for all $1 \leq i, j \leq d$,*

$$\lim_{t\to\infty} \frac{1}{t} M_{i,j}(t) = \left\langle \partial_j \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}},\ P_2 \mathcal{J}^{-1}\, \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\rangle + \left\langle \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}},\ P_2 \mathcal{J}^{-1}\, \partial_j \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\rangle = \partial_i \partial_j E(\mathbf{0}).$$

As a consequence, $\partial_i \partial_j E(\mathbf{0}) \in \mathbb{R}$ and $\mathbf{D} = \left(\partial_i \partial_j E(\mathbf{0})\right)_{d\times d}$ is positive definite. In particular,

$$\lim_{t\to\infty} \frac{1}{t} \sum_{x \in \mathbb{Z}^d} |x|^2\, \mathbb{E}\left(|\psi_t(x)|^2\right) = 2 \sum_{i=1}^{d} \left\langle \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}},\ P_2 \mathcal{J}^{-1}\, \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\rangle = \operatorname{tr} \mathbf{D} \in (0, \infty).$$

By (4.2.33), we have

$$M_{i,j}(t) \ = \ -\,\partial_i \partial_j \sum_{x\in\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot x} \mathbb{E}\left(|\psi_t(x)|^2\right)\Bigg|_{\mathbf{k}=\mathbf{0}} \ = \ -\,\partial_i \partial_j \left\langle \varphi_{\mathbf{0}},\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\, \Phi_{\mathbf{k}} \right\rangle\Big|_{\mathbf{k}=\mathbf{0}}. \tag{4.4.11}$$

The following decomposition of $M_{i,j}$ is essentially contained in [33]. We sketch the proof in Appendix A for reader's convenience.

Lemma 4.4.2. *For all $1 \le i, j \le d$ and $t \in \mathbb{R}^+$, $M_{i,j} = \sum_{n=1}^{5} N_n$, where*

$$N_1 = -\left\langle \varphi_{\mathbf{0}} \ , \ \partial_i \partial_j \Phi_{\mathbf{0}} \right\rangle; \tag{4.4.12}$$

$$N_2 = \int_0^t \left[\left\langle \partial_i \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-s \widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \, \partial_j \Phi_{\mathbf{0}} \right\rangle + \left\langle \partial_j \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-s \widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \, \partial_i \Phi_{\mathbf{0}} \right\rangle \right] \mathrm{d}s; \tag{4.4.13}$$

$$N_3 = \int_0^t \left\langle \partial_i \partial_j \, \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \, \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-s \widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \, \Phi_{\mathbf{0}} \right\rangle \mathrm{d}s; \tag{4.4.14}$$

$$N_4 = -\int_0^t \int_0^s \left[\left\langle \, \partial_i \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \, \varphi_{\mathbf{0}} \, , \ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \partial_j \widehat{\mathcal{L}}_{\mathbf{0}} \, \mathrm{e}^{-r \widehat{\mathcal{L}}_{\mathbf{0}}} \, (1 - Q_{\mathbf{0}}) \Phi_{\mathbf{0}} \right\rangle ; \right. \tag{4.4.15}$$

$$\left. + \left\langle \, \partial_j \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \, \varphi_{\mathbf{0}} \, , \ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \partial_i \widehat{\mathcal{L}}_{\mathbf{0}} \, \mathrm{e}^{-r \widehat{\mathcal{L}}_{\mathbf{0}}} \, (1 - Q_{\mathbf{0}}) \Phi_{\mathbf{0}} \right\rangle \right] \mathrm{d}r \, \mathrm{d}s \tag{4.4.16}$$

$$N_5 = -\int_0^t \int_0^s \left[\left\langle \, \partial_i \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \, \varphi_{\mathbf{0}} \, , \ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \partial_j \widehat{\mathcal{L}}_{\mathbf{0}} \, Q_{\mathbf{0}} \Phi_{\mathbf{0}} \right\rangle ; \right. \tag{4.4.17}$$

$$\left. + \left\langle \, \partial_j \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \, \varphi_{\mathbf{0}} \, , \ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}} (1 - Q_{\mathbf{0}}) \partial_i \widehat{\mathcal{L}}_{\mathbf{0}} \, Q_{\mathbf{0}} \Phi_{\mathbf{0}} \right\rangle \right] \mathrm{d}r \, \mathrm{d}s. \tag{4.4.18}$$

Combining the above decomposition and the contraction property of $\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}$ in Lemma 4.3.10, we have the following convergence of N_n, which implies Lemma 4.4.1 immediately.

Lemma 4.4.3. *Let $M_{i,j} = \sum_{n=1}^{5} N_n$ be given as in Lemma 4.4.2. Then*

$$\lim_{t \to \infty} \frac{1}{t} |N_n| = 0, \ \ n = 1, \cdots, 4. \tag{4.4.19}$$

$$\lim_{t \to \infty} \frac{1}{t} N_5 = \left\langle \, \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \, \varphi_{\mathbf{0}} \, , \ P_2 \mathcal{J}^{-1} \partial_j \widehat{\mathcal{K}}_{\mathbf{0}} \, \varphi_{\mathbf{0}} \right\rangle + \left\langle \, \partial_j \widehat{\mathcal{K}}_{\mathbf{0}} \, \varphi_{\mathbf{0}} \, , \ P_2 \mathcal{J}^{-1} \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \, \varphi_{\mathbf{0}} \right\rangle. \tag{4.4.20}$$

Proof. **Case** $n = 1$: Note that $\partial_i \partial_j \Phi_{\mathbf{0}} = \sqrt{\otimes \mathbf{p}} \ \partial_i \partial_j \widehat{\rho}_{0;\mathbf{k}} \big|_{\mathbf{k}=\mathbf{0}} \otimes \mathbb{1}$. Direct computation by (4.2.31) shows

$$\pi_\sigma \, \partial_i \partial_j \widehat{\rho}_{0;\mathbf{0}}(x) = -\sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} n_i n_j \psi_0(x - n) \overline{\psi_0(-n)}. \tag{4.4.21}$$

Therefore, by (4.4.12)

$$|N_1| = \left| \left\langle \delta_{\mathbf{0}} \otimes \overrightarrow{1} \otimes \mathbb{1} \ , \ \partial_i \partial_j \widehat{\rho}_{0;\mathbf{0}} \otimes \mathbb{1} \right\rangle \right| = \left| \sum_{n \in \mathbb{Z}^d} n_i n_j |\psi_0(n)|^2 \right| \le \sum_{n \in \mathbb{Z}^d} |n|^2 |\psi_0(n)|^2.$$

Clearly, $|N_1|$ is uniformly bounded in t by (4.4.8), which implies $\lim_{t\to\infty} \frac{1}{t}|N_1(t)| = 0$.

Case $n = 2$: By (4.2.31) and the same computation as in (4.4.21), we have $\partial_j \Phi_{\mathbf{0}} = \partial_j \widehat{\rho}_{0;\mathbf{k}}\big|_{\mathbf{k}=\mathbf{0}} \otimes \mathbb{1}$ with

$$\pi_\sigma \, \partial_j \, \widehat{\rho}_{0;\mathbf{0}}(x) = -\mathrm{i} \sum_{n \in \mathbf{p}\mathbb{Z}^d + \sigma} n_j \, \psi_0(x-n)\overline{\psi_0(-n)}. \tag{4.4.22}$$

By (4.4.8), (4.4.9) and direct computation, we obtain

$$\begin{aligned}
\left\|\partial_j \widehat{\rho}_{0;\mathbf{0}}\right\|^2_{\ell^2(\mathbb{Z}^d;\mathbb{C}^{\otimes\mathbf{p}})} \le & \sum_{\sigma\in\mathbb{Z}_{\mathbf{p}}} \sum_{x\in\mathbb{Z}^d} \left| \sum_{n\in\mathbf{p}\mathbb{Z}^d+\sigma} n_j \, \psi_0(x-n)\overline{\psi_0(-n)} \right|^2 \\
\le & \|\psi_0\|^2_{\ell^2} \sum_{\sigma\in\mathbb{Z}_{\mathbf{p}}} \left(\sum_{n\in\mathbf{p}\mathbb{Z}^d+\sigma} |n| \, |\psi_0(-n)| \right)^2 \\
\le & \|\psi_0\|^2_{\ell^2} \cdot \|x\psi_0\|^2_{\ell^1} < \infty.
\end{aligned}$$

By Lemma 4.2.10,

$$\left\|\partial_j \widehat{\mathcal{L}}_{\mathbf{0}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} = \left\|\partial_j \widehat{\mathcal{K}}_{\mathbf{0}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} \le \|\widehat{h}'\|_\infty.$$

By Lemma 4.3.10, we have

$$\begin{aligned}
& \int_0^t \left| \left\langle \partial_i \widehat{\mathcal{L}}^\dagger_{\mathbf{0}} \varphi_{\mathbf{0}} \ , \ \mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}} \, (1-Q_{\mathbf{0}}) \, \partial_j \Phi_{\mathbf{0}} \right\rangle \right| \mathrm{d}s \\
\le & \left\| \partial_i \widehat{\mathcal{K}}_{\mathbf{0}} \varphi_{\mathbf{0}} \right\| \cdot \|\partial_j \Phi_{\mathbf{0}}\| \cdot C_\epsilon \int_0^t \mathrm{e}^{-s(g-\epsilon)} \, \mathrm{d}s \\
\le & \|\widehat{h}'\|_\infty \cdot \sqrt{\otimes\mathbf{p}} \cdot \left\|\partial_j \widehat{\rho}_{0;\mathbf{0}}\right\| \cdot \frac{C_\epsilon}{g-\epsilon} < \infty.
\end{aligned}$$

Therefore, $\lim_{t\to\infty} \frac{1}{t}|N_2(t)| = 0$.

Case $n = 3$: N_3 can be estimated exact in the same way as N_2. Again by Lemma 4.2.10, we have

$$\left\|\partial_i \partial_j \widehat{\mathcal{L}}_{\mathbf{0}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} = \left\|\partial_i \partial_j \widehat{\mathcal{K}}_{\mathbf{0}}\right\|_{L^2(\widehat{M};\mathbb{C}^{\otimes\mathbf{p}})} \le \|\widehat{h}''\|_\infty.$$

By Lemma 4.3.10, we have

$$\sup_t |N_3(t)| \le \sup_t \int_0^t \left| \left\langle \partial_i\partial_j\, \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\varphi_{\mathbf{0}}\ ,\ \ \mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\,\Phi_{\mathbf{0}} \right\rangle \right| \mathrm{d}s$$
$$\le \|\widehat{h}''\|_\infty \cdot \sqrt{\otimes \mathbf{p}} \cdot \left\|\widehat{\rho}_{0;\mathbf{0}}\right\|_{\ell^2} \cdot \frac{C_\epsilon}{g-\epsilon} < \infty,$$

which gives $\lim\limits_{t\to\infty} \frac{1}{t}|N_3(t)| = 0$.

Case $n=4$: N_4 can be estimated by applying Lemma 4.3.10 twice:

$$\sup_t \int_0^t \int_0^s \left\langle\, \partial_i \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\partial_j\widehat{\mathcal{L}}_0\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}(1-Q_{\mathbf{0}})\,\Phi_0 \right\rangle \mathrm{d}r\,\mathrm{d}s$$
$$\le \left\|\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}\right\| \cdot \left\|\partial_j\widehat{\mathcal{L}}_0\right\| \cdot \|\Phi_0\| \cdot C_\epsilon^2 \sup_t \int_0^t \int_0^s \mathrm{e}^{-(s-r)(g-\epsilon)}\,\mathrm{e}^{-r(g-\epsilon)}\,\mathrm{d}r\,\mathrm{d}s$$
$$\le \|\widehat{h}'\|_\infty^2 \cdot \sqrt{\otimes \mathbf{p}} \cdot \left\|\widehat{\rho}_{0;\mathbf{0}}\right\|_{\ell^2} \cdot C_\epsilon^2 \cdot \left(\frac{1}{g-\epsilon} + \frac{1}{(g-\epsilon)^2}\right) < \infty,$$

and thus, $\lim\limits_{t\to\infty} \frac{1}{t}|N_4(t)| = 0$.

Case $n=5$: It remains to estimate $\frac{1}{t}N_5$. Recall we obtained $Q_{\mathbf{0}}\Phi_0 = \varphi_{\mathbf{0}}$ in (4.4.7). This

$$\frac{1}{t}\int_0^t \int_0^s \left\langle\, \partial_i \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\,\varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\partial_j\widehat{\mathcal{L}}_0\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,Q_{\mathbf{0}}\,\Phi_0 \right\rangle \mathrm{d}r\,\mathrm{d}s$$
$$= -\left\langle\, \partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}}\,,\ \left(\frac{1}{t}\int_0^t\int_0^s \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\mathrm{d}r\,\mathrm{d}s\right)\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}} \right\rangle,$$

since $\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}} \in \operatorname{ran}(1-Q_{\mathbf{0}})$, $(1-Q_{\mathbf{0}})\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}} = \partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}$.

Since $\operatorname{Re}\widehat{\mathcal{L}}_{\mathbf{0}} \ge 0$, by a standard contour integral argument, the following formula was obtained in [23, 33]

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t\int_0^s \Pi_2\mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\Pi_2\,\mathrm{d}r\,\mathrm{d}s = \Pi_2\left((1-Q_{\mathbf{0}})\widehat{\mathcal{L}}_{\mathbf{0}}(1-Q_{\mathbf{0}})\right)^{-1}\Pi_2 = \Pi_2\mathcal{J}^{-1}\Pi_2, \tag{4.4.23}$$

where $\mathcal{J}^{-1}$ is as in Lemma 4.3.9 . Recall that $\partial_i\widehat{\mathcal{K}}_{\mathbf{0}} \in \operatorname{Ran}(\Pi_2) \subseteq \operatorname{Ran}(P_2)$. Thus

$$\lim_{t\to\infty}\frac{1}{t}N_5 = \left\langle\, \partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}}\,,\ \Pi_2\mathcal{J}^{-1}\Pi_2\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}} \right\rangle + \left\langle\, \partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}}\,,\ \Pi_2\mathcal{J}^{-1}\Pi_2\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}} \right\rangle$$
$$= \left\langle\, \partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}}\,,\ P_2\mathcal{J}^{-1}\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}} \right\rangle + \left\langle\, \partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}}\,,\ P_2\mathcal{J}^{-1}\partial_i\widehat{\mathcal{K}}_{\mathbf{0}}\,\varphi_{\mathbf{0}} \right\rangle$$
$$= \partial_i\partial_j E(\mathbf{0}),$$

where the last line follows from the formula of $\partial_i\partial_j E(\mathbf{0})$ in (4.3.31). $\square$

4.4.3 Limiting behavior of $\mathbf{D}(\lambda)$ for small λ

The following lemma can be found in [33]. It will be the main tool for us to study the asymptotic behavior of $\mathbf{D}(\lambda)$.

Lemma 4.4.4 (Lemma D.1, [33])**.** *Let A and R be bounded operators on a Hilbert space $\mathcal{H}$. If A is normal,* $\operatorname{Re} A \geq 0$ *and* $\operatorname{Re} R \geq c > 0$*, then for any $\phi, \psi \in \mathcal{H}$,*

$$\lim_{\eta \to 0} \left\langle \phi,\ \left(\eta^{-1} A + R\right)^{-1} \psi \right\rangle_{\mathcal{H}} = \left\langle \Pi\phi,\ (\Pi R \Pi)^{-1}\, \Pi\psi \right\rangle_{\operatorname{ran}\Pi}$$

where $\Pi =$ projection onto the kernel of A.

Remark 4.4.5. A similar statement holds for a family of bounded operators R_η such that $\operatorname{Re} R_\eta \geq c > 0$ and $\lim_{\eta\to 0} R_\eta = R_0$ in the strong operator topology and $R_0 \geq c > 0$, i.e.,

$$\lim_{\eta \to 0} \left\langle \phi,\ \left(\eta^{-1} A + R_\eta\right)^{-1} \psi \right\rangle_{\mathcal{H}} = \left\langle \Pi\phi,\ (\Pi R_0 \Pi)^{-1}\, \Pi\psi \right\rangle_{\operatorname{ran}\Pi}.$$

$\triangle$

In view of Lemma 4.3.9, we want to have the block form of the above lemma.

Lemma 4.4.6. *Let A be a bounded self-adjoint operator on a Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ with the following block form:*

$$A = \begin{pmatrix} 0 & A_2 \\ A_2^\dagger & A_3 \end{pmatrix}, \quad A_3^\dagger = A_3. \tag{4.4.24}$$

Let $\Pi =$ projection onto the kernel of A, $\Pi_2 =$ projection onto the kernel of A_2 and $\widetilde{\Pi} =$ projection onto the kernel of $\Pi_2 A_3 \Pi_2$. For any $\varphi = \Pi_2\varphi$,

$$\Pi\varphi = 0 \quad \textit{if and only if} \quad \widetilde{\Pi}\varphi = 0.$$

Proof. For any $\varphi \in \mathcal{H}$, direct application of Lemma 4.4.4 to $I + \mathrm{i}\,\eta^{-1}A$ gives

$$\lim_{\eta\to 0}\left\langle \varphi,\ (I+\mathrm{i}\,\eta^{-1}A)^{-1}\varphi\right\rangle = \left\langle \Pi\varphi,\ (\Pi\, I\,\Pi)^{-1}\Pi\varphi\right\rangle = \|\Pi\varphi\|^2. \tag{4.4.25}$$

Let P_1, P_2 be the projection onto $\mathcal{H}_1, \mathcal{H}_2$ correspondingly and consider $\varphi \in \mathrm{ran}(\Pi_2)$. By the block form of A and Schur's formula, we have

$$\begin{aligned}\left\langle \varphi,\ (I+\mathrm{i}\,\eta^{-1}A)^{-1}\varphi\right\rangle &= \left\langle \varphi,\ (P_2+\mathrm{i}\eta^{-1}A_3+\eta^{-2}A_2^\dagger A_2)^{-1}\,\varphi\right\rangle \\ &= \left\langle \varphi,\ \Pi_2(P_2+\mathrm{i}\eta^{-1}A_3+\eta^{-2}A_2^\dagger A_2)^{-1}\Pi_2\,\varphi\right\rangle. \end{aligned}\tag{4.4.26}$$

If we apply Schur's formula one more time with respect to the decomposition $\mathcal{H}_2 = \mathrm{ran}(\Pi_2)\oplus \mathrm{ran}(\Pi_2^\perp)$ and notice that $\Pi_2 A_2^\dagger = A_2\Pi_2 = 0$, then we have

$$\left\langle \varphi,\ (I+\mathrm{i}\,\eta^{-1}A)^{-1}\varphi\right\rangle = \left\langle \varphi,\ \left(\mathrm{i}\eta^{-1}\Pi_2A_3\Pi_2 + \Pi_2 + \widetilde{A}\right)^{-1}\ \varphi\right\rangle$$

where $\widetilde{A} = \Pi_2A_3\Pi_2^\perp\left(\eta^2\Pi_2^\perp + \mathrm{i}\eta\Pi_2^\perp A_3\Pi_2^\perp + \Pi_2^\perp A_2^\dagger A_2\Pi_2^\perp\right)^{-1}\Pi_2^\perp A_3\Pi_2$. By (4.4.24), $\mathrm{Re}\,\widetilde{A} \geq 0$ on $\mathrm{ran}(\Pi_2)$, which implies $\mathrm{Re}(\Pi_2+\widetilde{A}) \geq 1 > 0$ on $\mathrm{ran}(\Pi_2)$.

Therefore, by Lemma 4.4.4 and Remark 4.4.5, we have that

$$\begin{aligned}&\lim_{\eta\to 0}\left\langle \varphi,\ (I+\mathrm{i}\,\eta^{-1}A)^{-1}\varphi\right\rangle \\ &= \lim_{\eta\to 0}\left\langle \varphi,\ \left(\mathrm{i}\eta^{-1}\Pi_2A_3\Pi_2 + \Pi_2 + \widetilde{A}\right)^{-1}\ \varphi\right\rangle \\ &= \left\langle \widetilde{\Pi}\varphi,\ \left(\widetilde{\Pi} + \widetilde{\Pi}\,\Pi_2A_3\Pi_2^\perp\left(\Pi_2^\perp A_2^\dagger A_2\Pi_2^\perp\right)^{-1}\Pi_2^\perp A_3\Pi_2\widetilde{\Pi}\right)^{-1}\ \widetilde{\Pi}\varphi\right\rangle, \end{aligned}\tag{4.4.27}$$

where $\widetilde{\Pi} =$ projection onto the kernel of $\Pi_2A_3\Pi_2$.

Putting (4.4.25) and (4.4.27) together, we have that

$$\left\langle \widetilde{\Pi}\varphi,\ \left(\widetilde{\Pi} + \widetilde{\Pi}\,\Pi_2A_3\Pi_2^\perp\left(\Pi_2^\perp A_2^\dagger A_2\Pi_2^\perp\right)^{-1}\Pi_2^\perp A_3\Pi_2\,\widetilde{\Pi}\right)^{-1}\ \widetilde{\Pi}\varphi\right\rangle = \|\Pi\varphi\|^2,$$

which completes the proof of Lemma 4.4.6. □

Now we can proceed to prove (4.1.15) in Theorem 4.1.11. As showed in Equation (4.3.31) and Lemma 4.4.1, the diffusion matrix $\mathbf{D}(\lambda)$ is independent of the initial condition $\psi_0 \in \ell^2(\mathbb{Z}^d)$. To study the asymptotic behavior of $\mathbf{D}(\lambda)$, it is enough to consider $\psi_0(x) = \delta_{\mathbf{0}}$, where we assume the ballistic motion holds in (4.1.14).

Proof of (4.1.15). We are going to apply Lemma 4.4.6 to A acting on $\widehat{\mathcal{H}}_1 \oplus \widehat{\mathcal{H}}_2$ given by:

$$A = P(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})P = \begin{pmatrix} 0 & P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2 \\ P_2\widehat{\mathcal{K}}_{\mathbf{0}}P_1 & P_2(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})P_2 \end{pmatrix}, \tag{4.4.28}$$

where $\widehat{\mathcal{H}}_i, P_i, i = 1, 2$ are as in (4.3.11) and $P = P_1 + P_2$. Let Π = projection onto the kernel of $P(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})P$, Π_2 = projection onto the kernel of $P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2$ and $\widetilde{\Pi}$ = projection onto the kernel of $\Pi_2(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})\Pi_2$.

Let $\widetilde{\phi}_j = \partial_j\widehat{\mathcal{K}}_{\mathbf{0}}\varphi_{\mathbf{0}}, j = 1 \cdots, d$, which are given as in (4.2.26). Recall that $\widetilde{\phi}_j \in \mathrm{Ker}(P_1\widehat{\mathcal{K}}_{\mathbf{0}}P_2)$, therefore $\widetilde{\phi}_j = \Pi_2\widetilde{\phi}_j$. Let $M_{i,j}$ be as in (4.4.10) and $\widehat{\rho}_{0;\mathbf{k}}$ be as in (4.2.31). By the decomposition in Lemma 4.4.2 at $\lambda = 0$, one can check that [2]

$$2\left\langle \widetilde{\phi}_j,\ \left(P + \eta^{-1}\mathrm{i}(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})\right)^{-1}\widetilde{\phi}_j \right\rangle = \eta^3 \int_0^\infty e^{-\eta t}\, M_{j,j}(t)\, \mathrm{d}t + O(\eta^2). \tag{4.4.29}$$

When $\lambda = 0$, $\widehat{\mathcal{L}}_{\mathbf{0}} = \mathrm{i}(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})$ is the unperturbed periodic operator on $\ell^2(\mathbb{Z}^d; \mathbb{C}^{\otimes \mathbf{p}})$. Setting $\eta = 2T^{-1}$ in (4.1.14), there is a $c > 0$ such that for all j and η small,

$$\eta^3 \int_0^\infty e^{-\eta t}\, M_{j,j}(t)\, \mathrm{d}t = \frac{8}{T^3}\int_0^\infty e^{-\frac{2t}{T}} \sum_{x\in\mathbb{Z}^d} x_j^2\, \mathbb{E}\left(|\psi_t(x)|^2\right)\, \mathrm{d}t \geq c > 0. \tag{4.4.30}$$

Put (4.4.25), (4.4.29) and (4.4.30) together, we have

$$\left\|\Pi\widetilde{\phi}_j\right\|^2 = \lim_{\eta\to 0}\left\langle \widetilde{\phi}_j,\ \left(P + \eta^{-1}\mathrm{i}(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})\right)^{-1}\widetilde{\phi}_j \right\rangle > 0.$$

Therefore, $\Pi\widetilde{\phi}_j \neq 0$ and Lemma 4.4.6 implies that $\widetilde{\Pi}\widetilde{\phi}_j \neq 0$.

Recall that $\widehat{\mathcal{L}}_{\mathbf{0}} = \mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}} + \mathrm{i}\lambda\widehat{\mathcal{V}} + B$ and $\Gamma_2 = P_2\left(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}} + \lambda^2\widehat{\mathcal{V}}\,(P_3\widehat{\mathcal{L}}_{\mathbf{0}}P_3)^{-1}\,\widehat{\mathcal{V}}\right)P_2$ as in (4.3.15). Let $R_\lambda = \Pi_2\widehat{\mathcal{V}}\left(P_3\widehat{\mathcal{L}}_{\mathbf{0}}P_3\right)^{-1}\widehat{\mathcal{V}}\Pi_2$ and $R_0 = \Pi_2\widehat{\mathcal{V}}\left(P_3(\mathrm{i}\widehat{\mathcal{K}}_{\mathbf{0}} + \mathrm{i}\widehat{\mathcal{U}})P_3\right)^{-1}\widehat{\mathcal{V}}\Pi_2$. Then $\Pi_2\Gamma_2\Pi_2 = \mathrm{i}\,\Pi_2P_2(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})P_2\Pi_2 + \lambda^2R_\lambda$ and $\lim_{\lambda\to 0} R_\lambda = R_0$ (in the strong operator

[2]This formula was obtained in [33], Section 4.7, where there is no error term $O(\eta^2)$. In [33], the choice $\psi_0 = \delta_{\mathbf{0}}$ implies that $M_{j,j}(0) = 0$ and $\widehat{\rho}_{0;\mathbf{0}} = \delta_{\mathbf{0}} \otimes \overrightarrow{1}$ and the proof is relatively simple. In the general $\mathbf{p}$-periodic case, the initial condition $\delta_{\mathbf{0}}$ no longer provides the simplified expressions of $M_{j,j}(0)$ and $\widehat{\rho}_{0;\mathbf{0}}$. We need the correction term for small η. The proof for the general case is essentially based on the same strategy for Lemma 4.4.3; we omit the details here.

topology). Applying Lemma 4.4.4 (and Remark 4.4.5) to $\Pi_2\Gamma_2\Pi_2$ on $\operatorname{ran}(\Pi_2)$, we obtain that, for any $1 \le i, j \le d$,

$$\begin{aligned}\lim_{\lambda\to 0} \lambda^2 \left\langle \widetilde{\phi}_i,\ (\Pi_2\Gamma_2\Pi_2)^{-1}\ \widetilde{\phi}_j \right\rangle &= \lim_{\lambda\to 0} \left\langle \widetilde{\phi}_i,\ \left(\mathrm{i}\,\lambda^{-2}\Pi_2(\widehat{\mathcal{K}}_{\mathbf{0}} + \widehat{\mathcal{U}})\Pi_2 + R_\lambda\right)^{-1}\ \widetilde{\phi}_j \right\rangle \\ &= \left\langle \widetilde{\Pi}\widetilde{\phi}_i,\ \left(\widetilde{\Pi}R_0\widetilde{\Pi}\right)^{-1}\ \widetilde{\Pi}\widetilde{\phi}_j \right\rangle.\end{aligned}$$

In particular, $\lim_{\lambda\to 0} \lambda^2 \left\langle \widetilde{\phi}_j,\ (\Pi_2\Gamma_2\Pi_2)^{-1}\ \widetilde{\phi}_j \right\rangle = \left\langle \widetilde{\Pi}\widetilde{\phi}_j,\ \left(\widetilde{\Pi}R_0\widetilde{\Pi}\right)^{-1}\ \widetilde{\Pi}\widetilde{\phi}_j \right\rangle > 0$.

By Lemma 4.3.9 and (4.3.31), we have

$$\lim_{\lambda\to 0} \lambda^2\partial_i\partial_j E(\mathbf{0}) = \left\langle \widetilde{\Pi}\widetilde{\phi}_j,\ \left(\widetilde{\Pi}R_0\widetilde{\Pi}\right)^{-1}\ \widetilde{\Pi}\widetilde{\phi}_i \right\rangle + \left\langle \widetilde{\Pi}\widetilde{\phi}_i,\ \left(\widetilde{\Pi}R_0\widetilde{\Pi}\right)^{-1}\ \widetilde{\Pi}\widetilde{\phi}_j \right\rangle =: \mathbf{D}^0_{ij}.$$

Let $\mathbf{D}^0 := (\mathbf{D}^0_{ij})_{d\times d}$. Then $\lim_{\lambda\to 0} \lambda^2\mathbf{D} = \mathbf{D}^0$ and $\langle \mathbf{k},\ \mathbf{D}^0\mathbf{k}\rangle > 0$ for any $\mathbf{0} \ne \mathbf{k} \in \mathbb{R}^d$ by the same argument for $\mathbf{D}$. As a consequence,

$$\lim_{\lambda\to 0} \lambda^2 \operatorname{tr}\mathbf{D} = \operatorname{tr}\mathbf{D}^0 > 0.$$

This completes the proof of Theorem 2.0.3. $\square$

CHAPTER 5

NUMERICAL ANALYSIS OF DIFFUSION IN MARKOV SCHRÖDINGER EQUATIONS

Recall that we are interested in solving a one dimensional, time-dependent Schrödinger equation of the form,

$$\begin{cases} \mathrm{i}\dfrac{\partial \psi_t(n)}{\partial t} = H_\alpha \psi_t(n) + \lambda v_n(\omega(t))\psi_t(n), \\ \quad \psi_0(n) = \delta_0(n). \end{cases} \tag{5.0.1}$$

Here, the unperturbed Hamiltonian H_α is given by either the dimer or trimmed Anderson model and the time dependent potential $v_n(\omega(t)) := \omega_n(t)$ is given by the "flip process". Briefly, the "flip process" is obtained by randomly selecting an initial state $\omega(0) \in \{-1, 1\}^{\mathbb{Z}}$ and assigning independent and identical Poisson processes to each site. The disorder $\omega(t)$ obtains time dependence by flipping the sign of $\omega_n(t)$ once the Poisson process at n fires. Another description of the "flip process" is given in Chapter 2.

For these two models we will numerically calculate the diffusion constant as a function of the disorder, $D(\lambda)$; with a particular interest in small values of λ. Section 5.1 outlines the methods used to calculate $D(\lambda)$, while Section 5.2 discusses the asymptotic behavior of $D(\lambda)$ for small λ. In the next chapter we will compare these results to those of the periodic case.

5.1 Numerical Method

The time dependence of the Hamiltonian,

$$H(t, \lambda) = H_\alpha + \lambda v(\omega(t)) \tag{5.1.1}$$

is contained solely in the "flip process", $v(\omega(t))$. By restricting the possible arrival times of each of the individual Poisson processes to the discrete set,

$$t \in \Delta t \cdot \mathbb{N} := \{\Delta t, 2\Delta t, \ldots, N\Delta t, \ldots\}, \qquad \Delta t \ll 1,$$

the evolution of the wave function from time t to $t + \Delta t$ is given by

$$\psi_{t+\Delta t} = \mathrm{e}^{-\mathrm{i}H(t)\Delta t}\psi_t. \tag{5.1.2}$$

Without knowing the eigenvalues of $H(t)$, calculating the exponential in Equation (5.1.2) can be extremely difficult and computationally expensive. To overcome this difficultly we will approximate the exponential with the Cayley transform,

$$\mathrm{e}^{-\mathrm{i}H(t)\Delta t} \approx \frac{1 - \frac{1}{2}\mathrm{i}H(t)\Delta t}{1 + \frac{1}{2}\mathrm{i}H(t)\Delta t}. \tag{5.1.3}$$

Note, the operator on the right hand side of Equation (5.1.3) is unitary. Combining Equations (5.1.2) and (5.1.3) yields the evolution equation,

$$\left(1 + \frac{1}{2}\mathrm{i}H(t)\Delta t\right)\psi_{t+\Delta t} = \left(1 - \frac{1}{2}\mathrm{i}H(t)\Delta t\right)\psi_t. \tag{5.1.4}$$

For a given value of λ, we solve Equation (5.0.1), via the evolution equation (5.1.4), for 32 trails. Each trial begins with $\psi_0 = \delta_0$ and is initially confined to a lattice of length 300. To minimize effects from the boundary the lattice is expanded by adding 150 sites to each end once the probability of finding the particle at either boundary becomes greater than 10^{-30}.

Once the wave function ψ_t is known for each of the 32 trials, we calculate the second moment as a function of time,

$$\left\langle X_t^2 \right\rangle := \sum_n |n|^2 \mathbb{E}(|\psi_t(n)|^2). \tag{5.1.5}$$

Here $\mathbb{E}(|\psi_t(n)|^2)$ denotes the average probability density over the 32 trials. This averaging removes any dependence on any specific realization of H_α and $v(\omega(t))$. Equipped with $\langle X_t^2 \rangle$, we calculate the diffusion constant as a function of time and disorder,

$$D(\lambda, t) := \frac{1}{t}\langle X_t^2 \rangle. \tag{5.1.6}$$

Finally, to remove time dependence we average $D(\lambda, t)$ over the tail end of each trial, i.e.,

$$D(\lambda) = \frac{1}{T}\int_{[t,t+T]} \mathrm{d}t'\, D(\lambda, t'). \tag{5.1.7}$$

5.2 Results

5.2.1 Dimer Model

For the dimer model we take the two site energies as $\varepsilon_a = 1, \varepsilon_b = 0$. This choice ensures superdiffusive scaling in the absence of disorder,

$$\left\langle X_t^2 \right\rangle \sim t^{3/2}. \tag{5.2.1}$$

Figure 5.1 shows the diffusion constant as a function of time for small values of λ. In figure 5.2 the average diffusion constant, Equation (5.1.7), is plotted as a function of λ. Importantly, these two figures show that the addition of disorder leads to diffusion and in the small λ limit the diffusion constant scales like $\lambda^{-1.093}$.

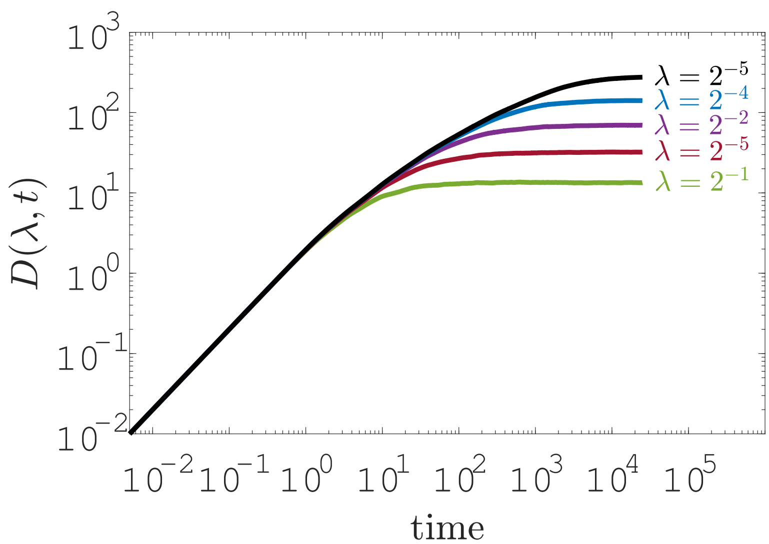

Figure 5.1: The diffusion constant as a function of time and disorder strength.

5.2.2 Trimmed Anderson Model

For the trimmed Anderson model we support the static random potential of H_α on $\Gamma = 2\mathbb{Z}$. In this case the second moment scales subdiffusively, see figure 2.3. This system diffuses for

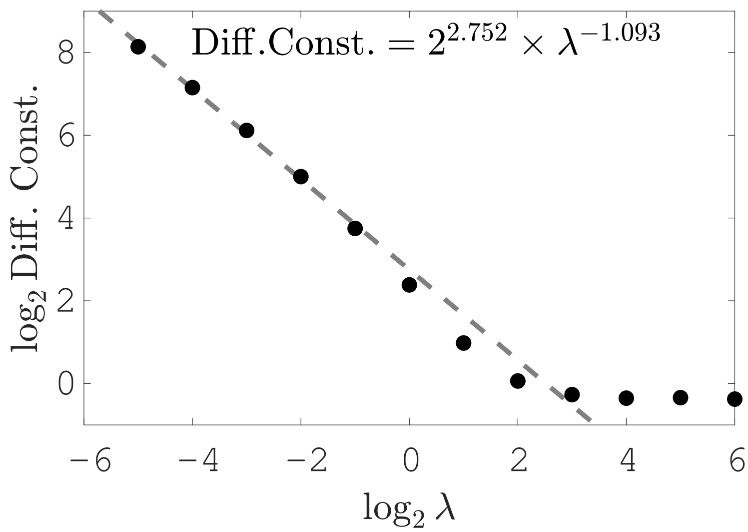

Figure 5.2: The average diffusion constant as a function of the disorder strength for the dimer model.

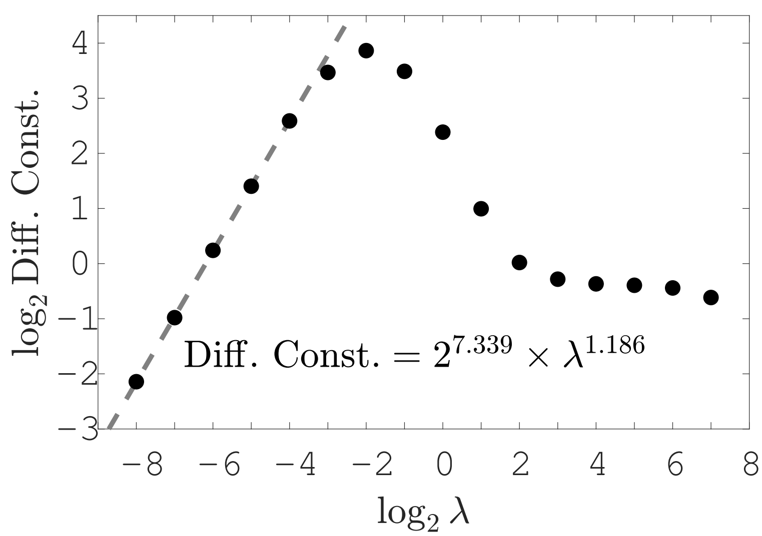

Figure 5.3: The average diffusion constant as a function of the disorder strength for the trimmed Anderson model.

any value of disorder. Plotting the average value of the diffusion constant vs disorder shows that in the small λ limit the diffusion constant scales like $\lambda^{1.186}$.

CHAPTER 6

CONCLUSIONS AND CONJECTURES

In light of the present work, it is natural to wonder whether a result similar to those presented in Theorem 4.1.11 hold for a general ergodic/deterministic potential U. In particular,

1. Under what assumptions will a potential, U, cause solutions to the Markov Schrödinger equation,
$$\begin{cases} \mathrm{i}\partial_t \psi_t(x) = H_0 \psi_t(x) + U\psi_t(x) + \lambda V_{\omega(t)} \psi_t(x), \\ \psi_0(x) \in \ell^2(\mathbb{Z}^d), \end{cases} \tag{6.0.1}$$
to display diffusive propagation over large time scales?

2. If diffusive propagation holds, what is the asymptotic behavior of the diffusion constant in the small λ limit?

Based on the behavior of the (6.0.1) with $U \equiv 0$ [23], U a random potential leading to localization [33], U periodic [34], and the anomalous cases (Chapter 5), we make the following conjecture:

Conjecture 6.0.1. For any bounded potential, U, and any coupling constant, $\lambda > 0$, there exist positive, finite upper and lower diffusion constants, $\overline{D}(U, \lambda)$ and $\underline{D}(U, \lambda)$, such that the solutions to equation (6.0.1) satisfy

$$\underline{D}(U, \lambda) := \liminf_{t \to \infty} \frac{1}{t} \sum_{x \in \mathbb{Z}^d} |x|^2 \mathbb{E}\left(|\psi_t(x)|^2\right) \leq \limsup_{t \to \infty} \frac{1}{t} \sum_{x \in \mathbb{Z}^d} |x|^2 \mathbb{E}\left(|\psi_t(x)|^2\right) =: \overline{D}(U, \lambda). \tag{6.0.2}$$

Furthermore, if

$$\lim_{t \to \infty} \frac{1}{t^\gamma} \sum_{x \in \mathbb{Z}^d} |x|^2 |\langle \delta_x, \mathrm{e}^{-\mathrm{i}(H_0 + U)} \delta_0 \rangle|^2 \in (0, \infty), \qquad \gamma \in [1, 2], \tag{6.0.3}$$

then

$$\overline{D}(U, \lambda) \sim O(\lambda^{2-2\gamma}) \qquad \text{and} \qquad \underline{D}(U, \lambda) \sim O(\lambda^{2-2\gamma}). \tag{6.0.4}$$

Remark 6.0.2. We have limited the transport exponent in the asymptotic formula (6.0.4) to the range $[1, 2]$. This lower bound is suggested by the trimmed Anderson model, where $\gamma = 0.07795$ and $D \sim \lambda^{1.186}$ instead of $D \sim \lambda^{1.8441}$ which (6.0.4) would predict. $\triangle$

We end with a conjecture about the almost Mathiue operator on $\ell^2(\mathbb{Z})$,

$$(H_\theta^{g,\alpha}\psi_t)(x) = \psi_t(x+1) + \psi_t(x-1) + 2g\cos 2\pi(\theta + x\alpha)\psi_t(x), \tag{6.0.5}$$

with parameters $g \in \mathbb{R}$ and $\theta, \alpha \in [0, 1]$:

Conjecture 6.0.3. For almost every $\theta, \alpha \in [0, 1]$, the AMO-Markovian equation has a diffusion constant $D(g, \lambda) \in (0, \infty)$ which is a smooth function for all $(g, \lambda) \in \mathbb{R} \times \mathbb{R}^+$. Moreover, $D(g, \lambda) \sim O(\lambda^2)$ for all $|g| > 1$ and $D(g, \lambda) \sim O(\lambda^{-2})$ for all $|g| < 1$.

APPENDICES

APPENDIX A

DECOMPOSITION OF THE SECOND MOMENTS AND THE PROOF OF LEMMA 4.4.2

The following facts will be used to simplify the expression of the second order partial derivative. Note that $\widehat{\mathcal{L}}_{\mathbf{0}}\,\varphi_{\mathbf{0}} = \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\,\varphi_{\mathbf{0}} \;=\; 0$, implies that $\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}$ and $\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}}$ act trivially on $\varphi_{\mathbf{0}}$ for any t, i.e.,

$$\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}\varphi_{\mathbf{0}} = \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}}\varphi_{\mathbf{0}} = \varphi_{\mathbf{0}} \tag{A.0.1}$$

and

$$\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}Q_{\mathbf{0}} = \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}}Q_{\mathbf{0}} = Q_{\mathbf{0}}. \tag{A.0.2}$$

On the other hand, recall the formula for differentiating a semi-group,

$$\partial_j\left(\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\right) \;=\; -\int_0^t \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{k}}}\,\partial_j\widehat{\mathcal{L}}_{\mathbf{k}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{k}}}\,\mathrm{d}s. \tag{A.0.3}$$

By (4.2.20) and (4.2.28), we have $\partial_j\widehat{\mathcal{L}}_{\mathbf{0}} = \mathrm{i}\,\partial_j\widehat{\mathcal{K}}_{\mathbf{0}} = -\partial_j\,\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}$. Because $\partial_j\widehat{\mathcal{K}}_{\mathbf{0}}$ maps $\widehat{\mathcal{H}}_0 \oplus \widehat{\mathcal{H}}_1$ to $\widehat{\mathcal{H}}_2$, we also have that

$$Q_{\mathbf{0}}\partial_j\widehat{\mathcal{L}}_{\mathbf{0}} = Q_{\mathbf{0}}\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} = 0; \tag{A.0.4}$$

$$\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{0}} = \mathrm{i}\partial_i\partial_j\widehat{\mathcal{K}}_{\mathbf{0}} = -\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} \text{ and } Q_{\mathbf{0}}\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{0}} = Q_{\mathbf{0}}\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger} = 0. \tag{A.0.5}$$

Direct computation from (4.4.11) gives

$$\begin{aligned}
M_{i,j}(t) =& -\,\partial_i\partial_j\left\langle\varphi_{\mathbf{0}},\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\,\Phi_{\mathbf{k}}\right\rangle\Big|_{\mathbf{k}=\mathbf{0}}\\
=& -\left\langle\varphi_{\mathbf{0}}\ ,\ \mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\partial_j\Phi_{\mathbf{0}}\right\rangle && \text{(A.0.6)}\\
& -\left\langle\varphi_{\mathbf{0}}\ ,\ \left(\partial_i\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}\right)_{|\mathbf{k}=\mathbf{0}}\,\partial_j\Phi_{\mathbf{0}}\right\rangle - \left\langle\varphi_{\mathbf{0}}\ ,\ \left(\partial_j\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}\right)_{|\mathbf{k}=\mathbf{0}}\,\partial_i\Phi_{\mathbf{0}}\right\rangle && \text{(A.0.7)}\\
& -\left\langle\varphi_{\mathbf{0}}\ ,\ \left(\partial_i\partial_j\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{0}}}\right)_{|\mathbf{k}=\mathbf{0}}\,\Phi_{\mathbf{0}}\right\rangle. && \text{(A.0.8)}
\end{aligned}$$

Clearly, (A.0.6) gives the expression for N_1 in (4.4.12). Now let's proceed to simplify the expression in (A.0.7). By the differential formula (A.0.3), we obtain

$$\begin{aligned}\left\langle \varphi_{\mathbf{0}}\,,\ \left(\partial_i\,\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\right)_{|\mathbf{k}=0}\,\partial_j\Phi_{\mathbf{0}}\right\rangle &= \left\langle \varphi_{\mathbf{0}}\,,\ \left(-\int_0^t \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\mathrm{d}s\right)\,\partial_j\Phi_{\mathbf{0}}\right\rangle \\ &= -\int_0^t \left\langle \varphi_{\mathbf{0}}\,,\ \ \partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\,\partial_j\Phi_{\mathbf{0}}\right\rangle\,\mathrm{d}s,\end{aligned}$$

where we use the fact by (A.0.2) that $\left\langle \varphi_{\mathbf{0}}\,,\ \ \partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,Q_{\mathbf{0}}\,\partial_j\Phi_{\mathbf{0}}\right\rangle = 0$. This gives the expression for N_2 in (4.4.13).

Simplifying (A.0.8) requires applying (A.0.3) twice. Differentiating (A.0.3) again yields,

$$\begin{aligned}\partial_i\partial_j\left(\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\right)\Big|_{\mathbf{k}=\mathbf{0}} &= -\int_0^t \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\mathrm{d}s \\ &\quad+\int_0^t\left(\int_0^{t-s}\mathrm{e}^{-(t-s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,\mathrm{d}r\right)\,\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\mathrm{d}s \\ &\quad+\int_0^t \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\left(\int_0^s \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,\mathrm{d}r\right)\,\mathrm{d}s.\end{aligned}$$

Therefore,

$$-\left\langle \varphi_{\mathbf{0}}\,,\ \left(\partial_i\partial_j\mathrm{e}^{-t\widehat{\mathcal{L}}_{\mathbf{k}}}\right)_{|\mathbf{k}=\mathbf{0}}\,\Phi_{\mathbf{0}}\right\rangle = \int_0^t \left\langle \varphi_{\mathbf{0}}\,,\ \ \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\partial_j\,\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\Phi_{\mathbf{0}}\right\rangle\,\mathrm{d}s \tag{A.0.9}$$

$$-\int_0^t\int_0^{t-s}\left\langle \varphi_{\mathbf{0}}\,,\ \ \mathrm{e}^{-(t-s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\Phi_{\mathbf{0}}\right\rangle\mathrm{d}r\,\mathrm{d}s \tag{A.0.10}$$

$$-\int_0^t\int_0^{s}\left\langle \varphi_{\mathbf{0}}\,,\ \ \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,\Phi_{\mathbf{0}}\right\rangle\mathrm{d}r\,\mathrm{d}s. \tag{A.0.11}$$

The expression on the right hand side of (A.0.9) leads to N_3 in (4.4.14) since

$$\left\langle \varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\partial_j\,\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\Phi_{\mathbf{0}}\right\rangle = \left\langle \partial_i\partial_j\,\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\varphi_{\mathbf{0}}\,,\ \ \mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\,\Phi_{\mathbf{0}}\right\rangle.$$

Expressions for (A.0.10) and (A.0.11) follow from (A.0.2) and (A.0.4) by direct computations. For (A.0.10) we have,

$$-\int_0^t\int_0^{t-s}\left\langle \varphi_{\mathbf{0}}\,,\ \ \mathrm{e}^{-(t-s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-s\widehat{\mathcal{L}}_{\mathbf{0}}}\,\Phi_{\mathbf{0}}\right\rangle\mathrm{d}r\,\mathrm{d}s$$

$$= -\int_0^t\int_0^{s}\Big[\left\langle \partial_i\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\,\varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}(1-Q_{\mathbf{0}})\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\Phi_{\mathbf{0}}\right\rangle \tag{A.0.12}$$

$$+\left\langle \partial_i\widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\,\varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}(1-Q_{\mathbf{0}})\partial_j\widehat{\mathcal{L}}_{\mathbf{0}}\,Q_{\mathbf{0}}\Phi_{\mathbf{0}}\right\rangle\Big]\,\mathrm{d}r\,\mathrm{d}s. \tag{A.0.13}$$

Similarily, for (A.0.11),

$$
\begin{aligned}
&-\int_0^t \int_0^s \Big\langle \varphi_{\mathbf{0}}\,,\ \ \mathrm{e}^{-(t-s)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_j \widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}\,\partial_i \widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,\Phi_{\mathbf{0}}\Big\rangle\,\mathrm{d}r\,\mathrm{d}s \\
&\qquad = -\int_0^t \int_0^s \Big[\Big\langle\,\partial_j \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\,\varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}(1-Q_{\mathbf{0}})\partial_i \widehat{\mathcal{L}}_{\mathbf{0}}\,\mathrm{e}^{-r\widehat{\mathcal{L}}_{\mathbf{0}}}\,(1-Q_{\mathbf{0}})\Phi_{\mathbf{0}}\Big\rangle \qquad \text{(A.0.14)} \\
&\qquad\quad + \Big\langle\,\partial_j \widehat{\mathcal{L}}_{\mathbf{0}}^{\dagger}\,\varphi_{\mathbf{0}}\,,\ \mathrm{e}^{-(s-r)\widehat{\mathcal{L}}_{\mathbf{0}}}(1-Q_{\mathbf{0}})\partial_i \widehat{\mathcal{L}}_{\mathbf{0}}\,Q_{\mathbf{0}}\Phi_{\mathbf{0}}\Big\rangle\Big]\,\mathrm{d}r\,\mathrm{d}s. \qquad \text{(A.0.15)}
\end{aligned}
$$

Clearly,

$$
N_4 = \text{(A.0.12)} + \text{(A.0.14)}, \quad N_5 = \text{(A.0.13)} + \text{(A.0.15)}. \tag{A.0.16}
$$

This completes the proof of Lemma 5.2.

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