# 博士論文

# Long-range scattering problem and continuum limit of discrete Schrödinger operators

# (離散シュレディンガー作用素の長距離散乱問題と連続極限)

氏名：只野　之英

January 9, 2019

# Contents

# Chapter 1

# Introduction

The Schrödinger equation on the Euclidean space $\mathbb{R}^d$

$$\begin{cases} i\partial_t u(t,x) = (-\Delta_x + V(t,x))u(t,x), & (t,x) \in \mathbb{R} \times \mathbb{R}^d, \\ u(0,x) = u_0(x), & x \in \mathbb{R}^d \end{cases} \tag{1.0.1}$$

has been one of the fundamental equations in quantum physics, and has been studied by not only many physicists but also mathematicians. If $V(t,x)$ does not depend on time $t$, i.e., $V(t,x) = V(x)$, it is well-known that the behavior of (1.0.1) is determined by the spectral analysis of the Schrödinger operators

$$-\Delta_x + V(x) \quad \text{on} \quad L^2(\mathbb{R}^d). \tag{1.0.2}$$

Spectral and scattering properties of (1.0.2) have studied deeply. In particular, there are a lot of remarkable results in the latter half of the twentieth century, and we can see those studies in [2] and [7].

On the other hand, discrete Schrödinger operators

$$H = H_0 + V = -\Delta_{disc} + V_{disc} \tag{1.0.3}$$

are derived from tight-binding approximation of Schrödinger operators which describe the Hamiltonian of electrons in solid state matters. In many cases, $\Delta_{disc}$ is regarded as the discrete Laplacian on the graph in consideration, and $V_{disc}$ as a real-valued function on the graph. It is known that the properties of discrete Schrödinger operators depend on the shape of graph.

*Example* 1.0.1. (1) One of the simplest models is the discrete Schrödinger operators on the square lattice $\mathbb{Z}^d$: For $u \in \ell^2(\mathbb{Z}^d)$

$$\begin{aligned} H_{sq}u(x) &= H_{sq,0}u(x) + Vu(x) \\ &= -\frac{1}{2d} \sum_{|y-x|=1} u(y) + V(x)u(x), \quad x \in \mathbb{Z}^d. \end{aligned}$$

(2) The discrete Schrödinger operators on the triangular lattice is given by

$$\begin{aligned} H_{tr}u(x) &= H_{tr,0}u(x) + Vu(x) \\ &= -\frac{1}{6} \sum_{j=1}^{6} u(x + n_j) + V(x)u(x), \quad x \in \mathbb{Z}^2 \end{aligned}$$

for $u \in \ell^2(\mathbb{Z}^2)$. Here $n_1 = (1,0)$, $n_2 = (-1,0)$, $n_3 = (0,1)$, $n_4 = (0,-1)$, $n_5 = (1,-1)$, $n_6 = (-1,1)$.

(3) The discrete Schrödinger operators on the hexagonal lattice describe a model of tight-binding Hamiltonians of graphene. For $u = {}^t(u_1, u_2) \in \ell^2(\mathbb{Z}^2; \mathbb{C}^2)$, we define

$$\begin{aligned} &H_{he}u(x_1, x_2) = H_{he,0}u(x_1, x_2) + Vu(x_1, x_2) \\ &= -\frac{1}{3} \begin{pmatrix} u_2(x_1, x_2) + u_2(x_1 - 1, x_2) + u_2(x_1, x_2 - 1) \\ u_1(x_1, x_2) + u_1(x_1 + 1, x_2) + u_1(x_1, x_2 + 1) \end{pmatrix} + \begin{pmatrix} V_1(x)u_1(x) \\ V_2(x)u_2(x) \end{pmatrix}. \end{aligned}$$

We note that each point $(x_1, x_2) \in \mathbb{Z}^2$ is equipped with two values $u_1(x_1, x_2)$ and $u_2(x_1, x_2)$. The former corresponds to the dots in the figure below and the latter to the squares.

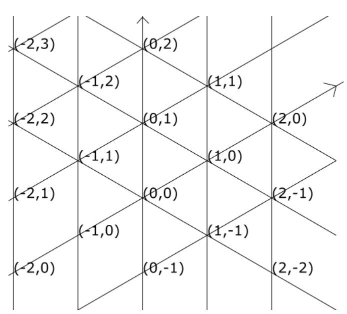


Figure 1.1: Triangular lattice.

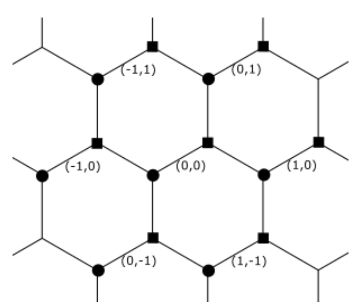


Figure 1.2: Hexagonal lattice.

We can find in [1] various examples of discrete Schrödinger operators, e.g., those on ladders, the diamond lattice, the Kagome lattice.

This thesis concerns a long-range scattering theory and continuum limit of discrete Schrödinger operators.

## 1.1 Backgrounds

### 1.1.1 Scattering problem

**· Known results on (1.0.2)**

The following results on the Schrödinger operators (1.0.2) are well-known (see Dereziński-Gérard [3] and Yafaev [10]).

- If $V(x)$ is short-range, i.e., there exist $\rho > 1$ and $C > 0$ such that $|V(x)| \leq C(1+|x|)^{-\rho}$, then the wave operators

$$W^{\pm} := \text{s-}\lim_{t\to\pm\infty} e^{it(-\Delta_x+V(x))}e^{-it(-\Delta_x)} \tag{1.1.1}$$

  exist and they are asymptotically complete, i.e., the range $\operatorname{Ran} W^{\pm}$ of $W^{\pm}$ equals to the absolutely continuous subspace $\mathcal{H}_{ac}(-\Delta_x + V(x))$ of $-\Delta_x + V(x)$.

- If $V(x)$ is long-range, i.e., there exist $\rho \in (0,1]$ and $C > 0$ such that $|V(x)| \leq C(1+|x|)^{-\rho}$, it may occur that $W^{\pm}$ do not exist. However, if we assume in addition differential condition on $V(x)$, there exist "modified wave operators" and they are "asymptotically complete".

Since each element of the absolutely continuous subspace is called a scattering state, it follows that if (1.1.1) exist and are asymptotically complete, $W^{\pm}$ give one-to-one correspondings of the scattering states of $-\Delta_x$ and $-\Delta_x + V(x)$. This is regarded as an analogue of the classical scattering problem; if $V(x)$ decays at infinity, then it is reasonable to expect that every classical orbit associated to the Hamiltonian $|\xi|^2 + V(x)$ which scatters into infinity can be approximated by some free orbit.

The second result is also related to the classical scattering problem. In fact, there are several kinds of modified wave operators and each of them is constructed from solutions which derive from classical scattering. For example, Isozaki-Kitada modifiers [4] require outgoing and incoming solutions of the eikonal equation

$$|\nabla_x\varphi(x,\xi)|^2 + V(x) = |\xi|^2, \quad (x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d. \tag{1.1.2}$$

**· Known results on discrete Schrödinger operators**

Similarly to the Schrödinger operators, a short-range scattering theory for discrete Schrödinger operators on general lattices works well: If $V$ is short-range, i.e., there exist $\rho > 1$ and $C > 0$ such that $|V(x)| \leq C(1+|x|)^{-\rho}$, then the wave operators

$$W^{\pm} := \text{s-}\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}$$

exist and they are asymptotically complete, i.e., $\operatorname{Ran} W^{\pm} = \mathcal{H}_{ac}(H)$.

On the other hand, there is a known result by Nakamura [5] on a long-range scattering theory for discrete Schrödinger operators on the square lattice. Nakamura [5] considered the Hamiltonian $h_{sq}(x,\xi) = h_{sq,0}(\xi)+\tilde{V}(x)$, $(x,\xi) \in \mathbb{R}^d \times \mathbb{T}^d$, where $h_{sq,0}$ is a real-valued smooth function on the torus $\mathbb{T}^d$ given by the representation of $H_{sq,0}$ via the discrete Fourier transform (see (2.1.2)). Then modified wave operators are made from solutions of the Hamilton-Jacobi equation

$$\partial_t\phi(t,\xi) = h_{sq}(\nabla_\xi\phi(t,\xi),\xi).$$

### 1.1.2 Continuum limit of discrete Schrödinger operators

Discrete Schrödinger operators have another derivation: a discrete approximation of Schrödinger operators (1.0.2). In particular, it is a reasonable observation that the discrete Schrödinger operators on the square lattice $h\mathbb{Z}^d = \{hn \mid n \in \mathbb{Z}^d\}$ with width $h > 0$

$$\begin{aligned} H_h u(x) :=& h^{-2}\sum_{j=1}^{d}(2u(x) - u(x+he_j) - u(x-he_j)) \\ &+ V(x)u(x),\ x \in h\mathbb{Z}^d,\ u \in \ell^2(h\mathbb{Z}^d) \end{aligned} \tag{1.1.3}$$

seems to converge to the Schrödinger operator $H = -\Delta + V(x)$. In fact, in physics research, Schrödinger equations (1.0.1) are usually solved approximately by numerical computations on the lattice. Furthermore, in mathematics, numerical analysis studies conditions for numerical solutions to be really approximations of the rigorous solutions.

Our interest is to study a continuum limit of the discrete Schrödinger operators (1.1.3) from the view point of the spectral theory. We refer to Rabinovich [6] as a known result that (1.1.3) tends to the Schrödinger operator (1.0.2) in the sense of their spectra.

## 1.2 Organization of this thesis

The organization of this thesis is as follows. Chapter 2 concerns a long-range scattering theory for discrete Schrödinger operators of the form

$$Hu(x) = \sum_{y \in \mathbb{Z}^d} f(y)u(x-y) + V(x)u(x),\ u \in \ell^2(\mathbb{Z}^d), \tag{1.2.1}$$

including those on the square and triangular lattices. We prove that, if $V$ satisfies a long-range condition (2.1.3), then modified wave operators with Isozaki-Kitada modifiers exist and they are asymptotically complete. We also show that Isozaki-Kitada modifiers are constructed from solutions to the eikonal equation

$$h_0(\nabla_\xi \varphi(x,\xi)) + \tilde{V}(x) = h_0(\xi),$$

where $h_0(\xi) = \sum_{x \in \mathbb{Z}^d} e^{-ix\cdot\xi} f(x)$ and $\tilde{V} \in C^\infty(\mathbb{R}^d)$ is a suitable smooth continuation of $V$. In Chapter 3, we consider a long-range scattering theory for discrete Schrödinger operators on the hexagonal lattice, i.e., the graphene. Since discrete Schrödinger operators on graphene act on the Hilbert space $\ell^2(\mathbb{Z}^2;\mathbb{C}^2)$, the argument of Chapter 2 cannot be applied directly. However, we show that if we employ the argument of diagonalization of the free operator $H_{he,0}$, we can reduce a long-range scattering problem of $H_{he}$ to that of a direct sum of operators of the form (1.2.1). Chapter 4 is devoted to a continuum limit of (1.1.3). Choosing a suitable operator $P_h : L^2(\mathbb{R}^d) \to \ell^2(h\mathbb{Z}^d)$, we prove that $P_h^*(H_h - \mu)^{-1}P_h \to (H-\mu)^{-1}$ as $h \to 0$ in the operator norm topology. We note that this convergence is valid if, roughly speaking, $V$ is bounded from below and diverges at most exponentially at infinity. As a corollary of the main theorem, we show that the Hausdorff distance between the spectra of $H_h$ and $H$ tends to 0 as $h \to 0$.

## Acknowledgments

The author would like to thank his supervisor Shu Nakamura for helpful discussions and comments, and his encouragement. He would also like to thank Hiroshi Isozaki for kind discussions.

# Bibliography


[1] K. Ando, H. Isozaki, H. Morioka: Spectral properties of Schrödinger operators on perturbed lattices. Ann. Henri Poincaré **17** (2016), 2103-2171.

[2] H. L. Cycon, R. G. Froese, W. Kirsch, B. Simon, Schrödinger Operators. Springer Verlag (1987)

[3] J. Dereziński, C. Gérard: Scattering Theory of Classical and Quantum $N$-Particle Systems. Springer Verlag, 1997.

[4] H. Isozaki, H. Kitada: Modified wave operators with time-independent modifiers. J. Fac. Sci. Uni. Tokyo Sect. IA Math. **32** (1985), no. 1, 77-104.

[5] S. Nakamura: Modified wave operators for discrete Schrödinger operators with long-range perturbations. J. Math. Phys. **55** (2014), 112101 (8 pages).

[6] V. Rabinovich: Wiener algebra of operators on the lattice $(\mu\mathbb{Z})^n$ depending on the small parameter $\mu > 0$. Complex Variables and Elliptic Equations **58** (2013), No. 6, 751–766.

[7] M. Reed, B. Simon: The Methods of Modern Mathematical Physics, Volume III, Scattering Theory. Academic Press, 1979.

[8] Y. Tadano: Long-range scattering for discrete Schrödinger operators. To appear in Ann. Henri Poincaré (preprint, arXiv:1605.02466).

[9] Y. Tadano: Long-range scattering theory of discrete Schrödinger operators on the hexagonal lattice. Preprint, arXiv:1811.11527.

[10] D. R. Yafaev: Mathematical scattering theory. Analytic theory. Mathematical Surveys and Monographs, 158. American Mathematical Society, Providence, RI, 2010.

# Chapter 2

# Long-range scattering for discrete Schrödinger operators

## 2.1 Introduction

We consider a class of generalized discrete Schrödinger operators $H_0$ and $H$ on $\mathcal{H} = \ell^2(\mathbb{Z}^d)$, $d \geq 1$,

$$\begin{cases} H_0 u[x] = \displaystyle\sum_{y \in \mathbb{Z}^d} f[y] u[x-y], \\ Hu[x] = H_0 u[x] + V[x] u[x], \end{cases} \tag{2.1.1}$$

where $f \in \mathscr{S}(\mathbb{Z}^d) := \{u \in \ell^2(\mathbb{Z}^d) \mid u[x] = \mathcal{O}(\langle x \rangle^{-\infty})\}$, $\langle x \rangle := (1 + |x|^2)^{\frac{1}{2}}$, satisfies $f[-x] = \overline{f[x]}$, $x \in \mathbb{Z}^d$, and $V$ is a real-valued bounded function on $\mathbb{Z}^d$. Then $H_0$ and $H$ are bounded selfadjoint operators on $\mathcal{H}$.

We define the discrete Fourier transform $F$ by

$$Fu(\xi) = (2\pi)^{-\frac{d}{2}} \sum_{x \in \mathbb{Z}^d} e^{-ix\cdot\xi} u[x], \quad \xi \in \mathbb{T}^d = [-\pi, \pi)^d$$

for $u \in \ell^1(\mathbb{Z}^d)$. Then $F$ is continuously extended to a unitary operator from $\mathcal{H}$ to $L^2(\mathbb{T}^d)$ and

$$H_0 u[x] = F^* \left( h_0(\cdot) Fu(\cdot) \right) [x],$$

where

$$h_0(\xi) := \sum_{x \in \mathbb{Z}^d} e^{-ix\cdot\xi} f[x], \quad \xi \in \mathbb{T}^d = [-\pi, \pi)^d. \tag{2.1.2}$$

The above condition on $f$ implies $h_0$ is a real-valued smooth function on $\mathbb{T}^d$. We denote by $v(\xi)$ and $A(\xi)$ the generalized velocity and the Hessian of $h_0$, respectively:

$$v(\xi) = \nabla_\xi h_0(\xi),$$
$$A(\xi) = {}^t\nabla_\xi \nabla_\xi h_0(\xi) = (\partial_{\xi_j}\partial_{\xi_k} h_0(\xi))_{1\le j,k\le d}.$$

The set of threshold energies is denoted by $\mathcal{T}$,

$$\mathcal{T} = \{h_0(\xi) \mid \xi \in \mathbb{T}^d, v(\xi) = 0\}.$$

We note $\mathcal{T}$ has Lebesgue measure 0 by Sard's theorem. We first assume the condition below.

**Assumption 2.1.1.** The sets $\{\xi \in \mathbb{T}^d \mid v(\xi) = 0\}$ and $\{\xi \in \mathbb{T}^d \mid \det A(\xi) = 0\}$ have $d$-dimensional Lebesgue measure zero.

The above assumption implies the absence of point and singular continuous spectrum. The following assertion is a generalized version of [13, Theorem 12.3.2].

**Proposition 2.1.2.** *Suppose that the set $\{\xi \in \mathbb{T}^d \mid v(\xi) = 0\}$ has $d$-dimensional Lebesgue measure zero. Then $H_0$ has purely absolutely continuous spectrum and $\sigma_{\mathrm{ac}}(H_0) = h_0(\mathbb{T}^d)$, where $\sigma_{\mathrm{ac}}(H_0)$ denotes the absolutely continuous spectrum of $H_0$.*

*Proof.* Fix a point $\xi_0 \in W := \{\xi \in \mathbb{T}^d \mid v(\xi) \neq 0\}$. Then it suffices to prove $C_c^\infty(U) \subset \mathcal{H}_{ac}(FH_0F^*)$ for some neighborhood $U \subset W$ of $\xi_0$; for any $f \in C_c^\infty(U)$,

$$\mathcal{B}(\sigma(H_0)) \to \mathbb{R},\ B \mapsto \int_{h_0^{-1}(B)\cap \operatorname{supp} f} |f(\xi)|^2 d\xi$$

is an absolutely continuous Borel measure. The claim is proved by taking a local coordinate $U \ni x \mapsto (y(x), h_0(x)) \in \mathbb{R}^{d-1} \times \mathbb{R}$. □

If $V[x]$ decays at infinity, then $V$ is a compact operator on $\mathcal{H}$ and hence $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0) = \sigma_{ac}(H_0) = h_0(\mathbb{T}^d)$, where $\sigma_{\mathrm{ess}}(H)$ and $\sigma_{\mathrm{ess}}(H_0)$ denotes the essential spectrum of $H$ and $H_0$, respectively. We suppose a long-range condition on $V$.

**Assumption 2.1.3.** There exist $\tilde{V} \in C^\infty(\mathbb{R}^d;\mathbb{R})$ and $\varepsilon \in (0, 1]$ such that $\tilde{V}|_{\mathbb{Z}^d} = V$ and

$$|\partial_x^\alpha \tilde{V}(x)| \le C_\alpha \langle x\rangle^{-|\alpha|-\varepsilon}, \quad x \in \mathbb{R}^d,\ \alpha \in \mathbb{Z}_+^d,$$

where $\mathbb{Z}_+ = \{0, 1, 2, \cdots\}$.

Under Assumptions 2.1.1 and 2.1.3, the singular continuous spectrum of $H$ is empty (see, e.g., [12]). In the following, we write $V$ for $\tilde{V}$ without confusion.

*Remark* 2.1.4. Assumption 2.1.3 is equivalent to the following condition used in [11],

$$|\tilde{\partial}_x^\alpha V\,[x]\,| \le C'_\alpha \langle x\rangle^{-|\alpha|-\varepsilon}, \quad x \in \mathbb{R}^d,\ \alpha \in \mathbb{Z}_+^d,$$

where $\tilde{\partial}_x^\alpha = \tilde{\partial}_{x_1}^{\alpha_1} \cdots \tilde{\partial}_{x_d}^{\alpha_d}$, and $\tilde{\partial}_{x_j} V\,[x] = V\,[x] - V\,[x - e_j]$ is the difference operator with respect to the $j$-th variable. Here $\{e_j\}$ is the standard orthogonal basis of $\mathbb{R}^d$. See [11, Lemma 2.1] for the detail.

In Section 2.2, we construct modified wave operators with time-independent modifiers, which are proposed by Isozaki and Kitada [6], so called Isozaki-Kitada modifiers. Isozaki-Kitada modifiers are formally defined by

$$W_J^{\pm} = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} J e^{-itH_0}.$$

We construct $J$ as an operator of the form

$$Ju\,[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(\varphi(x,\xi) - y\cdot\xi)} u[y] d\xi, \tag{2.1.3}$$

where the phase function $\varphi$ is a solution to the eikonal equation

$$h_0(\nabla_x \varphi(x,\xi)) + V(x) = h_0(\xi) \tag{2.1.4}$$

in the "outgoing" and "incoming" regions and considered in Appendix 2.4.

The next theorem is our main result.

**Theorem 2.1.5.** *Under Assumptions 2.1.1 and 2.1.3, there exists an operator $J$ of the form (2.1.3) such that, for any $\Gamma \Subset h_0(\mathbb{T}^d)\backslash\mathfrak{T}$, the modified wave operators*

$$W_J^{\pm}(\Gamma) := \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} J e^{-itH_0} E_{H_0}(\Gamma) \tag{2.1.5}$$

*exist, where $E_{H_0}$ denotes the spectral measure of $H_0$. Furthermore, the following properties hold:*

*i) Intertwining property: $HW_J^{\pm}(\Gamma) = W_J^{\pm}(\Gamma)H_0$.*

*ii) Partial isometries: $\|W_J^{\pm}(\Gamma)u\| = \|E_{H_0}(\Gamma)u\|$.*

*iii) Asymptotic completeness:* $\operatorname{Ran} W_J^{\pm}(\Gamma) = E_H(\Gamma)\mathcal{H}_{\mathrm{ac}}(H)$.

*Examples* 2.1.6. i) In [11], a long-range scattering theory of the standard difference Laplacian $H_0 u[x] = -\frac{1}{2}\sum_{|y-x|=1} u[y]$, $x \in \mathbb{Z}^d$ is considered. In this case, $h_0(\xi) = -\sum_{j=1}^{d} \cos \xi_j$ satisfies Assumption 2.1.1.

ii) A model for 2-dimensional triangle lattice is expressed by the operator $H_0 u[x] = -\frac{1}{6}\sum_{j=1}^{6} u[x+n_j]$, $x \in \mathbb{Z}^2$, where $n_1 = (1,0)$, $n_2 = (-1,0)$, $n_3 = (0,1)$, $n_4 = (0,-1)$, $n_5 = (1,-1)$, $n_6 = (-1,1)$ (see, e.g., [2]). Since

$$h_0(\xi) = -\frac{1}{3}(\cos \xi_1 + \cos \xi_2 + \cos(\xi_1 - \xi_2))$$

in this case, Assumption 2.1.1 is satisfied.

Scattering theory for Schrödinger operators on $\mathbb{R}^d$ has been extensively studied ( [1], [5], [15], [16]). If the perturbation is long-range, i.e., $V(x) = O(\langle x\rangle^{-\varepsilon})$, $0 < \varepsilon \le 1$, then the scattering theory needs a modification ( [5], [6], [16]). Discrete Schrödinger operator describes the state of electrons in solid matters with graph structure. Spectral properties of discrete Schrödinger operators have been studied in [2], [4], [7], [11], [12], [14].

The main idea of the construction of modifiers is similar to [11]. We translate $H$ into an operator on the flat torus $\mathbb{T}^d$ via discrete Fourier transform and consider the corresponding classical mechanics on $\mathbb{T}^d$. The proof is mainly based on [6]. We use the time-decaying method to construct the phase function $\varphi$ in the definition of $J$, and then the stationary phase method and the Enss method to prove the existence and completeness of modified wave operators. The construction of $\varphi$ is given in Appendix 2.4, which follows the argument of [8]. The main properties of $\varphi$ is summarized in Proposition 2.2.1. In Section 2, we prepare some lemmas for the proof of Theorem 2.1.5. The Poisson summation formula is used to prove that pseudo-difference operators on $\mathbb{Z}^d$ are translated to pseudo-differential operators on $\mathbb{T}^d$ modulo smoothing operators (see the proof of Lemma 2.2.3 in Appendix 2.5). This enables us to get over the difficulty derived from the discreteness of $\mathbb{Z}^d$. In Section 3, we prove Theorem 2.1.5.

## 2.2 Preliminaries

We first state a proposition on the Hamilton flow generated by $h(x,\xi) := h_0(\xi) + V(x)$, which is proved in Appendix 2.4. Here we note that $h_0$, $v$ and $A$ are extended periodically in $\xi$ from $\mathbb{T}^d = [-\pi,\pi)^d$ to $\mathbb{R}^d$, and we identify integrations on $\mathbb{T}^d$ with those on $[-\pi,\pi)^d$. We also note that the following proposition concerns functions on $\mathbb{R}^d \times \left(\mathbb{R}^d \backslash v^{-1}(0)\right)$, not on $\mathbb{Z}^d \times \left(\mathbb{T}^d \backslash v^{-1}(0)\right)$.

We fix $\chi \in C^\infty(\mathbb{R}^d)$ such that

$$\chi(x) = \begin{cases} 0 & \text{if } |x| \le 1, \\ 1 & \text{if } |x| \ge 2, \end{cases} \tag{2.2.1}$$

and we define $\cos(x, y) := \frac{x \cdot y}{|x||y|}$ for $x, y \in \mathbb{R}^d \backslash \{0\}$. The following assertion is an analogue of [6, Theorem 2.5].

**Proposition 2.2.1.** *There exists a real-valued function $\varphi \in C^\infty(\mathbb{R}^d \times (\mathbb{R}^d \backslash v^{-1}(0)))$ satisfying the following properties: Set $a > 0$. Let $\varphi_a \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ be defined by*

$$\varphi_a(x, \xi) = (\varphi(x, \xi) - x \cdot \xi)\chi\left(\frac{v(\xi)}{a}\right) + x \cdot \xi. \tag{2.2.2}$$

(1) *The function $\varphi_a$ satisfies*

$$\varphi_a(x, \xi + 2\pi m) = \varphi_a(x, \xi) + 2\pi x \cdot m, \quad m \in \mathbb{Z}^d, \tag{2.2.3}$$

$$|\partial_x^\alpha \partial_\xi^\beta \left[\varphi_a(x, \xi) - x \cdot \xi\right]| \le C_{\alpha\beta, a} \langle x \rangle^{1-\varepsilon-|\alpha|}, \tag{2.2.4}$$

$$|{}^t\nabla_x \nabla_\xi \varphi_a(x, \xi) - I| < \frac{1}{2} \tag{2.2.5}$$

*for $(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$, where $|M| := \left(\sum_{j,k=1}^d |M_{jk}|^2\right)^{\frac{1}{2}}$ for a matrix $M$.*

(2) *We set*

$$J_a u\,[x] := (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y \in \mathbb{Z}^d} e^{i(\varphi_a(x,\xi) - y \cdot \xi)} u[y] d\xi. \tag{2.2.6}$$

*Then*

$$(HJ_a - J_a H_0)u\,[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y \in \mathbb{Z}^d} e^{i(\varphi_a(x,\xi) - y \cdot \xi)} s_a(x, \xi) u\,[y]\, d\xi, \tag{2.2.7}$$

*where*

$$\begin{aligned} s_a(x, \xi) &:= e^{-i\varphi_a(x,\xi)} H(e^{i\varphi_a(\cdot,\xi)})\,[x] - h_0(\xi) \\ &= \sum_{z \in \mathbb{Z}^d} f[z] e^{i(\varphi_a(x-z,\xi) - \varphi_a(x,\xi))} + V\,[x] - h_0(\xi) \end{aligned} \tag{2.2.8}$$

*satisfies for $|x| \ge 1$ and $|v(\xi)| \ge a$*

$$|\partial_\xi^\beta s_a(x, \xi)| \le \begin{cases} C_{\beta,a} \langle x \rangle^{-1-\varepsilon}, & |\cos(x, v(\xi))| \ge \frac{1}{2}, \\ C_{\beta,a} \langle x \rangle^{-\varepsilon}, & |\cos(x, v(\xi))| \le \frac{1}{2}. \end{cases} \tag{2.2.9}$$

We note that $\varphi_a$ satisfies the eikonal equation (2.1.4) on $\{(x,\xi) \mid |x| \geq R_a, |v(\xi)| \geq a, |\cos(x, v(\xi))| \geq \frac{1}{2}\}$ and that the property is used for the proof of (2.2.9) in the $|\cos(x, v(\xi))| \geq \frac{1}{2}$ case (see Proposition 2.4.9 and (2.4.51)).

In the rest of this section, we prepare some lemmas for the proof of properties ii) and iii). We choose $\gamma \in C_c^\infty(h_0(\mathbb{T}^d)\setminus\mathcal{T})$ and $\rho_\pm \in C^\infty([-1,1];[0,1])$ such that

$$\begin{aligned}
&\rho_+(\sigma) + \rho_-(\sigma) = 1, \\
&\rho_+(\sigma) = 1, \quad \sigma \in \left[\frac{1}{4}, 1\right], \\
&\rho_-(\sigma) = 1, \quad \sigma \in \left[-1, -\frac{1}{4}\right].
\end{aligned}$$

Using $\gamma$ and $\rho_\pm$, we define operators with cutoffs in the energy and the direction of $x$ and $v(\xi)$. We set symbols $p_\pm$ and operators $P_\pm$, $\tilde{P}_\pm$ and $E_\pm(t)$ by

$$p_\pm(y,\xi) = \gamma(h_0(\xi))\chi(y)\rho_\pm(\cos(y, v(\xi))), \tag{2.2.10}$$

$$P_\pm u\,[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\xi} p_\pm(y,\xi) u\,[y]\, d\xi, \tag{2.2.11}$$

$$\tilde{P}_\pm u\,[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(x\cdot\xi - \varphi_a(y,\xi))} p_\pm(y,\xi) u\,[y]\, d\xi, \tag{2.2.12}$$

$$E_\pm(t) = J_a e^{-itH_0} \tilde{P}_\pm, \quad t \in \mathbb{R}, \tag{2.2.13}$$

where $J_a$ is defined by (2.2.6).

We consider properties of these operators. We use the stationary phase method as in the pseudo-differential operator calculus (see, e.g., [17]). The following two Lemmas correspond to [6, Proposition 3.4] and [6, Lemma 3.7], and the proofs are given in Appendix 2.5 (see also [3] and [6]).

**Lemma 2.2.2.** *$J_a$, $P_\pm$ and $\tilde{P}_\pm$ are bounded operators on $\mathcal{H}$.*

**Lemma 2.2.3.** *$\gamma(H_0) - P_+ - P_-$, $P_\pm^* - P_\pm$, $E_\pm(0) - P_\pm$, $J_a^* J_a - I$ and $J_a J_a^* - I$ are compact operators on $\mathcal{H}$.*

The next lemma, corresponding to [6, Proposition 3.8], is an analogue of the intertwining property of wave operators.

**Lemma 2.2.4.** *For any $s \in \mathbb{R}$,*

$$\operatorname*{s-lim}_{t\to\pm\infty} e^{itH_0} J_a^* E_\pm(t-s) = e^{isH_0} \tilde{P}_\pm. \tag{2.2.14}$$

*Proof.* The definition of $E_\pm(t)$ implies

$$\begin{aligned} e^{itH_0}J_a^*E_\pm(t-s) &= e^{itH_0}J_a^*J_a e^{-i(t-s)H_0}\tilde{P}_\pm \\ &= e^{itH_0}(J_a^*J_a - I)e^{-itH_0}e^{isH_0}\tilde{P}_\pm + e^{isH_0}\tilde{P}_\pm. \end{aligned}$$

Since $e^{-itH_0}u \to 0$ weakly as $t \to \pm\infty$ for any $u \in \mathcal{H} = \mathcal{H}_{\mathrm{ac}}(H_0)$, Lemma 2.2.3 implies that the first term converges strongly to 0 as $t \to \pm\infty$. □

Next we prove the norm convergence of $\lim_{t\to\pm\infty} e^{itH}E_\pm(t)$. If we set

$$G_\pm(t) := (\frac{d}{idt} + H)E_\pm(t) = (HJ_a - J_aH_0)E_\pm(t),$$

then we have

$$e^{itH}E_\pm(t) - P_\pm = E_\pm(0) - P_\pm + i\int_0^t e^{i\tau H}G_\pm(\tau)d\tau.$$

The following proposition is analogous to [6, Theorem 3.5], and proves $G_\pm(t)$ is integrable in $\{\pm t \geq 0\}$, respectively.

**Proposition 2.2.5.** *$G_\pm(t)$ is norm continuous and compact for any $t \in \mathbb{R}$. Furthermore, $G_\pm(t)$ satisfies*

$$\|G_\pm(t)\| \leq C\langle t\rangle^{-1-\varepsilon}, \ \pm t \geq 0. \tag{2.2.15}$$

*In particular, $e^{itH}E_\pm(t) - P_\pm$ converges to a compact operator with respect to the norm topology as $t \to \pm\infty$, respectively.*

*Proof.* Let

$$\Phi(x,y,\xi;t) := \varphi_a(x,\xi) - th_0(\xi) - \varphi_a(y,\xi).$$

Then the definition (2.2.13) of $E_\pm(t)$ implies

$$\begin{aligned} G_\pm(t)u[x] &= (HJ_a - J_aH_0)e^{-itH_0}\tilde{P}_\pm u[x] \\ &= (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i\Phi(x,y,\xi;t)}s_a(x,\xi)p_\pm(y,\xi)u[y]d\xi. \end{aligned}$$

The norm continuity of $G_\pm(t)$ is obvious. Furthermore, (2.2.9) implies the compactness of $HJ_a - J_aH_0$ by the similar argument in the proof of Lemma 2.2.3, hence $G_\pm(t)$ is compact.

Let us prove (2.2.15). We consider the + case only. The other case is proved similarly. We use another decomposition $\rho^{\pm} \in C^{\infty}([-1,1];[0,1])$ which is different from $\rho_{\pm}$ in that

$$\rho^{+}(\sigma) + \rho^{-}(\sigma) = 1,$$
$$\rho^{+}(\sigma) = \begin{cases} 1, & \sigma \geq \frac{3}{4}, \\ 0, & \sigma \leq \frac{1}{2}. \end{cases}$$

We define

$$s_{-}(x,\xi) := s_a(x,\xi)\chi_{\{x\neq 0\}}\rho^{-}(\cos(x, v(\xi))),$$
$$s_{+}(x,\xi) := s_a(x,\xi) - s_{-}(x,\xi).$$

We then decompose $G_+$ as

$$\begin{aligned} G_+(t)u[x] &= (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i\Phi(x,y,\xi;t)}(s_+p_+ + s_-p_+)(x,y,\xi)u[y]d\xi \\ &=: (F_+(t)+F_-(t))u[x]. \end{aligned} \tag{2.2.16}$$

Now we claim that for any $t \geq 0$ and $\ell \geq 0$,

$$\|F_+(t)\| \leq C\langle at\rangle^{-1-\varepsilon}, \tag{2.2.17}$$
$$\|F_-(t)\| \leq C_\ell\langle at\rangle^{-\ell}. \tag{2.2.18}$$

If (2.2.17) and (2.2.18) hold, then (2.2.15) follows from (2.2.16).

For the proof of (2.2.17), we let

$$\phi(t;y,\xi) := th_0(\xi) + \varphi_a(y,\xi)$$

and set

$$L_1 := \langle\nabla_\xi\phi\rangle^{-2}(1 - \nabla_\xi\phi\cdot D_\xi).$$

Then (2.2.4) implies on the support of $s_+(x,\xi)p_+(y,\xi)$,

$$\langle\nabla_\xi\phi\rangle^{-1} \leq C\langle|y| + t|v(\xi)|\rangle^{-1}.$$

Thus, for any $\ell \in \mathbb{Z}_+$, we have

$$\begin{aligned}
F_+(t)u[x] &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} L_1^\ell(e^{-i\phi(t;y,\xi)}) e^{i\varphi_a(x,\xi)} s_+(x,\xi)p_+(y,\xi)u[y]d\xi \\
&= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{-i\phi(t;y,\xi)} ({}^tL_1)^\ell (e^{i\varphi_a(x,\xi)} s_+(x,\xi)p_+(y,\xi))u[y]d\xi \\
&= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i\Phi(t;y,\xi)} \{e^{-i\varphi_a(x,\xi)} ({}^tL_1)^\ell (e^{i\varphi_a(x,\xi)} s_+p_+)\}u[y]d\xi.
\end{aligned}$$

The function in $\{\}$ is a finite sum of functions of the form $s_j^\ell(x,\xi)p_j^\ell(y,\xi;t)$ such that

$$\begin{cases} |\partial_\xi^\beta s_j^\ell(x,\xi)| \le C_\beta \langle x\rangle^{\ell-1-\varepsilon}, \\ |\partial_\xi^\beta p_j^\ell(y,\xi;t)| \le C_\beta \langle |y| + t|v(\xi)|\rangle^{-\ell}. \end{cases} \tag{2.2.19}$$

Indeed, (2.2.19) follows from (2.2.9) and (2.2.10). Letting

$$\begin{aligned}
S_j^\ell u[x] &:= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(\varphi_a(x,\xi)-y\cdot\xi)} s_j^\ell(x,\xi)u[y]d\xi, \\
P_j^\ell(t)u[x] &:= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(x\cdot\xi-\varphi_a(y,\xi))} p_j^\ell(y,\xi;t)u[y]d\xi,
\end{aligned}$$

we have

$$F_+(t) = \sum_j S_j^\ell e^{-itH_0} P_j^\ell(t).$$

Furthermore, we have by (2.2.19) and the argument in the proof of Lemma 2.2.2

$$\begin{aligned}
&\|\langle x\rangle^{1+\varepsilon-\ell} S_j^\ell\| < \infty, \\
&\|P_j^\ell(t)\| \le C_\ell \langle at\rangle^{-\ell}.
\end{aligned}$$

Thus we obtain

$$\|\langle x\rangle^{1+\varepsilon-\ell} F_+(t)\| \le C'_\ell \langle at\rangle^{-\ell}$$

for any $\ell \in \mathbb{Z}_+$. Interpolation with respect to $\ell$ implies (2.2.17).

For the proof of (2.2.18), we note on the support of $s_-(x,\xi)p_+(y,\xi)$,

$$\langle \nabla_\xi \Phi\rangle^{-1} \le C\langle |x-y| + t|v(\xi)|\rangle^{-1}.$$

Letting

$$L_2 := \langle \nabla_\xi \Phi \rangle^{-2}(1 + \nabla_\xi \Phi \cdot D_\xi),$$

we have

$$\begin{aligned} F_-(t)u[x] &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y \in \mathbb{Z}^d} e^{i\Phi(x,y,\xi;t)} ({}^tL_2)^\ell (s_-(x,\xi)p_+(y,\xi))u[y]d\xi \\ &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y \in \mathbb{Z}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(y,\xi))} e^{-ith_0(\xi)} ({}^tL_2)^\ell (s_-p_+)u[y]d\xi \end{aligned}$$

for any $\ell \in \mathbb{Z}_+$. Since

$$q^\ell(x,y,\xi;t) := e^{-ith_0(\xi)} ({}^tL_2)^\ell (s_-(x,\xi)p_+(y,\xi))$$

satisfies

$$|\partial_\xi^\beta q^\ell(x,y,\xi;t)| \le C_{\ell,\beta} \langle tv(\xi) \rangle^{|\beta|-\ell}$$

for any $\ell \in \mathbb{Z}_+$, we obtain (2.2.18) by the argument in the proof of Lemma 2.2.2. □

The next proposition claims that any particle in the energy $\Gamma$ does not stay in any bounded domain in $x$.

**Proposition 2.2.6.** *For any $R > 0$ and $\ell \ge 0$,*

$$\|\chi_{\{|x|<R\}} E_\pm(s)\| \le C_{\ell,R} \langle s \rangle^{-\ell}, \quad \pm s \ge 0. \tag{2.2.20}$$

*Proof.* We prove (2.2.20) for the + case only. We first note

$$E_+(s)u[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y \in \mathbb{Z}^d} e^{i\Phi(x,y,\xi;s)} p_+(y,\xi)u[y]d\xi,$$

where $\Phi(x,y,\xi;t) = \varphi_a(x,\xi) - th_0(\xi) - \varphi_a(y,\xi)$. We observe that on the support of $p_+(y,\xi)$,

$$|sv(\xi) + \nabla_\xi \varphi_a(y,\xi)| \ge c(|y| + s|v(\xi)|)$$

for large $s$. Then, if $|x| \le R$, we have for $s > 0$ large enough

$$|\nabla_\xi \Phi(x,y,\xi;s)| \ge c(|y| + s|v(\xi)|), \quad (y,\xi) \in \operatorname{supp} p_+.$$

Similarly to the proof of (2.2.18), we obtain (2.2.20). □

## 2.3 Proof of Theorem 2.1.5

### 2.3.1 Existence of modified wave operators

We prove the existence of the limit (2.1.5) for the + case only. The other case is proved similarly. First we fix $\Gamma \Subset h_0(\mathbb{T}^d)\backslash\mathcal{T}$. We remark that, for any $u \in \mathcal{H}$ such that $Fu \in C^\infty(\mathbb{T}^d)$ and $\operatorname{supp} Fu \subset h_0^{-1}(\Gamma)$, we have

$$JE_{H_0}(\Gamma)u = J_a u \tag{2.3.1}$$

for some small enough $a > 0$. Then, to prove the existence of the limit (2.1.5), it suffices to show that

$$\begin{aligned} &\int_0^\infty \left\| \frac{d}{dt}\left(e^{itH} J e^{-itH_0} E_{H_0}(\Gamma)u\right)\right\| dt \qquad (2.3.2)\\ &= \int_0^\infty \left\| \frac{d}{dt}\left(e^{itH} J_a e^{-itH_0} u\right)\right\| dt \\ &= \int_0^\infty \|e^{itH}(HJ_a - J_a H_0)e^{-itH_0}u\| dt \\ &= \int_0^\infty \|(HJ_a - J_a H_0)e^{-itH_0}u\| dt \end{aligned}$$

is finite for such $u$. The last equality follows from the fact that $e^{itH}$ is a unitary operator. Furthermore, by Assumption 2.1.1 and a partition of unity on $\mathbb{T}^d$, we may assume that $Fu \in C^\infty(\mathbb{T}^d)$ has a sufficiently small support in $\{\xi \in h_0^{-1}(\Gamma) \mid \det A(\xi) \neq 0\}$.

Let $w(t) := (HJ_a - J_a H_0)e^{-itH_0}u$. Then (2.2.7) implies

$$w(t)[x] = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi) - th_0(\xi))} s_a(x,\xi) Fu(\xi) d\xi.$$

Now we use the stationary phase method. The stationary point $\xi = \xi(x,t)$ is determined by

$$\frac{1}{t}\nabla_\xi \varphi_a(x,\xi) - v(\xi) = 0. \tag{2.3.3}$$

We define

$$D_t := \{x \in \mathbb{Z}^d \mid \exists \xi \in \operatorname{supp} Fu \text{ s.t. (2.3.3) holds}\}.$$

By (2.2.4), there exists an open set $U \Subset \{\xi \in h_0^{-1}(\Gamma) \mid \det A(\xi) \neq 0\}$ such that $\operatorname{supp} Fu \Subset U$ and that for $t > 0$ large enough,

$$D_t \subset \left\{x \mid \frac{x}{t} \in v(U)\right\} =: D_t'.$$

On $(D'_t)^c$, the non stationary phase method implies

$$|w(t)[x]| \leq C_\ell \langle |x| + t\rangle^{-\ell}, \quad x \in \mathbb{Z}^d, \ t > 0$$

for any $\ell \geq 0$. Thus we learn for any $\ell \geq 0$

$$\|\chi_{(D'_t)^c} w(t)\| \leq C'_\ell t^{-\ell}. \tag{2.3.4}$$

On $D'_t$, the stationary phase method implies

$$w(t)[x] = t^{-\frac{d}{2}} A(t,x) s_a(x, \xi(x,t)) Fu(\xi(x,t)) + t^{-\frac{d}{2}-1} r(t,x),$$

where $A(t,x)$ is uniformly bounded in $x$ and $t$ with $x \in D'_t$, and

$$|r(t,x)| \leq C \sup_{|\beta| \leq d+3} \sup_{\xi \in \operatorname{supp} Fu} |\partial_\xi^\beta s_a(x,\xi)|.$$

Since $\cos(x, v(\xi)) \geq \frac{1}{2}$ for $x \in D'_t$ and $\xi \in \operatorname{supp} Fu$ if $t$ is sufficiently large, we have by (2.2.9)

$$|s_a(x, \xi(x,t))| \leq C \langle x\rangle^{-1-\varepsilon},$$
$$|r(t,x)| \leq C \langle x\rangle^{-1-\varepsilon}.$$

We note $|x| \sim t$ on $D'_t$ and the Lebesgue measure of $D'_t$ is bounded by $Ct^d$. Thus we learn

$$\|\chi_{D'_t} w(t)\| \leq \left( \int_{D'_t} \left( Ct^{-\frac{d}{2}} \langle x\rangle^{-1-\varepsilon}\right)^2 dx \right)^{\frac{1}{2}} \leq C' t^{-1-\varepsilon}. \tag{2.3.5}$$

Hence (2.3.4) and (2.3.5) imply

$$\|w(t)\| \leq \|\chi_{D'_t} w(t)\| + \|\chi_{(D'_t)^c} w(t)\| \leq C'' t^{-1-\varepsilon},$$

which proves (2.3.2) is finite. □

### 2.3.2 Proof of the properties i), ii) and iii)

*Proof of i).* The intertwining property is proved similarly to the short-range case (see, e.g., [15]). □

*Proof of ii).* It suffices to show $\|W_J^\pm(\Gamma)u\| = \|u\|$ for $Fu \in C^\infty(\mathbb{T}^d)$ with $\operatorname{supp} Fu \subset h_0^{-1}(\Gamma)$. For such $u$, $Ju = J_a u$ holds for small $a > 0$. Thus letting $u_t = e^{-itH_0}u$, we learn

$$\|W_J^\pm(\Gamma)u\|^2 = \lim_{t\to\pm\infty} \|J_a u_t\|^2 = \lim_{t\to\pm\infty} ((J_a^* J_a - I)u_t, u_t) + \|u\|^2.$$

Using $\text{w-lim}_{t\to\pm\infty} u_t = 0$ and Lemma 2.2.3, we have $\lim_{t\to\pm\infty}(J_a^* J_a - I)u_t = 0$. This proves $W_J^\pm(\Gamma)$ are partial isometries. □

*Proof of iii).* We prove the asymptotic completeness of $W_J^+(\Gamma)$ only. Since intertwining property implies $\operatorname{Ran} W_J^+(\Gamma) \subset E_H(\Gamma)\mathcal{H}_{\mathrm{ac}}(H)$, it suffices to prove $\operatorname{Ran} W_J^+(\Gamma) \supset E_H(\Gamma)\mathcal{H}_{\mathrm{ac}}(H)$.

We fix $v \in \mathcal{H}_{\mathrm{ac}}(H)$ and $\gamma \in C^\infty(\mathbb{R})$ so that $\gamma(H)v = v$ and $\operatorname{supp}\gamma \subset \Gamma$. We set $v_t := e^{-itH}v$ for simplicity. Then we show that $E_H(\Gamma)\mathcal{H}_{\mathrm{ac}}(H) \subset \operatorname{Ran} W_J^+(\Gamma)$ follows from

$$\lim_{s\to\infty}\limsup_{t\to\infty}\|v_s - e^{i(t-s)H}E_+(t-s)v_s\| = 0. \tag{2.3.6}$$

First, we observe

$$\begin{aligned}&\|e^{itH_0}J_a^* e^{-itH}v - e^{isH_0}\tilde{P}_+ v_s\|\\ &\le \|e^{itH_0}J_a^*\left[v_t - E_+(t-s)v_s\right]\| + \|e^{itH_0}J_a^* E_+(t-s)v_s - e^{isH_0}\tilde{P}_+ v_s\|.\end{aligned}$$

Lemma 2.2.4 implies the second term tends to 0 as $t \to \infty$. The first term is estimated by (2.3.6) since

$$\begin{aligned}&\|e^{itH_0}J_a^*\left[v_t - E_+(t-s)v_s\right]\|\\ &\le \|e^{itH_0}J_a^*\|\|v_t - E_+(t-s)v_s\|\\ &= \|J_a^*\|\|e^{i(t-s)H}(v_t - E_+(t-s)v_s)\|\\ &= \|J_a^*\|\|v_s - e^{i(t-s)H}E_+(t-s)v_s\|.\end{aligned}$$

Thus we have

$$\lim_{s\to\infty}\limsup_{t\to\infty}\|e^{itH_0}J_a^* e^{-itH}v - e^{isH_0}\tilde{P}_+ v_s\| = 0.$$

This implies $\left\{e^{itH_0}J_a^* e^{-itH}v\right\}_{t\ge 0}$ is a Cauchy sequence in $\mathcal{H}$, equivalently, there exists the limit

$$\lim_{t\to\infty} e^{itH_0}J_a^* e^{-itH}v =: \Omega^a v.$$

Hence we obtain for sufficiently small $a > 0$,

$$v = W_J^+(\Gamma)\Omega^a v \in \operatorname{Ran} W_J^+(\Gamma).$$

In the rest of the proof, we show (2.3.6). Since $v_s = \gamma(H)v_s$, we have

$$\begin{aligned}v_s - e^{i(t-s)H}E_+(t-s)v_s =& \gamma(H)v_s - e^{i(t-s)H}E_+(t-s)v_s\\ =& (\gamma(H) - \gamma(H_0))v_s\\ &+ (\gamma(H_0) - P_+ - P_-)v_s\\ &+ (P_+ - e^{i(t-s)H}E_+(t-s))v_s + P_- v_s.\end{aligned} \tag{2.3.7}$$

We note $\text{w-lim}_{s\to\infty} v_s = 0$ and $\gamma(H)-\gamma(H_0)$ is compact by the compactness of $H - H_0 = V$. We also note $\gamma(H_0) - P_+ - P_-$ is compact by Lemma 2.2.3, and $P_+ - e^{i(t-s)H}E_+(t-s)$ converges to a compact operator independent of $s$ as $t \to \infty$ by Proposition 2.2.5. Thus the terms on the RHS of (2.3.7) except the last one converge to 0.

To estimate the last term of (2.3.7), we observe

$$\begin{aligned}\|P_- v_s\|^2 =&(P_-^* P_- v_s, v_s) \\ =&((P_-^* - P_-)P_- v_s, v_s) \\ &+ ((P_- - e^{-isH}E_-(-s))P_- v_s, v_s) \\ &+ (P_- v_s, E_-(-s)^* v).\end{aligned} \tag{2.3.8}$$

By the similar argument as above, we learn the first and second terms of (2.3.8) converge to 0 as $s \to \infty$. The third term of (2.3.8) is bounded by

$$\begin{aligned}&|(P_- v_s, E_-(-s)^* v)| \\ &= |(P_- v_s, E_-(-s)^*(\chi_{\{|x|\geq R\}} + \chi_{\{|x|<R\}})v)| \\ &\leq \|E_-(-s)P_- v_s\|\|\chi_{\{|x|\geq R\}}v\| + \|P_- v_s\|\|\chi_{\{|x|<R\}}E_-(-s)\|\|v\| \\ &\leq C_v(\|\chi_{\{|x|\geq R\}}v\| + \|\chi_{\{|x|<R\}}E_-(-s)\|)\end{aligned} \tag{2.3.9}$$

for any $R > 0$. Using (2.2.20) and $\lim_{R\to\infty} \|\chi_{\{|x|\geq R\}}v\| = 0$, we learn that (2.3.9) converges to 0 as $s \to \infty$. Hence we obtain (2.3.6). □

## 2.4 Appendix: Classical mechanics and the construction of phase function

In this appendix, we use the following notations: For $\rho \in (0,1)$, we define

$$\begin{aligned}h(x,\xi) =&h_0(\xi) + V(x), \\ V_\rho(t,x) =&V(x)\chi(\rho x)\chi\left(\frac{\langle \log\langle t\rangle\rangle x}{\langle t\rangle}\right), \\ h_\rho(t,x,\xi) =&h_0(\xi) + V_\rho(t,x), \\ \nabla_x^2 V_\rho(t,x) =&{}^t\nabla_x \nabla_x V_\rho(t,x),\end{aligned}$$

where $\chi \in C^\infty(\mathbb{R}^d)$ is a fixed function satisfying (2.2.1). Let $\varepsilon$ be as in Assumption 2.1.3. We fix $\varepsilon_0, \varepsilon_1 > 0$ such that $\varepsilon_0 + \varepsilon_1 < \varepsilon$.

The construction of time-decaying potential is same as Isozaki and Kitada [6], and is first used by Kitada and Yajima [9]. One of the merits of this construction is that $V_\rho$ decays with respect to time $t$ almost same as position $x$. The next lemma follows from Assumption 2.1.3 with elementary computations.

**Lemma 2.4.1.** *For any $t \in \mathbb{R}$, $x \in \mathbb{R}^d$ and multi-index $\alpha$,*

$$|\partial_x^\alpha V_\rho(t,x)| \le C_\alpha \min\{\rho^{\varepsilon_0}\langle t\rangle^{-|\alpha|-\varepsilon_1}, \langle x\rangle^{-|\alpha|-\varepsilon}\}, \tag{2.4.1}$$

*where $C_\alpha$'s are independent of $x$, $t$ and $\rho$.*

Let $(q,p)(t,s) = (q,p)(t,s;x,\xi)$ be the solution to the canonical equation associated to the Hamiltonian $h_\rho$:

$$\begin{cases} \partial_t q(t,s) = \nabla_\xi h_\rho(t, p(t,s), q(t,s)), \\ \partial_t p(t,s) = -\nabla_x h_\rho(t, p(t,s), q(t,s)), \\ (q,p)(s,s) = (x,\xi). \end{cases}$$

This can be rewritten in the integral form:

$$q(t,s) = x + \int_s^t v(p(\tau,s))d\tau, \tag{2.4.2}$$

$$p(t,s) = \xi - \int_s^t \nabla_x V_\rho(\tau, q(\tau,s))d\tau. \tag{2.4.3}$$

Before proving Proposition 2.2.1, let us describe the outline of this section. First, we see in Proposition 2.4.2 that $q(t,s) \sim x + (t-s)v(\xi)$ and $p(t,s) \sim \xi$ for sufficiently small $\rho > 0$. Then we construct a solution $\phi(t;x,\xi)$ of the Hamilton-Jacobi equation (2.4.30) by the method of characteristics. Also estimates for $y(s,t;x,\xi)$ and $\eta(t,s;x,\xi)$, characterized by (2.4.21) and (2.4.22), respectively, are given in Proposition 2.4.3. Using the above $\phi$, we define functions $\phi_\pm(x,\xi)$ by (2.4.33), and we confirm that $\phi_\pm$ satisfies the eikonal equation (2.1.4) and the estimate (2.2.4) in outgoing and incoming region, respectively. Finally, we construct a function $\varphi(x,\xi)$ such that Proposition 2.2.1 holds with $\phi_\pm$ and phase-space cutoffs.

Now, we start with estimates for classical orbits $(q,p)(t,s;x,\xi)$. The following proposition is the corresponding result of [6, Proposition 2.1].

**Proposition 2.4.2.** *For $\rho > 0$ small enough, there exist $C_\ell > 0$ ($\ell \in \mathbb{Z}_+$)*

*such that, for any $x, \xi \in \mathbb{R}^d$, $0 \le \pm s \le \pm t$ and multi-indices $\alpha$ and $\beta$,*

$$|p(s,t;x,\xi) - \xi| \le C_0 \rho^{\varepsilon_0} \langle s \rangle^{-\varepsilon_1}, \tag{2.4.4}$$

$$|p(t,s;x,\xi) - \xi| \le C_0 \rho^{\varepsilon_0} \langle s \rangle^{-\varepsilon_1}, \tag{2.4.5}$$

$$|\partial_x^\alpha \left[\nabla_x q(s,t;x,\xi) - I\right]| \le C_{|\alpha|} \rho^{\varepsilon_0} \langle s \rangle^{-\varepsilon_1}, \tag{2.4.6}$$

$$|\partial_x^\alpha \nabla_x p(s,t;x,\xi)| \le C_{|\alpha|} \rho^{\varepsilon_0} \langle s \rangle^{-1-\varepsilon_1}, \tag{2.4.7}$$

$$|\partial_x^\alpha \partial_\xi^\beta \left[\nabla_x q(t,s;x,\xi) - I\right]| \le C_{|\alpha|+|\beta|} \rho^{\varepsilon_0} \langle s \rangle^{-1-\varepsilon_1} |t-s|, \tag{2.4.8}$$

$$|\partial_x^\alpha \partial_\xi^\beta \nabla_x p(t,s;x,\xi)| \le C_{|\alpha|+|\beta|} \rho^{\varepsilon_0} \langle s \rangle^{-1-\varepsilon_1}, \tag{2.4.9}$$

$$|\partial_\xi^\beta \left[\nabla_\xi q(t,s;x,\xi) - (t-s)A(\xi)\right]| \le C_{|\beta|} \rho^{\varepsilon_0} \langle s \rangle^{-\varepsilon_1} |t-s|, \tag{2.4.10}$$

$$|\partial_\xi^\beta \left[\nabla_\xi p(t,s;x,\xi) - I\right]| \le C_{|\beta|} \rho^{\varepsilon_0} \langle s \rangle^{-\varepsilon_1}, \tag{2.4.11}$$

$$\begin{aligned} &|\partial_x^\alpha \partial_\xi^\beta \left[q(t,s;x,\xi) - x - (t-s)v(p(t,s;x,\xi))\right]| \\ &\qquad \le C_{|\alpha|+|\beta|} \rho^{\varepsilon_0} \min\{|t-s|\langle s \rangle^{-\varepsilon_1}, \langle t \rangle^{1-\varepsilon_1}\}. \end{aligned} \tag{2.4.12}$$

*Here, $|x| = \left(\sum_{j=1}^d |x_j|^2\right)^{\frac{1}{2}}$ for a vector $x$ and $|M| = \left(\sum_{j,k=1}^d |M_{jk}|^2\right)^{\frac{1}{2}}$ for a matrix $M$.*

*Proof.* We prove in the $0 \le s \le t$ case. The other case is proved similarly. The proof is decomposed into 5 steps.

Step 1: Proof of (2.4.4) and (2.4.5). The inequalities (2.4.4) and (2.4.5) are shown by (2.4.1) and

$$p(t,t') - \xi = -\int_{t'}^{t} \nabla_x V_\rho(\tau, q(\tau,t'))d\tau, \quad t,t' \in \mathbb{R}.$$

Step 2: Proof of (2.4.6) and (2.4.7). We use the induction with respect to $|\alpha|$. First we prove (2.4.6) and (2.4.7) for $\alpha = 0$. Differentiating (2.4.2) and (2.4.3) in $x$, we have

$$\begin{cases} \nabla_x q(s,t) = I + \int_t^s A(p(\tau,t))\nabla_x p(\tau,t)d\tau, \\ \nabla_x p(s,t) = -\int_t^s \nabla_x^2 V_\rho(\tau, q(\tau,t))\nabla_x q(\tau,t)d\tau. \end{cases}$$

Letting

$$\begin{aligned} Q_0(s) &:= \nabla_x q(s,t) - I, \\ P_0(s) &:= \nabla_x p(s,t), \end{aligned}$$

we observe

$$\begin{cases} Q_0(s) = \int_t^s A(p(\tau,t))P_0(\tau)d\tau, \\ P_0(s) = -\int_t^s \nabla_x^2 V_\rho(\tau, q(\tau,t))Q_0(\tau)d\tau - \int_t^s \nabla_x^2 V_\rho(\tau, q(\tau,t))d\tau. \end{cases} \tag{2.4.13}$$

Thus combining the two equations in (2.4.13), we learn

$$P_0(s) = B_t(P_0(\cdot))(s) + R_0(s),$$

where

$$B_t(P(\cdot))(s) := -\int_t^s \nabla_x^2 V_\rho(\tau, q(\tau,t)) \left[\int_t^\tau A(p(\sigma,t))P(\sigma)d\sigma\right] d\tau,$$
$$R_0(s) := -\int_t^s \nabla_x^2 V_\rho(\tau, q(\tau,t))d\tau.$$

Let $\|M(\cdot)\|_0 := \sup_{0\le s\le t}\langle s\rangle^{1+\varepsilon_1}|M(s)|$ for $M \in C([0,t]\,; M_d(\mathbb{R}))$. Then (2.4.1) implies

$$\begin{aligned}|B_t(P(\cdot))(s)| &\le \int_s^t C_2\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}\int_\tau^t |P(\sigma)|d\sigma d\tau \\ &\le C_2\rho^{\varepsilon_0}\|P\|_0\int_s^\infty \langle\tau\rangle^{-2-\varepsilon_1}\int_\tau^\infty \langle\sigma\rangle^{-1-\varepsilon_1}d\sigma d\tau \\ &\le C_2C'\rho^{\varepsilon_0}\langle s\rangle^{-1-2\varepsilon_1}\|P\|_0, \\ |R_0(s)| &\le \int_s^t C_2\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}d\tau \le C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1}.\end{aligned}$$

If $\rho \le (2C_2C')^{-\frac{1}{\varepsilon_0}}$, the operator norm $\|B_t\|_0$ of $B_t$ with respect to $\|\cdot\|_0$ is bounded by $\frac{1}{2}$. Hence we obtain

$$\|P_0(\cdot)\|_0 = \|(1-B_t)^{-1}(R_0(\cdot))\|_0 \le \frac{1}{1-\|B_t\|_0}\|R_0(\cdot)\|_0 \le 2C\rho^{\varepsilon_0}, \quad (2.4.14)$$

which proves (2.4.7) for $\alpha = 0$. The inequality (2.4.6) for $\alpha = 0$ follows directly from (2.4.13) and (2.4.14).

Next we confirm the induction is valid. We fix $\alpha \in \mathbb{Z}_+^d\backslash\{0\}$ and assume that (2.4.6) and (2.4.7) hold for $\alpha'$ with $|\alpha'| < |\alpha|$. Differentiating (2.4.13), we have

$$\left\{\begin{array}{l}\partial_x^\alpha Q_0(s) = \int_t^s A(p(\tau,t))\partial_x^\alpha P_0(\tau)d\tau + R_{0,1}(s), \\ \partial_x^\alpha P_0(s) = -\int_t^s \nabla_x^2 V_\rho(\tau, q(\tau,t))\partial_x^\alpha Q_0(\tau)d\tau \\ \qquad\qquad\qquad\qquad +R_{0,21}(s) + R_{0,22}(s),\end{array}\right. \quad (2.4.15)$$

where

$$R_{0,1}(s) := \sum_{0 \lneq \alpha' \leq \alpha} \binom{\alpha}{\alpha'} \int_t^s \partial_x^{\alpha'} \left[A(p(\tau,t))\right] \partial_x^{\alpha-\alpha'} P_0(\tau) d\tau,$$

$$R_{0,21}(s) := - \sum_{0 \lneq \alpha' \leq \alpha} \binom{\alpha}{\alpha'} \int_t^s \partial_x^{\alpha'} \left[\nabla_x^2 V_\rho(\tau, q(\tau,t))\right] \partial_x^{\alpha-\alpha'} Q_0(\tau) d\tau,$$

$$R_{0,22}(s) := - \int_t^s \partial_x^{\alpha} \left[\nabla_x^2 V_\rho(\tau, q(\tau,t))\right] d\tau,$$

and $\binom{\alpha}{\alpha'} := \prod_{j=1}^d \frac{\alpha_j!}{\alpha'_j!(\alpha_j-\alpha'_j)!}$. By (2.4.1) and assumptions of the induction, we have

$$|R_{0,1}(s)| \leq C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1},$$

$$|R_{0,21}(s)| \leq \int_s^t C\rho^{\varepsilon_0}\langle \tau\rangle^{-2-\varepsilon_1} \cdot C\rho^{\varepsilon_0}\langle \tau\rangle^{-\varepsilon_1} d\tau \leq C\rho^{\varepsilon_0}\langle s\rangle^{-1-2\varepsilon_1},$$

$$|R_{0,22}(s)| \leq \int_s^t C\rho^{\varepsilon_0}\langle \tau\rangle^{-2-\varepsilon_1} d\tau \leq C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1}.$$

The similar argument as for $\alpha = 0$ implies $\|\partial_x^\alpha P_0(\cdot)\|_0 \leq C_\alpha \rho^{\varepsilon_0}$ and (2.4.6).

Step 3: Proof of (2.4.10) and (2.4.11). We use the induction with respect to $|\beta|$. First we consider the $\beta = 0$ case. Similarly to Step 2, we have

$$\begin{cases} \nabla_\xi q(t,s) = \int_s^t A(p(\tau,s)) \nabla_\xi p(\tau,s) d\tau, \\ \nabla_\xi p(t,s) = I - \int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s)) \nabla_\xi q(\tau,s) d\tau, \end{cases}$$

equivalently,

$$\begin{cases} Q'(t) = \int_s^t A(p(\tau,s)) P'(\tau) d\tau - \int_s^t (A(p(\tau,s)) - A(\xi)) d\tau, \\ P'(t) = -\int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s)) Q'(\tau) d\tau \\ \qquad\qquad - \int_s^t (\tau - s) \nabla_x^2 V_\rho(\tau, q(\tau,s)) A(\xi) d\tau, \end{cases} \tag{2.4.16}$$

where

$$Q'(t) := \nabla_\xi q(t,s) - (t-s)A(\xi),$$
$$P'(t) := \nabla_\xi p(t,s) - I.$$

By (2.4.16), we have

$$P'(t) = B_s(P'(\cdot))(t) + R'(t),$$

where

$$R'(t) := -\int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s)) \int_s^\tau A(p(\sigma,s))d\sigma d\tau.$$

Letting $\|M(\cdot)\|_1 := \sup_{t\geq s}|M(t)|$ for $M \in C([s,\infty)\,;M_d(\mathbb{R}))$, we have

$$\begin{aligned}
|B_s(P(\cdot))(t)| &\leq \int_s^t C_2\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}\int_s^\tau |P(\sigma)|d\sigma d\tau \\
&\leq C_2\rho^{\varepsilon_0}\|P\|_1\int_s^t \langle\tau\rangle^{-2-\varepsilon_1}(\tau-s)d\tau \\
&\leq C_2C'\rho^{\varepsilon_1}\langle s\rangle^{-\varepsilon_1}\|P\|_1, \\
|R'(t)| &\leq \int_s^t C\rho^{\varepsilon_1}\langle\tau\rangle^{-2-\varepsilon_1}(\tau-s)d\tau \leq C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}.
\end{aligned}$$

Thus, if $\rho \leq (2C_2C')^{-\varepsilon_0}$, we obtain

$$\|P'(\cdot)\|_1 = \|(1-B_s)^{-1}R'(\cdot)\|_1 \leq \frac{1}{1-\|B_s\|_1}\|R'(\cdot)\|_1 \leq 2C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}. \tag{2.4.17}$$

This proves (2.4.11) for $\beta = 0$. The inequality (2.4.10) for $\beta = 0$ follows from (2.4.5), (2.4.16) and (2.4.17).

Next we prove the induction works. Differentiating (2.4.16), we have

$$\begin{cases} \partial_\xi^\beta Q'(t) = \int_s^t A(p(\tau,s))\partial_\xi^\beta P'(\tau)d\tau + R'_{11}(t) + R'_{12}(t), \\ \partial_\xi^\beta P'(t) = -\int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s))\partial_\xi^\beta Q'(\tau)d\tau + R'_{21}(t) + R'_{22}(t), \end{cases} \tag{2.4.18}$$

where

$$\begin{aligned}
R'_{11}(t) &:= \sum_{0\lneq\beta'\leq\beta}\binom{\beta}{\beta'}\int_s^t \partial_\xi^{\beta'}\left[A(p(\tau,s))\right]\partial_\xi^{\beta-\beta'}P'(\tau)d\tau, \\
R'_{12}(t) &:= \int_s^t \partial_\xi^\beta\left[A(p(\tau,s)) - A(\xi)\right]d\tau, \\
R'_{21}(t) &:= -\sum_{0\lneq\beta'\leq\beta}\binom{\beta}{\beta'}\int_s^t \partial_\xi^{\beta'}\left[\nabla_x^2 V_\rho(\tau,q(\tau,s))\right]\partial_\xi^{\beta-\beta'}Q'(\tau)d\tau, \\
R'_{22}(t) &:= -\int_s^t (\tau-s)\partial_\xi^\beta\left[\nabla_x^2 V_\rho(\tau,q(\tau,s))A(\xi)\right]d\tau.
\end{aligned}$$

Thus we have

$$\partial_\xi^\beta P'(t) = B_s(\partial_\xi^\beta P'(\cdot))(t) - \int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s))(R'_{11}(\tau) + R'_{12}(\tau))d\tau \\ + R'_{21}(t) + R'_{22}(t).$$

If (2.4.10) and (2.4.11) are true for $\beta'$ with $|\beta'| < |\beta|$, we learn

$$\begin{aligned} |R'_{11}(t)| &\le C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}|t-s|, \\ |R'_{12}(t)| &\le C \sup_{|\beta'|\le|\beta|}\int_s^t |\partial_\xi^{\beta'}[p(\tau,s)-\xi]|d\tau \le C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}|t-s|, \\ |R'_{21}(t)| &\le \int_s^t C\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}\cdot C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}|\tau-s|d\tau \le C\rho^{2\varepsilon_0}\langle s\rangle^{-2\varepsilon_1}, \\ |R'_{22}(t)| &\le \int_s^t C\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}|\tau-s|d\tau \le C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}. \end{aligned}$$

Using the similar argument as for $\beta = 0$, we obtain (2.4.10) and (2.4.11) for any $\beta$.

Step 4: Proof of (2.4.8) and (2.4.9). We use the induction with respect to $|\alpha| + |\beta|$. In the $\alpha = \beta = 0$ case, differentiation in $x$ implies

$$\begin{cases} \nabla_x q(t,s) = I + \int_s^t A(p(\tau,s))\nabla_x p(\tau,s)d\tau, \\ \nabla_x p(t,s) = -\int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s))\nabla_x q(\tau,s)d\tau. \end{cases}$$

Letting

$$\begin{aligned} Q(t) &:= \nabla_x q(t,s) - I, \\ P(t) &:= \nabla_x p(t,s), \end{aligned}$$

we observe

$$\begin{cases} Q(t) = \int_s^t A(p(\tau,s))P(\tau)d\tau, \\ P(t) = -\int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s))Q(\tau)d\tau - \int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s))d\tau. \end{cases} \tag{2.4.19}$$

This implies

$$P(t) = B_s(P(\cdot))(t) + R(t),$$

where

$$R(t) := -\int_s^t \nabla_x^2 V_\rho(\tau, q(\tau,s))d\tau.$$

Since

$$|R(t)| \le \int_s^t C_2\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}d\tau \le C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1},$$

we have

$$\|P(\cdot)\|_1 = \|(1-B_s)^{-1}R\|_1 \le 2C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1},$$

which proves (2.4.9) for $\alpha = \beta = 0$. The inequality (2.4.8) follows from (2.4.9) and (2.4.19).

We prove the induction with respect to $|\alpha|+|\beta|$ works. By (2.4.19), we have

$$\begin{cases} \partial_x^\alpha\partial_\xi^\beta Q(t) = \int_s^t A(p(\tau,s))\partial_x^\alpha\partial_\xi^\beta P(\tau)d\tau + R_1(t), \\ \partial_x^\alpha\partial_\xi^\beta P(t) = -\int_s^t \nabla_x^2 V_\rho(\tau,q(\tau,s))\partial_x^\alpha\partial_\xi^\beta Q(\tau)d\tau \\ \qquad\qquad\qquad\qquad\qquad\qquad +R_{21}(t)+R_{22}(t), \end{cases} \tag{2.4.20}$$

where

$$R_1(t) := \sum_{\substack{\alpha'\le\alpha,\beta'\le\beta,\\ |\alpha'+\beta'|\ge 1}} \binom{\alpha}{\alpha'}\binom{\beta}{\beta'}\int_s^t \partial_x^{\alpha'}\partial_\xi^{\beta'}\left[A(p(\tau,s))\right]\partial_x^{\alpha-\alpha'}\partial_\xi^{\beta-\beta'}P(\tau)d\tau,$$

$$R_{21}(t) \\ := -\sum_{\substack{\alpha'\le\alpha,\beta'\le\beta,\\ |\alpha'+\beta'|\ge 1}} \binom{\alpha}{\alpha'}\binom{\beta}{\beta'}\int_s^t \partial_x^{\alpha'}\partial_\xi^{\beta'}\left[\nabla_x^2 V_\rho(\tau,q(\tau,s))\right]\partial_x^{\alpha-\alpha'}\partial_\xi^{\alpha-\beta'}Q(\tau)d\tau,$$

$$R_{22}(t) := -\int_s^t \partial_x^\alpha\partial_\xi^\beta\left[\nabla_x^2 V_\rho(\tau,q(\tau,s))\right]d\tau.$$

Thus we learn

$$\partial_x^\alpha\partial_\xi^\beta P(t) = B_s(\partial_x^\alpha\partial_\xi^\beta P(\cdot))(t) - \int_s^t \nabla_x^2 V_\rho(\tau,q(\tau,s))R_1(\tau)d\tau \\ + R_{21}(t)+R_{22}(t).$$

By (2.4.10),(2.4.11) and assumptions of the induction, we have

$$|R_1(t)| \le C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1}|t-s|,$$

$$|R_{21}(t)| \le \int_s^t C\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}\cdot C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1}|\tau-s|d\tau \le C\rho^{2\varepsilon_0}\langle s\rangle^{-1-2\varepsilon_1},$$

$$|R_{22}(t)| \le \int_s^t C\rho^{\varepsilon_0}\langle\tau\rangle^{-2-\varepsilon_1}d\tau \le C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1}.$$

Similarly to the argument for $\alpha = \beta = 0$, we obtain (2.4.8) and (2.4.9) for any $\alpha$ and $\beta$.

Step 5: Proof of (2.4.12). By (2.4.2) and (2.4.3), we have

$$\begin{aligned} q(t,s;x,\xi) &= x + \int_s^t v(p(\tau,s))d\tau \\ &= x + \int_s^t v\left(p(t,s) + \int_\tau^t \nabla_x V_\rho(\sigma, q(\sigma,s))d\sigma\right) d\tau. \end{aligned}$$

Thus

$$\begin{aligned} &q(t,s;x,\xi) - x - (t-s)v(p(t,s)) \\ &= \int_s^t \left[ v\left(p(t,s) + \int_\tau^t \nabla_x V_\rho(\sigma, q(\sigma,s))d\sigma\right) - v(p(t,s))\right] d\tau. \end{aligned}$$

This equality and (2.4.8)-(2.4.11) imply (2.4.12). □

Similarly to [6, Proposition 2.2], we observe that, if $\rho$ is small enough, the maps

$$\begin{aligned} y &\mapsto q(s,t;y,\xi), \\ \eta &\mapsto p(t,s;x,\eta) \end{aligned}$$

have the corresponding inverses.

**Proposition 2.4.3.** *Fix $\rho > 0$ so that $C_0\rho^{\varepsilon_0} < \frac{1}{2}$ holds, where $C_0$ is the constant in Proposition 2.4.2. Then, for $x, \xi \in \mathbb{R}^d$ and $0 \le \pm s \le \pm t$, there exist $y(s,t) = y(s,t;x,\xi) \in \mathbb{R}^d$ and $\eta(t,s) = \eta(t,s;x,\xi) \in \mathbb{R}^d$ such that*

$$\begin{cases} q(s,t;y(s,t;x,\xi),\xi) = x, & (2.4.21) \\ p(t,s;x,\eta(t,s;x,\xi)) = \xi, & (2.4.22) \end{cases}$$

*and*

$$\begin{cases} q(t,s;x,\eta(t,s;x,\xi)) = y(s,t;x,\xi), & (2.4.23) \\ p(s,t;y(s,t;x,\xi),\xi) = \eta(t,s;x,\xi). & (2.4.24) \end{cases}$$

*Furthermore, for any $x, \xi \in \mathbb{R}^d$, $0 \le \pm s \le \pm t$ and multi-indices $\alpha$ and $\beta$,*

$$|\partial_x^\alpha [\nabla_x y(s,t;x,\xi) - I]| \le C'_\alpha \rho^{\varepsilon_0} \langle s\rangle^{-\varepsilon_1}, \tag{2.4.25}$$

$$|\partial_x^\alpha \partial_\xi^\beta \nabla_x \eta(t,s;x,\xi)| \le C'_{\alpha\beta} \rho^{\varepsilon_0} \langle s\rangle^{-1-\varepsilon_1}, \tag{2.4.26}$$

$$|\partial_\xi^\beta [\eta(t,s;x,\xi) - \xi]| \le C'_\beta \rho^{\varepsilon_0} \langle s\rangle^{-\varepsilon_1}, \tag{2.4.27}$$

$$\begin{aligned} &|\partial_\xi^\beta [y(s,t;x,\xi) - x - (t-s)v(\xi)]| \\ &\le C'_\beta \rho^{\varepsilon_0} \min\{|t-s|\langle s\rangle^{-\varepsilon_1}, \langle t\rangle^{1-\varepsilon_1}\}. \end{aligned} \tag{2.4.28}$$

*Proof.* Step 1. By $|\nabla_x q(s,t;x,\xi) - I| < \frac{1}{2}$, $|\nabla_\xi p(t,s;x,\xi) - I| < \frac{1}{2}$ and Schwartz's global inversion theorem ( [5, Proposition A.7.1]), we have the existence and uniqueness of $y(s,t;x,\xi)$ and $\eta(t,s;x,\xi)$ satisfying (2.4.21) and (2.4.22). The equalities (2.4.23) and (2.4.24) are shown by (2.4.21) and (2.4.22).

Step 2: Proof of (2.4.25). Differentiation of (2.4.21) in $x$ implies

$$\nabla_x q(s,t;y(s,t),\xi)\nabla_x y(s,t) = I. \tag{2.4.29}$$

We have by (2.4.6)

$$\begin{aligned}|\nabla_x y(s,t) - I| &= |(\nabla_x q(s,t;y(s,t),\xi))^{-1} - I| \\ &\leq C|\nabla_x q(s,t;y(s,t),\xi) - I| \\ &\leq C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}.\end{aligned}$$

Differentiating (2.4.29), we have for $\alpha \neq 0$

$$\begin{aligned}&\nabla_x q(s,t;y(s,t),\xi)\partial_x^\alpha \nabla_x y(s,t) \\ &= -\sum_{0\lneq\alpha'\leq\alpha} \binom{\alpha}{\alpha'} \partial_x^{\alpha'} \left[\nabla_x q(s,t;y(s,t),\xi)\right] \partial_x^{\alpha-\alpha'} \nabla_x y(s,t).\end{aligned}$$

Using (2.4.6) and the induction with respect to $|\alpha|$, we observe that the RHS of the above equality is bounded by $C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}$. Thus we have $|\partial_x^\alpha \nabla_x y(s,t)| \leq C'_\alpha \rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}$.

Step 3: Proof of (2.4.27). By (2.4.24), we observe for $\beta = 0$

$$\begin{aligned}|\eta(t,s) - \xi| &= |p(s,t;y(s,t),\xi) - \xi| \\ &= \left|\int_s^t \nabla_x V_\rho(\tau, q(\tau,t;y(s,t),\xi))d\tau\right| \\ &\leq C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}.\end{aligned}$$

In the case of $|\beta| = 1$, we have by differentiation of (2.4.22) in $\xi$

$$\nabla_\xi p(t,s;x,\eta(t,s))\nabla_\xi \eta(t,s) = I.$$

Similarly to Step 2, we obtain by (2.4.11)

$$\begin{aligned}|\nabla_\xi \eta(t,s) - I| &\leq C|\nabla_\xi p(t,s;x,\eta(t,s)) - I| \\ &\leq C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}.\end{aligned}$$

In the other cases, we learn by (2.4.22)

$$
\begin{aligned}
&\nabla_\xi p(t,s;x,\eta(t,s))\partial_\xi^\beta \nabla_\xi \eta(t,s)\\
&= - \sum_{0 \lneq \beta' \le \beta} \binom{\beta}{\beta'} \partial_\xi^{\beta'} [\nabla_\xi p(t,s;x,\eta(t,s))] \partial_\xi^{\beta-\beta'} \nabla_\xi \eta(t,s), \quad \beta \neq 0.
\end{aligned}
$$

The induction with respect to $|\beta|$ and (2.4.11) imply each term in the RHS is bounded by $C\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1}$. Thus (2.4.27) holds for any $\beta$.

Step 4: Proof of (2.4.26). Differentiating (2.4.22) in $x$, we have

$$
\nabla_x p(t,s;x,\eta(t,s)) + \nabla_\xi p(t,s;x,\eta(t,s)) \nabla_x \eta(t,s) = 0.
$$

This equality and (2.4.9) imply

$$
\begin{aligned}
|\nabla_x \eta(t,s)| &= |(\nabla_\xi p(t,s;x,\eta(t,s)))^{-1} \nabla_x p(t,s;x,\eta(t,s))|\\
&\le C|\nabla_x p(t,s;x,\eta(t,s))|\\
&\le C\rho^{\varepsilon_0}\langle s\rangle^{-1-\varepsilon_1},
\end{aligned}
$$

which proves (2.4.26) for $\alpha=\beta=0$. If $\alpha+\beta\neq 0$, we have

$$
\begin{aligned}
&\nabla_\xi p(t,s;x,\eta(t,s))\partial_x^\alpha \partial_\xi^\beta \nabla_x \eta(t,s)\\
&= - \partial_x^\alpha \partial_\xi^\beta [\nabla_x p(t,s;x,\eta(t,s))]\\
&\quad - \sum_{\substack{\alpha' \le \alpha, \beta' \le \beta,\\ |\alpha'+\beta'| \ge 1}} \binom{\alpha}{\alpha'} \binom{\beta}{\beta'} \partial_x^{\alpha'} \partial_\xi^{\beta'} [\nabla_\xi p(t,s;x,\eta(t,s))] \partial_x^{\alpha-\alpha'} \partial_\xi^{\beta-\beta'} \nabla_x \eta(t,s).
\end{aligned}
$$

Thus (2.4.26) is proved by (2.4.27), (2.4.9), (2.4.11) and the induction with respect to $|\alpha|+|\beta|$.

Step 5: Proof of (2.4.28). Similarly to the proof of (2.4.12) in Proposition 2.4.2, we have

$$
\begin{aligned}
&y(s,t) - x - (t-s)v(\xi)\\
&= q(t,s;x,\eta(t,s)) - x - (t-s)v(p(t,s;x,\eta(t,s)))\\
&= \int_s^t \left[ v\left(\xi + \int_\tau^t \nabla_x V_\rho(\sigma, q(\sigma,s;x,\eta(t,s)))d\sigma\right) - v(\xi)\right] d\tau.
\end{aligned}
$$

Using this equality, (2.4.10) and (2.4.27), we obtain (2.4.28). □

We define

$$
\phi(t;x,\xi) := u(t;x,\eta(t,0;x,\xi)),
$$

where

$$u(t;x,\eta) := x\cdot\eta + \int_0^t \{h_\rho - x\cdot\nabla_x h_\rho\}(\tau, q(\tau,0;x,\eta), p(\tau,0;x,\eta))d\tau.$$

Then a direct calculus implies that $\phi$ satisfies the Hamilton-Jacobi equation

$$\begin{cases} \partial_t\phi(t;x,\xi) = h_\rho(t, \nabla_\xi\phi(t;x,\xi), \xi), \\ \phi(0;x,\xi) = x\cdot\xi, \end{cases} \tag{2.4.30}$$

and the relation between $\phi$ and the functions $y$ and $\eta$ in Proposition 2.4.3:

$$\begin{cases} \nabla_x\phi(t;x,\xi) = \eta(t,0;x,\xi), \\ \nabla_\xi\phi(t;x,\xi) = y(0,t;x,\xi). \end{cases} \tag{2.4.31}$$

*Remark* 2.4.4. The relation (2.4.31) and Proposition 2.4.3 imply the estimate

$$|\partial_x^\alpha\partial_\xi^\beta\,[\nabla_x y(s,t;x,\xi) - I]\,| \le C'_{|\alpha|+|\beta|}\rho^{\varepsilon_0}\langle s\rangle^{-\varepsilon_1} \tag{2.4.32}$$

holds for $|\beta|\ge 1$. Hence (2.4.25) is extended to (2.4.32) for any $\alpha$ and $\beta$.

Now, we construct outgoing and incoming solutions of the eikonal equation (2.1.4).

**Lemma 2.4.5.** *The limits*

$$\phi_\pm(x,\xi) := \lim_{t\to\pm\infty}(\phi(t;x,\xi) - \phi(t;0,\xi)) \tag{2.4.33}$$

*exist, are smooth in* $\mathbb{R}^{2d}$ *and*

$$\phi_\pm(x,\xi+2\pi m) = \phi_\pm(x,\xi) + 2\pi x\cdot m, \quad x,\xi\in\mathbb{R}^d,\ m\in\mathbb{Z}^d. \tag{2.4.34}$$

*Proof.* We define

$$R(t,x,\xi) := \phi(t;x,\xi) - \phi(t;0,\xi).$$

Then we have

$$\begin{aligned} \nabla_x R(t,x,\xi) &= \eta(t,0;x,\xi) = p(0,t;y(0,t;x,\xi),\xi) \\ &= \xi + \int_0^t (\nabla_x V_\rho)(\tau, q(\tau,t;y(0,t;x,\xi),\xi))d\tau \\ &= \xi + \int_0^t (\nabla_x V_\rho)(\tau, q(\tau,0;x,\eta(t,0;x,\xi)))d\tau. \end{aligned}$$

Since

$$|\partial_x^\alpha \partial_\xi^\beta [(\nabla_x V_\rho)(\tau, q(\tau, 0; x, \eta(t, 0; x, \xi)))]| \leq C_{\alpha\beta} \langle \tau \rangle^{-1-\varepsilon_1},$$

$\nabla_x R(t, x, \xi)$ converges to a smooth function uniformly in $(x, \xi) \in \mathbb{R}^{2d}$. Thus

$$\partial_\xi^\beta R(t, x, \xi) = x \cdot \int_0^1 \nabla_x \partial_\xi^\beta R(t, \theta x, \xi) d\theta \tag{2.4.35}$$

converges locally uniformly in $\mathbb{R}^{2d}$. This implies the smoothness of $\phi_\pm$.

It is easy to see (2.4.34) if we remark

$$\begin{aligned} \eta(t, 0; x, \xi + 2\pi m) &= \eta(t, 0; x, \xi) + 2\pi m, \\ q(t, 0; x, \xi + 2\pi m) &= q(t, 0; x, \xi) \end{aligned}$$

for $x, \xi \in \mathbb{R}^d$, $t \in \mathbb{R}$ and $m \in \mathbb{Z}^d$. □

Next we consider properties of $\phi_\pm$ in the "outgoing" and "incoming" regions. We prepare improved estimates of Proposition 2.4.2 for an orbit which is outgoing or incoming.

**Lemma 2.4.6.** *Let $(q, p)(t) = (q, p)(t, 0; x, \xi)$ be an orbit satisfying (2.4.2) and (2.4.3). Suppose*

$$|q(\tau)| \geq b|\tau| + d, \quad \pm\tau \geq 0$$

*for some $b > 0$ and $d \geq 0$. Then there exist $l_{\alpha\beta}, l_\beta \geq 2$ such that for $\pm t \geq 0$ and $\alpha$, $\beta \in \mathbb{N}_{\geq 0}^d$,*

$$|p(t) - \xi| \leq C b^{-1} \langle d \rangle^{-\varepsilon}, \tag{2.4.36}$$

$$|\partial_x^\alpha \partial_\xi^\beta [\nabla_x q(t) - I]| \leq C_{\alpha\beta} b^{-l_{\alpha\beta}} \langle d \rangle^{-1-|\alpha|-\varepsilon} |t|, \tag{2.4.37}$$

$$|\partial_x^\alpha \partial_\xi^\beta \nabla_x p(t)| \leq C_{\alpha\beta} b^{-l_{\alpha\beta}} \langle d \rangle^{-1-|\alpha|-\varepsilon}, \tag{2.4.38}$$

$$|\partial_\xi^\beta [\nabla_\xi q(t) - tA(\xi)]| \leq C_\beta b^{-l_\beta} \langle d \rangle^{-\varepsilon} |t|, \tag{2.4.39}$$

$$|\partial_\xi^\beta [\nabla_\xi p(t) - I]| \leq C_\beta b^{-l_\beta} \langle d \rangle^{-\varepsilon}. \tag{2.4.40}$$

*Proof.* We calculate similarly to Proposition 2.4.2, whereas we use the following estimate instead:

$$|\partial_x^\alpha V_\rho(t, q(t))| \leq C_\alpha \langle q(t) \rangle^{-|\alpha|-\varepsilon} \leq C_\alpha \langle b|t| + d \rangle^{-|\alpha|-\varepsilon}.$$

□

The next lemma gives improved estimates of Proposition 2.4.3 for outgoing or incoming orbits.

**Lemma 2.4.7.** *Let $b, d \geq 0$, $b \neq 0$ and $x$, $\xi \in \mathbb{R}^d$ satisfy*

$$|q(\tau, 0; x, \eta(t, 0; x, \xi))| \geq b|\tau| + d, \quad 0 \leq \pm\tau \leq \pm t$$

*for any $\pm t \geq 0$. Then there exist $l'_{\alpha\beta}, l'_\beta \geq 2$ such that, for $\pm t \geq 0$,*

$$|\partial_x^\alpha \partial_\xi^\beta [\nabla_x \eta(t, 0; x, \xi)]| \leq C_{\alpha\beta} b^{-l'_{\alpha\beta}} \langle d \rangle^{-1-|\alpha|-\varepsilon}, \tag{2.4.41}$$

$$|\partial_\xi^\beta [\eta(t, 0; x, \xi) - \xi]| \leq C_\beta b^{-l'_\beta} \langle d \rangle^{-\varepsilon}. \tag{2.4.42}$$

*Proof.* The proofs are similar to those of (2.4.26) and (2.4.27) if we use

$$|\partial_x^\alpha V_\rho(\tau, q(\tau, 0; x, \eta(t, 0; x, \xi)))| \leq C_\alpha \langle b|\tau| + d \rangle^{-|\alpha|-\varepsilon}, \quad 0 \leq \pm\tau \leq \pm t.$$

□

Using the above two lemmas, we have the estimate of $\phi_\pm(x, \xi) - x \cdot \xi$ on the outgoing and incoming region, respectively. See [6, Proposition 2.4] for the case of Schrödinger operators.

**Proposition 2.4.8.**

$$|\partial_x^\alpha \partial_\xi^\beta [\phi_\pm(x, \xi) - x \cdot \xi]| \leq C_{\alpha\beta} |v(\xi)|^{-l_{\alpha\beta}} \langle x \rangle^{1-|\alpha|-\varepsilon} \tag{2.4.43}$$

*on $\{(x, \xi) \mid |x|^{\varepsilon_1} |v(\xi)|^{1-\varepsilon_1} \geq C_{\varepsilon_1}, \pm\cos(x, v(\xi)) \geq 0\}$, respectively.*

*Proof.* On $\{(x, \xi) \mid x, v(\xi) \neq 0, \ \pm\cos(x, v(\xi)) \geq 0\}$, (2.4.4), (2.4.5) and (2.4.12) imply for $0 \leq \pm\tau \leq \pm t$,

$$\begin{aligned} |q(\tau, 0; x, \eta(t, 0; x, \xi))| \geq& |x + \tau v(p(\tau, 0; x, \eta(t, 0; x, \xi)))| - C_0 \langle \tau \rangle^{1-\varepsilon_1} \\ =& |x + \tau v(p(\tau, t; y(0, t; x, \xi), \xi))| - C_0 \langle \tau \rangle^{1-\varepsilon_1} \\ \geq& |x + \tau v(\xi)| - C\langle \tau \rangle^{1-\varepsilon_1} - C_0 \langle \tau \rangle^{1-\varepsilon_1} \\ \geq& \frac{1}{\sqrt{2}}(|x| + |\tau v(\xi)|) - C\langle \tau \rangle^{1-\varepsilon_1}. \end{aligned}$$

If we remark

$$|x| + |\tau v(\xi)| \geq \left(\frac{1}{\varepsilon_1}|x|\right)^{\varepsilon_1} \left(\frac{1}{1-\varepsilon_1}|\tau v(\xi)|\right)^{1-\varepsilon_1} = \frac{|x|^{\varepsilon_1} |v(\xi)|^{1-\varepsilon_1}}{\varepsilon_1^{\varepsilon_1}(1-\varepsilon_1)^{1-\varepsilon_1}} |\tau|^{1-\varepsilon_1},$$

we learn for $|x|^{\varepsilon_1}|v(\xi)|^{1-\varepsilon_1} \geq C_{\varepsilon_1}$

$$|q(\tau, 0; x, \eta(t, 0; x, \xi))| \geq \frac{1}{2}(|x| + |\tau v(\xi)|), \quad 0 \leq \pm\tau \leq \pm t. \tag{2.4.44}$$

Hence the proposition is proved by (2.4.44), (2.4.31), (2.4.33), (2.4.35) and Lemma 2.4.7. □

The following proposition says $\phi_\pm$ is a solution to the eikonal equation (2.1.4).

**Proposition 2.4.9.** *For any $a > 0$, there exists $R_a > 1$ such that $\phi_\pm$ satisfies the eikonal equation*

$$h(x, \nabla_x \phi_\pm(x, \xi)) = h_0(\xi) \tag{2.4.45}$$

*on the outgoing (or incoming) region*

$$\{(x, \xi) \mid |x| \geq R_a, \ |v(\xi)| \geq a, \pm\cos(x, v(\xi)) \geq 0\},$$

*respectively.*

*Proof.* By (2.4.31) and (2.4.33), we have

$$\nabla_x \phi_\pm(x, \xi) = \lim_{t \to \pm\infty} \eta(t, 0; x, \xi) = \lim_{t \to \pm\infty} p(0, t; y(0, t; x, \xi), \xi).$$

If $|x| \geq 2\rho^{-1}$, then we have by the definition of $V_\rho$

$$h(x, \nabla_x \phi_\pm(x, \xi)) = \lim_{t \to \pm\infty} h_\rho(0, x, p(0, t; y(0, t; x, \xi), \xi)). \tag{2.4.46}$$

Now we claim

$$\begin{aligned} E(\tau) &:= h_\rho(\tau, q(\tau, t; y(0, t; x, \xi), \xi), p(\tau, t; y(0, t; x, \xi), \xi)) \\ &= h_\rho(\tau, q(\tau, 0; x, \eta(t, 0; x, \xi)), p(\tau, 0; x, \eta(t, 0; x, \xi))) \end{aligned}$$

is a constant for $0 \leq \pm\tau \leq \pm t$. A direct calculus implies

$$\begin{aligned} \frac{dE}{d\tau}(\tau) &= \partial_t h_\rho(\tau, q(\tau, 0; x, \eta(t, 0; x, \xi)), p(\tau, 0; x, \eta(t, 0; x, \xi))) \\ &= \partial_t V_\rho(\tau, q(\tau, 0; x, \eta(t, 0; x, \xi))). \end{aligned}$$

We note (2.4.44) holds on $\{(x, \xi) \mid |x| \geq R_a, \ |v(\xi)| \geq a, \ \pm\cos(x, v(\xi)) \geq 0\}$ for $R_a$ large enough, and hence

$$\begin{aligned} |q(\tau, 0; x, \eta(t, 0; x, \xi))| &\geq \frac{1}{2}(R_a + a|\tau|) \\ &\geq 2\max\{\rho^{-1}, \frac{\langle\tau\rangle}{\langle\log\langle\tau\rangle\rangle}\}, \quad 0 \leq \pm\tau \leq \pm t. \end{aligned}$$

We also note $\partial_t V_\rho(t,x) = 0$ if $|x| \geq 2\max\{\rho^{-1}, \frac{\langle t\rangle}{\langle \log\langle t\rangle\rangle}\}$. Thus we have $\frac{dE}{d\tau}(\tau) = 0$ if $0 \leq \pm\tau \leq \pm t$, in particular,

$$\begin{aligned} h_\rho(0,x,p(0,t;y(0,t;x,\xi),\xi)) &= E(0) = E(t) \\ &= h_\rho(t,y(0,t;x,\xi),\xi). \end{aligned} \tag{2.4.47}$$

Hence, (2.4.46) and (2.4.47) imply

$$h(x,\nabla_x\phi_\pm(x,\xi)) = \lim_{t\to\pm\infty} h_\rho(t,y(0,t;x,\xi),\xi) = h_0(\xi).$$

□

*Proof of Proposition 2.2.1.* Let $\varphi \in C^\infty(\mathbb{R}^d \times (\mathbb{R}^d \backslash v^{-1}(0)))$ be defined by

$$\begin{aligned} \varphi(x,\xi) = (\phi_+(x,\xi) - x\cdot\xi)\chi_+(x,\xi) \\ + (\phi_-(x,\xi) - x\cdot\xi)\chi_-(x,\xi) + x\cdot\xi, \end{aligned} \tag{2.4.48}$$

where

$$\chi_\pm(x,\xi) = \chi\left(\mu|v(\xi)|^\ell x\right)\psi_\pm(\cos(x,v(\xi))) \tag{2.4.49}$$

and $\psi_\pm \in C^\infty([-1,1];[0,1])$ satisfy

$$\psi_\pm(\sigma) = \begin{cases} 1, & \pm\sigma \geq \frac{1}{2}, \\ 0, & \pm\sigma \leq 0. \end{cases}$$

If $\mu$ and $\ell$ are fixed so that $\mu$ is sufficiently small and that $\ell$ is sufficiently large, then $\varphi$ satisfies (2.2.3), (2.2.4) and (2.2.5).

Finally we prove (2.2.9). Let $s_a$ be defined by (2.2.8). We decompose $s_a$ by

$$s_a(x,\xi) = s_a^1(x,\xi) + s_a^2(x,\xi), \tag{2.4.50}$$

where

$$\begin{aligned} s_a^1(x,\xi) &= \sum_{z\in\mathbb{Z}^d} f[z]\, e^{i(\varphi_a(x-z,\xi)-\varphi_a(x,\xi))} - h_0(\nabla_x\varphi_a(x,\xi)), \\ s_a^2(x,\xi) &= h(x,\nabla_x\varphi_a(x,\xi)) - h_0(\xi). \end{aligned}$$

For $s_a^2$, (2.4.45) and Assumption 2.1.3 imply for $|x| \geq R_a$ and $\beta$,

$$\partial_\xi^\beta s_a^2(x,\xi) = \begin{cases} 0, & |\cos(x,v(\xi))| \geq \frac{1}{2}, \\ \mathcal{O}(\langle x\rangle^{-\varepsilon}), & |\cos(x,v(\xi))| \leq \frac{1}{2}. \end{cases} \tag{2.4.51}$$

For $s_a^1$, we have

$$s_a^1(x,\xi) = \sum_{z\in\mathbb{Z}^d} f[z]\left(e^{i(\varphi_a(x-z,\xi)-\varphi_a(x,\xi))} - e^{-iz\cdot\nabla_x\varphi_a(x,\xi)}\right)$$
$$= \sum_{z\in\mathbb{Z}^d} f[z]\, e^{-iz\cdot\nabla_x\varphi_a(x,\xi)}\left(e^{i\Phi_a(x,\xi,z)} - 1\right),$$

where

$$\Phi_a(x,\xi,z) = \varphi_a(x-z,\xi) - \varphi_a(x,\xi) + z\cdot\nabla_x\varphi_a(x,\xi)$$
$$= z\cdot\left(\int_0^1 \theta_1 \int_0^1 \nabla_x^2\varphi_a(x-\theta_1\theta_2 z,\xi)d\theta_2 d\theta_1\right)z.$$

By (2.2.4), we observe

$$|\partial_\xi^\beta[e^{-iz\cdot\nabla_x\varphi_a(x,\xi)}]| \leq C_\beta\langle z\rangle^{|\beta|}$$

and

$$|\partial_\xi^\beta\Phi_a(x,\xi,z)| \leq C_\beta|z|^2\int_0^1\theta_1\int_0^1\langle x-\theta_1\theta_2 z\rangle^{-1-\varepsilon}d\theta_2 d\theta_1$$
$$\leq C_\beta\langle x\rangle^{-1-\varepsilon}\langle z\rangle^{3+\varepsilon}.$$

Thus we obtain

$$|\partial_\xi^\beta s_a^1(x,\xi)| \leq C_\beta\langle x\rangle^{-1-\varepsilon}. \tag{2.4.52}$$

Hence (2.2.9) is proved by (2.4.50), (2.4.51) and (2.4.52). □

## 2.5 Appendix: Proofs of Lemmas 2.2.2 and 2.2.3

### 2.5.1 Proof of Lemma 2.2.2

First we remark that $J_a, P_\pm, \tilde{P}_\pm$ and their formal adjoint operators

$$J_a^* u[x] = (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(x\cdot\xi-\varphi_a(y,\xi))}u[y]d\xi,$$

$$P_\pm^* u[x] = (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\xi}p_\pm(x,\xi)u[y]\,d\xi,$$

$$\tilde{P}_\pm^* u[x] = (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(\varphi_a(x,\xi)-y\cdot\xi)}p_\pm(x,\xi)u[y]\,d\xi$$

map from $\mathscr{S}(\mathbb{Z}^d)$ to itself.

Letting $L := \langle x-y\rangle^{-2}(1+(x-y)\cdot D_\xi)$, $D_\xi := \frac{1}{i}\nabla_\xi$, we easily see $L\left(e^{i(x-y)\cdot\xi}\right) = e^{i(x-y)\cdot\xi}$. Thus we have

$$\begin{aligned}P_\pm u\,[x] =&(2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} L^k\left(e^{i(x-y)\cdot\xi}\right)p_\pm(y,\xi)u\,[y]\,d\xi\\ =&(2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\xi}(L^*)^k\left(p_\pm(y,\xi)\right)u\,[y]\,d\xi\end{aligned}$$

for any $k\in\mathbb{N}_{\geq 0}$. We define $|p_\pm| := \sup_{|\beta|\leq d+1}\sup_{(x,\xi)\in\mathbb{Z}^d\times\mathbb{T}^d}|\partial_\xi^\beta p_\pm(x,\xi)|$. Then we learn that, setting $k=d+1$,

$$|P_\pm u\,[x]\,| \leq C|p_\pm|\sum_{y\in\mathbb{Z}^d}\langle x-y\rangle^{-d-1}|u[x]|.$$

This and Young's inequality imply $\|P_\pm u\| \leq C|p_\pm|\|u\|$, where $\|u\| := \left(\sum_{x\in\mathbb{Z}^d}|u[x]|^2\right)^{\frac{1}{2}}$. Hence $P_\pm$ are bounded.

Next we prove $\tilde{P}_\pm$ are bounded. A direct calculus implies

$$\begin{aligned}\tilde{P}_\pm^*\tilde{P}_\pm u[x] &= (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(y,\xi))}p_\pm(x,\xi)p_\pm(y,\xi)u\,[y]\,d\xi\\ &= (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\eta(\xi;x,y)}p_\pm(x,\xi)p_\pm(y,\xi)u\,[y]\,d\xi,\end{aligned}$$

where $\eta$ in the last equality is defined by

$$\eta(\xi;x,y) := \int_0^1 \nabla_x\varphi_a(y+\theta(x-y),\xi)d\theta. \tag{2.5.1}$$

Then (2.2.5) implies $\eta(\cdot;x,y):\mathbb{T}^d\to\mathbb{T}^d$ has its inverse map $\xi(\cdot;x,y)$. Changing the variable $\xi$ to $\eta$, we have

$$\tilde{P}_\pm^*\tilde{P}_\pm u[x] = (2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\eta}r(x,y,\eta)u\,[y]\,d\eta,$$

where

$$r(x,y,\eta) = p_\pm(x,\xi(\eta;x,y))p_\pm(y,\xi(\eta;x,y))\left|\det\left(\frac{d\xi}{d\eta}\right)\right|.$$

Since (2.2.4) implies

$$\left|\partial_\eta^\beta\left[\det\left(\frac{d\xi}{d\eta}\right)-1\right]\right|\le C_\beta\langle x\rangle^{-\varepsilon}, \tag{2.5.2}$$

the similar argument for $P_\pm$ proves the boundedness of $\tilde{P}_\pm^*\tilde{P}_\pm$. Thus, for $u\in\mathscr{S}(\mathbb{Z}^d)$, we obtain

$$\|\tilde{P}_\pm u\|^2=|(\tilde{P}_\pm^*\tilde{P}_\pm u,u)|\le\|\tilde{P}_\pm^*\tilde{P}_\pm\|\|u\|^2,$$

which implies $\tilde{P}_\pm$ are bounded. The boundedness of $J_a$ is proved similarly. □

### 2.5.2 Proof of Lemma 2.2.3

Since

$$\gamma(H_0)-P_+-P_-=\gamma(H_0)(1-\chi),$$

the compactness of the support of $1-\chi$ implies $P_++P_--\gamma(H_0)$ is a finite rank operator, in particular, a compact operator.

We show $P_\pm^*-P_\pm$ are compact. We observe

$$\begin{aligned}
&(P_\pm^*-P_\pm)u[x]\\
&=(2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d}e^{i(x-y)\cdot\xi}(p_\pm(x,\xi)-p_\pm(y,\xi))u\,[y]\,d\xi\\
&=(2\pi)^{-d}\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d}e^{i(x-y)\cdot\xi}(x-y)\cdot\int_0^1\nabla_x p_\pm(y+\theta(x-y),\xi)d\theta\,u[y]d\xi\\
&=(2\pi)^{-d}i\int_{\mathbb{T}^d}\sum_{y\in\mathbb{Z}^d}e^{i(x-y)\cdot\xi}\int_0^1\nabla_\xi\cdot\nabla_x p_\pm(y+\theta(x-y),\xi)d\theta\,u[y]d\xi,
\end{aligned}$$

where the last equality follows from integral by parts in $\xi$. Since

$$\begin{aligned}
\left|\int_0^1\partial_\xi^\beta[\nabla_\xi\cdot\nabla_x p_\pm(y+\theta(x-y),\xi)]d\theta\right|&\le C_\beta\int_0^1\langle y+\theta(x-y)\rangle^{-1}d\theta\\
&\le C'_\beta\langle x\rangle^{-1},
\end{aligned}$$

similar argument in Lemma 2.2.2 proves $\langle x\rangle(P_\pm^*-P_\pm)$ are bounded. By the compactness of $\langle x\rangle^{-1}$ as an operator on $\mathcal{H}$, $P_\pm^*-P_\pm=\langle x\rangle^{-1}\cdot\langle x\rangle(P_\pm^*-P_\pm)$ are compact.

We next prove the compactness of $E_\pm(0) - P_\pm$. Using (2.5.1), we have

$$\begin{aligned} E_\pm(0)u[x] &= J_a \tilde{P}_\pm u[x] \\ &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(y,\xi))} p_\pm(y,\xi) u\,[y]\,d\xi \\ &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\eta} p_\pm(y,\xi(\eta)) \left|\det\left(\frac{d\xi}{d\eta}\right)\right| u\,[y]\,d\eta. \end{aligned}$$

Thus

$$(E_\pm(0) - P_\pm)u[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\eta} r(x,y,\eta) u\,[y]\,d\eta,$$

where

$$r(x,y,\eta) = p_\pm(y,\xi(\eta)) \left|\det\left(\frac{d\xi}{d\eta}\right)\right| - p_\pm(y,\eta).$$

By (2.5.2), we have $|\partial_\eta^\beta[r(x,y,\eta)]| \le C_\beta \langle x\rangle^{-\varepsilon}$, and hence $\langle x\rangle^\varepsilon(E_\pm(0) - P_\pm)$ are bounded. This proves $E_\pm(0) - P_\pm$ are compact.

The compactness of $J_a J_a^* - I$ is proved similarly to that of $E_\pm(0) - P_\pm$, since

$$\begin{aligned} (J_a J_a^* - I)u[x] &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(y,\xi))} u\,[y]\,d\xi - u[x] \\ &= (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y\in\mathbb{Z}^d} e^{i(x-y)\cdot\eta} \left(\left|\det\left(\frac{d\xi}{d\eta}\right)\right| - 1\right) u\,[y]\,d\eta. \end{aligned}$$

Finally, we prove $J_a^* J_a - I$ is compact. Now we mimic the proof of [12, Lemma 7.1]. For $f \in L^2(\mathbb{T}^d)$, we denote

$$\begin{aligned} L_a f(\xi) &= F J_a^* J_a F^* f(\xi) \\ &= (2\pi)^{-d} \sum_{x\in\mathbb{Z}^d} \int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(x,\eta))} f(\eta) d\eta, \\ \tilde{L}_a f(\xi) &= (2\pi)^{-d} \int_{\mathbb{R}^d} \int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(x,\eta))} f(\eta) d\eta dx. \end{aligned}$$

First we show that, for any $\psi \in C^\infty(\mathbb{T}^d)$ with sufficiently small support,

$$K_{a,\psi} := \psi \circ (L_a - \tilde{L}_a)$$

is a compact operator on $L^2(\mathbb{T}^d)$. We define $\Pi : L^1(\mathbb{R}^d) \to L^1(\mathbb{T}^d)$ by

$$\Pi f(\xi) := \sum_{m\in\mathbb{Z}^d} f(\xi + 2\pi m).$$

Then (2.2.3) implies

$$\begin{aligned}\Pi\tilde{L}_a f(\xi) =&(2\pi)^{-d} \sum_{m\in\mathbb{Z}^d} \int_{\mathbb{R}^d}\int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi+2\pi m)-\varphi_a(x,\eta))} f(\eta) d\eta dx \\ =&(2\pi)^{-d} \sum_{m\in\mathbb{Z}^d} \int_{\mathbb{R}^d}\int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi)+2\pi x\cdot m-\varphi_a(x,\eta))} f(\eta) d\eta dx.\end{aligned}$$

Using Poisson's summation formula

$$\sum_{m\in\mathbb{Z}^d} e^{2\pi i x\cdot m} = \sum_{m\in\mathbb{Z}^d} \delta_{x-m} \tag{2.5.3}$$

in the sense of distribution, we have

$$\Pi\tilde{L}_a f(\xi) =(2\pi)^{-d} \sum_{x\in\mathbb{Z}^d} \int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi)-\varphi_a(x,\eta))} f(\eta) d\eta = L_a f(\xi).$$

Thus we learn

$$\begin{aligned}K_{a,\psi} f(\xi) =&\psi \circ (\Pi\tilde{L}_a - \tilde{L}_a) f(\xi) \\ =&\sum_{m\in\mathbb{Z}^d\setminus\{0\}} \psi(\xi) \int_{\mathbb{R}^d}\int_{\mathbb{T}^d} e^{i(\varphi_a(x,\xi+2\pi m)-\varphi_a(x,\eta))} f(\eta) d\eta dx \\ =&\int_{\mathbb{T}^d} k_{a,\psi}(\xi,\eta) f(\eta) d\eta,\end{aligned}$$

where the integral kernel

$$k_{a,\psi}(\xi,\eta) = \sum_{m\in\mathbb{Z}^d\setminus\{0\}} \psi(\xi) \int_{\mathbb{R}^d} e^{i(\varphi_a(x,\xi+2\pi m)-\varphi_a(x,\eta))} dx$$

is smooth. This implies the compactness of $K_{a,\psi}$.

In order to show the compactness of $\psi \circ (\tilde{L}_a - I)$, we note

$$\tilde{L}_a f(\xi) = (2\pi)^{-d} \int_{\mathbb{R}^d}\int_{\mathbb{T}^d} e^{i\int_0^1 \nabla_\xi \varphi_a(x,\eta+\theta(\xi-\eta))d\theta\cdot(\xi-\eta)} f(\eta) d\eta dx.$$

Letting

$$y(x;\xi,\eta) := \int_0^1 \nabla_\xi \varphi_a(x,\eta+\theta(\xi-\eta))d\theta,$$

we observe $y(\cdot;\xi,\eta)$ has its inverse map by (2.2.5). Thus we have

$$\tilde{L}_a f(\xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} \int_{\mathbb{T}^d} e^{iy\cdot(\xi-\eta)} \left| \det\left(\frac{dx}{dy}\right) \right| f(\eta) d\eta dy.$$

This equality and

$$\left| \partial_y^\alpha \partial_\xi^\beta \partial_\eta^\gamma \left[ \det\left(\frac{dx}{dy}\right) - 1 \right] \right| \leq C_{\alpha\beta\gamma} \langle y \rangle^{-|\alpha|-\varepsilon}$$

imply the compactness of $\psi \circ (\tilde{L}_a - I)$.

Hence, with the help of a partition of unity $\{\psi_j\}_{j=1}^J$ on $\mathbb{T}^d$, we observe

$$J_a^* J_a - I = F^*(L_a - I)F = F^* \sum_{j=1}^J \left( K_{a,\psi_j} + \psi_j \circ (\tilde{L}_a - I) \right) F$$

is compact. □

# Bibliography


[1] W. Amrein, A. Boutet de Monvel, V. Georgescu: $C_0$-groups, commutator methods and spectral theory of $N$-body Hamiltonians. Progress in Mathematics, 135. Birkhäuser Verlag, Basel, 1996.

[2] K. Ando, H. Isozaki, H. Morioka: Spectral properties of Schrödinger operators on perturbed lattices. Ann. Henri Poincaré **17** (2016), 2103–2171.

[3] K. Asada, D. Fujiwara: On some oscillatory integral transformations in $L^2(\mathbb{R}^n)$. Japan. J. Math. (N.S.) **4** (1978), no. 2, 299–361.

[4] A. Boutet de Monvel, J. Sahbani: On the spectral properties of discrete Schrödinger operators: (The multi-dimensional case). Rev. Math. Phys. **11** (1999), 1061–1078.

[5] J. Dereziński, C. Gérard: Scattering Theory of Classical and Quantum $N$-Particle Systems. Springer Verlag, 1997.

[6] H. Isozaki, H. Kitada: Modified wave operators with time-independent modifiers. J. Fac. Sci. Univ. Tokyo Sect. IA Math. **32** (1985), no. 1, 77–104.

[7] H. Isozaki, I. Korotyaev: Inverse Problems, Trace Formulae for Discrete Schorödinger Operators. Ann. Henri Poincaré **13** (2012), 751–788.

[8] H. Kitada: Scattering theory for Schrödinger equations with time-dependent potentials of long-range type. J. Fac. Sci. Univ. Tokyo Sect. IA Math. **29** (1982), 353–369.

[9] H. Kitada, K. Yajima: A scattering theory for time-dependent long-range potentials. Duke Math. J. **49** (1982), 341–376.

[10] H. Kitada, K. Yajima: Remarks on our paper "A scattering theory for time-dependent long-range potentials". Duke Math. J. **50** (1983), 1005–1016.

[11] S. Nakamura: Modified wave operators for discrete Schrödinger operators with long-range perturbations. J. Math. Phys. **55** (2014), 112101 (8 pages).

[12] S. Nakamura: Microlocal properties of scattering matrices. Comm. Partial Differential Equations 41 (2016), 894–912.

[13] C. R. de Oliveira: Intermediate Spectral Theory and Quantum Dynamics. Birkhäuser Verlag AG, 2009.

[14] D. Parra, S. Richard: Spectral and scattering theory for Schrödinger operators on perturbed topological crystals. Rev. Math. Phys. **30** (2018), 1850009-1 – 1850009-39.

[15] M. Reed, B. Simon: The Methods of Modern Mathematical Physics, Volume III, Scattering Theory, Academic Press, 1979.

[16] D. R. Yafaev: Mathematical scattering theory. Analytic theory. Mathematical Surveys and Monographs, 158. American Mathematical Society, Providence, RI, 2010.

[17] M. Zworski: Semiclassical Analysis. Graduate Studies in Mathematics, Volume 138. American Mathematical Society, Providence, 2012.

# Chapter 3

# Long-range scattering theory for discrete Schrödinger operators on graphene

## 3.1 Introduction

The aim of this chapter is to consider a long-range scattering theory for discrete Schrödinger operators on graphene, that is, the hexagonal lattice. Unlike discrete Schrödinger operators on the square and triangular lattices, operators on the hexagonal lattice cannot be represented as an operator on the space of $\mathbb{C}^1$-valued functions on $\mathbb{Z}^2$, but $\mathbb{C}^2$-valued. Because of this aspect, a long-range scattering theory for this model cannot be treated as in the last chapter. In this chapter, we generalize the results of the last chapter, and in particular we construct Isozaki-Kitada modifiers for the hexagonal lattice. For a short-range scattering theory for discrete Schrödinger operators on general lattices, including the hexagonal lattice, see [14]. See also [3] and [4] for spectral properties of discrete Schrödinger operators on general lattices.

Let $\mathcal{H} = \ell^2(\mathbb{Z}^2; \mathbb{C}^2)$. For $u \in \mathcal{H}$, we use the notation $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$, $u_1, u_2 \in \ell^2(\mathbb{Z}^2)$. The unperturbed discrete Schrödinger operator $H_0$ on graphene is described as the negative of the difference Laplacian

$$H_0 u[x] = - \begin{pmatrix} u_2[x] + u_2[x - e_1] + u_2[x - e_2] \\ u_1[x] + u_1[x + e_1] + u_1[x + e_2] \end{pmatrix}, \quad x \in \mathbb{Z}^2, u \in \mathcal{H}, \quad (3.1.1)$$

where $e_1 = (1, 0)$, $e_2 = (0, 1)$. The derivation of $H_0$ is found in e.g. [2]

and [3]. As is seen later, $H_0$ has purely absolutely continuous spectrum and $\sigma(H_0) = \sigma_{ac}(H_0) = [-3, 3]$.

For a function $V : \mathbb{Z}^2 \to \mathbb{R}^2$, the corresponding multiplication operator is also denoted by $V$:

$$Vu[x] = \begin{pmatrix} V_1[x]u_1[x] \\ V_2[x]u_2[x] \end{pmatrix}, \tag{3.1.2}$$

where $V_1[x]$ and $V_2[x]$ are the first and second value of $V[x]$. We set $H = H_0 + V$. It is known that if $V$ is short-range, i.e., $|V[x]| \le C\langle x\rangle^{-\rho}$ for some $C > 0$ and $\rho > 1$, where $\langle x\rangle := (1 + |x|^2)^{\frac{1}{2}}$, the wave operators

$$W^{\pm} = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH}e^{-itH_0}$$

exist and $W^{\pm}$ are asymptotically complete, i.e., the range of $W^{\pm}$ equals to the absolutely continuous subspace of $H$. In this chapter, we assume the long-range condition below.

**Assumption 3.1.1.** The function $V$ has the following representation

$$V_1 = V_\ell + V_{s,1},\ V_2 = V_\ell + V_{s,2},$$

where $V_\ell$ and $V_{s,j}$ satisfy

$$|\tilde{\partial}^\alpha V_\ell[x]| \le C_\alpha \langle x\rangle^{-|\alpha|-\rho}, \quad x \in \mathbb{Z}^2,\ \alpha \in \mathbb{Z}_+^2,$$
$$|V_{s,j}[x]| \le C\langle x\rangle^{-1-\rho}, \quad x \in \mathbb{Z}^2,\ j = 1, 2$$

for some $\rho \in (0, 1]$ and $C_\alpha, C > 0$. Here $\tilde{\partial}^\alpha = \tilde{\partial}_{x_1}^{\alpha_1}\tilde{\partial}_{x_2}^{\alpha_2}$, $\tilde{\partial}_{x_j}W[x] := W[x] - W[x - e_j]$.

*Remark* 3.1.2. The above assumption is invariant under the choice of isomorphism between the set of vertices of the hexagonal lattice and $\mathbb{Z}^2 \times \{1, 2\}$ invariant under the canonical $\mathbb{Z}^2$ action. In particular, it follows that the difference between each pair of the nearest vertices is short-range. We note that the pair of potentials $V_1[x] = \langle x\rangle^{-1}$ and $V_2[x] = -\langle x\rangle^{-1}$, an analog of Wigner-von Neumann potentials, is not allowed under the above assumption. We also note that, for 1-dimensional discrete Schrödinger operators, embedded eigenvalues can occur even if $|V[x]| \le C\langle x\rangle^{-1}$, $x \in \mathbb{Z}$ for some $C > 0$ (see [11]).

We give notations for the description of the main theorem. Let $\mathcal{T} = \{0, \pm 1, \pm 3\}$ be the set of threshold energies. For a selfadjoint operator $S$ and an Borel set $I \subset \mathbb{R}$, $E_S(I)$ denotes the spectral projection of $S$ onto $I$ and $\mathcal{H}_{ac}(S)$ denotes the absolutely continuous subspace of $S$. The main theorem of this chapter is the following.

**Theorem 3.1.3.** *Assume that $V$ satisfies Assumption 3.1.1. Then for any open set $\Gamma \Subset [-3,3]\backslash\mathcal{T}$, one can construct a Fredholm operator $J$ on $\mathcal{H}$ such that there exist modified wave operators*

$$W_J^{\pm}(\Gamma) := \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} J e^{-itH_0} E_{H_0}(\Gamma) \tag{3.1.3}$$

*and the following properties hold:*
*i)Intertwining property* $HW_J^{\pm}(\Gamma) = W_J^{\pm}(\Gamma)H_0$.
*ii)Partial isometries* $\|W_J^{\pm}(\Gamma)u\| = \|E_{H_0}(\Gamma)u\|$.
*iii)Asymptotic completeness* $\operatorname{Ran} W_J^{\pm}(\Gamma) = E_H(\Gamma)\mathcal{H}_{ac}(H)$.

The above theorem is an analog of [12] and Theorem 2.1.5 in the sense of a long-range scattering theory for discrete Schrödinger operators. For a long-range scattering theory for Schrödinger operators on the Euclidean space, see e.g. [6], [18] and references therein.

We observe spectral properties of the free operator $H_0$, and we show an abstract form of the operator $J$ in (3.1.3). By $\mathcal{F} : \mathcal{H} \to L^2(\mathbb{T}^2;\mathbb{C}^2)$, $\mathbb{T}^2 := [-\pi,\pi)^2$, we denote the discrete Fourier transform

$$\mathcal{F}u(\xi) = \begin{pmatrix} Fu_1(\xi) \\ Fu_2(\xi) \end{pmatrix}, \quad \xi \in \mathbb{T}^2, \tag{3.1.4}$$
$$Fu_j(\xi) = (2\pi)^{-1} \sum_{x\in\mathbb{Z}^2} e^{-ix\cdot\xi} u_j[x], \quad j = 1,2.$$

Then $\mathcal{F}\circ H_0 \circ \mathcal{F}^*$ is a multiplier by the matrix

$$H_0(\xi) = \begin{pmatrix} 0 & \overline{\alpha(\xi)} \\ \alpha(\xi) & 0 \end{pmatrix}, \tag{3.1.5}$$

where $\alpha(\xi) := -(1 + e^{i\xi_1} + e^{i\xi_2})$. Note that for each $\xi \in \mathbb{T}^2$, $H_0(\xi)$ is an Hermitian matrix.

In order to determine the spectrum $\sigma(H_0)$ of $H_0$, we consider the diagonalization of matrix at each point in the momentum space $\mathbb{T}^2$. We set a unitary matrix

$$U(\xi) := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -\frac{\overline{\alpha(\xi)}}{|\alpha(\xi)|} \\ \frac{\alpha(\xi)}{|\alpha(\xi)|} & 1 \end{pmatrix}, \quad \xi \in \mathbb{T}^2\backslash\{\alpha^{-1}(0)\}.$$

Then $H_0(\xi)$ is diagonalized by $U(\xi)$; setting $p(\xi) := |\alpha(\xi)|$, we have

$$\tilde{H}_0(\xi) := U(\xi)^* H_0(\xi) U(\xi) = \begin{pmatrix} p(\xi) & 0 \\ 0 & -p(\xi) \end{pmatrix}, \ \xi \in \mathbb{T}^2\backslash\{\alpha^{-1}(0)\}.$$

Since $\alpha^{-1}(0) = \{(\pm\frac{2}{3}\pi, \mp\frac{2}{3}\pi)\}$, $\tilde{H}_0(\xi)$ and $U(\xi)$ are defined a.e. in $\mathbb{T}^2$. Furthermore $p$ is smooth outside $\alpha^{-1}(0)$ and the set of its critical points

$$\begin{aligned}\mathrm{Cr} :=&\{\xi \in \mathbb{T}^2\backslash\alpha^{-1}(0) \mid \nabla_\xi p(\xi) = 0\} \\ =&\{(0,0), (-\pi, 0), (0, -\pi), (-\pi, -\pi)\}\end{aligned} \tag{3.1.6}$$

has Lebesgue measure zero. Thus $H_0$ has purely absolutely continuous spectrum (see Proposition 2.2.1) and

$$\sigma(H_0) = \overline{p(\mathbb{T}^2\backslash\alpha^{-1}(0)) \cup (-p(\mathbb{T}^2\backslash\alpha^{-1}(0)))} = [-3, 3]. \tag{3.1.7}$$

Using the above $U$, $J$ is formally represented as

$$J = \mathcal{F}^* U(\cdot)\mathcal{F} \circ \begin{pmatrix} J_+ & 0 \\ 0 & J_- \end{pmatrix} \circ \mathcal{F}^* U(\cdot)^* \mathcal{F},$$

where

$$J_\pm u[x] = (2\pi)^{-1} \int_{\mathbb{T}^2} e^{i\varphi_\pm(x,\xi)} F u(\xi) d\xi$$

and $\varphi_\pm(x,\xi)$, $(x,\xi) \in \mathbb{R}^2 \times \mathbb{T}^2$, are outgoing and incoming solution of the eikonal equation

$$p(\nabla_x \varphi) + \tilde{V}_\ell(x) = p(\xi),$$

where $\tilde{V}_\ell$ is a suitable smooth extension of $V_\ell$ onto $\mathbb{R}^2$. However there are two technical difficulties. One is the singularity of $p(\xi)$ at $\alpha^{-1}(0)$. The other is the singularity of $U(\xi)$. The latter is more crucial because we cannot prove that the difference $V_\ell - \mathcal{F}^* U \mathcal{F} \circ V_\ell \circ \mathcal{F}^* U^* \mathcal{F}$ is short-range due to the singularity of $U(\xi)$. We will avoid the above difficulties in Subsection 3.2.1.

We describe the outline of this chapter. The essential idea of proof is as follows; in order to make the above long-range scattering problem easier, we replace the free operator $H_0$ to a modified free operator $H_0'$ witch can be diagonalized in the whole momentum space $\mathbb{T}^2$. In Subsection 3.2.1, we construct the modified free operator $H_0'$, and the property of $H_0'$ is written in Lemma 3.2.1. Considering the long-range scattering theory for $H_0'$ instead of $H_0$, we can reduce the problem of long-range scattering for operators on $\mathcal{H}$ to that for operators on $\ell^2(\mathbb{Z}^2)$. Then we will see in Subsection 3.3.1 that the result of the last chapter is applicable to the above setting. Subsection 3.3.2 concerns a short-range scattering theory. This step is treated with the limiting absorption principle and Kato's smooth perturbation theory. We also use a pseudodifferential calculus prepared in Subsection 3.2.2. In Appendix 3.4, we show the limiting absorption principle by using the Mourre theory.

## 3.2 Preliminaries

### 3.2.1 Construction of the modified free operator

Let us fix the open interval $\Gamma \Subset [-3,3]\backslash\mathcal{T}$ as in Theorem 3.1.3 and $\delta := \mathrm{dist}(0,\Gamma) = \inf_{\lambda\in\Gamma}|\lambda|$. We construct a modified free operator

$$H_0' := \mathcal{F}^* \circ H_0'(\cdot) \circ \mathcal{F},$$

where $H_0'(\xi) \in C^\infty(\mathbb{T}^2; M_2(\mathbb{C}))$ is a simple symmetric matrix for each $\xi \in \mathbb{T}^2$. We will choose $H_0'(\xi)$ so that $H_0'$ has the same spectral projection as $H_0$ in $[-3, -\frac{\delta}{2}] \cup [\frac{\delta}{2}, 3]$.

Let $\kappa \in C^\infty(\mathbb{R}_{\geq 0}; \mathbb{R}_{\geq 0})$ be fixed such that $\operatorname{supp}\kappa \subset [0, \frac{\delta^2}{4})$ and $0 < E + \kappa(E)^2 < \frac{\delta^2}{4}$ for $E \in [0, \frac{\delta^2}{4})$. Let us define

$$H'(\xi) := \begin{pmatrix} \kappa(p(\xi)^2) & \overline{\alpha(\xi)} \\ \alpha(\xi) & -\kappa(p(\xi)^2) \end{pmatrix}. \tag{3.2.1}$$

Then $H'(\xi)$ has two eigenvalues

$$\lambda_\pm(\xi) := \pm\left(\kappa(p(\xi)^2)^2 + p(\xi)^2\right)^{\frac{1}{2}} \tag{3.2.2}$$

and the corresponding eigenvectors are

$$f_+(\xi) = \begin{pmatrix} \kappa(p(\xi)^2) + \lambda_+(\xi) \\ \alpha(\xi) \end{pmatrix},\ f_-(\xi) = \begin{pmatrix} -\overline{\alpha(\xi)} \\ \kappa(p(\xi)^2) + \lambda_+(\xi) \end{pmatrix}.$$

Therefore letting

$$\begin{aligned} U'(\xi) :=& \frac{1}{C(\xi)} \begin{pmatrix} \kappa(p(\xi)^2) + \lambda_+(\xi) & -\overline{\alpha(\xi)} \\ \alpha(\xi) & \kappa(p(\xi)^2) + \lambda_+(\xi) \end{pmatrix}, \\ C(\xi) :=& \left\{ p(\xi)^2 + \left[\kappa(p(\xi)^2) + \lambda_+(\xi)\right]^2 \right\}^{\frac{1}{2}}, \end{aligned} \tag{3.2.3}$$

we learn that $U'(\xi)$ is a unitary matrix-valued smooth function on $\mathbb{T}^2$ and

$$\tilde{H}_0'(\xi) := U'(\xi)^* H_0'(\xi) U'(\xi) = \begin{pmatrix} \lambda_+(\xi) & 0 \\ 0 & \lambda_-(\xi) \end{pmatrix}. \tag{3.2.4}$$

Note that $\lambda_\pm(\xi) = \pm p(\xi)$ for $\xi \in p^{-1}\left((\frac{\delta}{2}, 3]\right)$ by the condition of $\kappa$. Thus we obtain the following lemma.

**Lemma 3.2.1.** *Let*

$$H_0' := \mathcal{F}^* H_0'(\cdot)\mathcal{F},\ \tilde{H}_0' := \mathcal{F}^* \tilde{H}_0'(\cdot)\mathcal{F},\ U' := \mathcal{F}^* U'(\cdot)\mathcal{F} \tag{3.2.5}$$

*and*

$$\lambda_\pm := F^* \lambda_\pm(\cdot) F. \tag{3.2.6}$$

*Then*

$$\tilde{H}_0' = (U')^* H_0' U' = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \tag{3.2.7}$$

$$E_{H_0}(I) = E_{H_0'}(I), \quad I \Subset (-\infty, -\frac{\delta}{2}) \cup (\frac{\delta}{2}, \infty). \tag{3.2.8}$$

*In particular,*

$$e^{-itH_0} E_{H_0}(\Gamma) = e^{-itH_0'} E_{H_0'}(\Gamma), \quad t \in \mathbb{R}, \tag{3.2.9}$$

$$\chi(H_0) = \chi(H_0'), \quad \chi \in C_c^\infty(\Gamma). \tag{3.2.10}$$

### 3.2.2 Pseudodifferential calculus

In this subsection we prepare an assertion concerning the boundedness of pseudodifference operators on $\mathbb{Z}^d$, $d \geq 1$. This lemma is an analog of symbol calculus of pseudodifferential operators on $\mathbb{T}^2$. The proof is given in Appendix 3.5. See also [16, Theorem 4.7.10].

**Lemma 3.2.2.** *Let $m_1, m_2 \in \mathbb{R}$, $a : \mathbb{T}^d \times \mathbb{Z}^d \to \mathbb{C}$, $b : \mathbb{Z}^d \to \mathbb{C}$, and*

$$\mathrm{Op}(a)u[x] = (2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{y \in \mathbb{Z}^d} e^{i(x-y)\cdot\xi} a(\xi, y) u[y] d\xi,$$

$$\mathrm{Op}(b)u[x] = b[x]u[x].$$

*Suppose that $a(\cdot, y) \in C^\infty(\mathbb{T}^d)$ for $y \in \mathbb{Z}^d$ and $|\partial_\xi^\alpha a(\xi, y)| \leq C_\alpha \langle y \rangle^{-m_1}$, $|\tilde{\partial}_{x_j} b[x]| \leq C\langle x \rangle^{-m_2}$ for $x \in \mathbb{Z}^2$, $j = 1, \ldots, d$, where $\tilde{\partial}_{x_j} b[x] = b[x] - b[x - e_j]$. Then, $\langle x \rangle^p [\mathrm{Op}(b), \mathrm{Op}(a)] \langle x \rangle^q$ is a bounded operator on $\ell^2(\mathbb{Z}^d)$ if $p + q = m_1 + m_2$.*

## 3.3 Proof of Theorem 3.1.3

First note that the properties i) and ii) are satisfied if the limits (3.1.3) exist. See [7] and [18] for the proofs.

We denote by $V_\ell$ the multiplication operator by $\begin{pmatrix} V_\ell[x] \\ V_\ell[x] \end{pmatrix}$ if there is no risk of confusion. Let

$$H'_\ell := H'_0 + U' V_\ell \left(U'\right)^* = U' \left(\tilde{H}'_0 + V_\ell\right) \left(U'\right)^* . \tag{3.3.1}$$

Then it suffices to prove the following two assertions.

**Theorem 3.3.1.** *One can construct a Fredholm operator $J$ such that there exist modified wave operators*

$$W'^{,\pm}_{J,\ell}(\Gamma) := \operatorname*{s-lim}_{t\to\pm\infty} e^{itH'_\ell} J e^{-itH'_0} E_{H'_0}(\Gamma) \tag{3.3.2}$$

*exist and* $\operatorname{Ran} W'^{,\pm}_{J,\ell}(\Gamma) = E_{H'_\ell}(\Gamma)\mathcal{H}_{ac}(H'_\ell)$*.*

**Theorem 3.3.2.** *There exist the wave operators*

$$W'^{,\pm}_{s}(\Gamma) := \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} e^{-itH'_\ell} E^{ac}_{H'_\ell}(\Gamma), \tag{3.3.3}$$

*where $E^{ac}_{H'_\ell}(\Gamma)$ denotes the spectral projection of $H'_\ell$ onto the absolutely continuous subspace in $\Gamma$, and* $\operatorname{Ran} W'^{,\pm}_{s}(\Gamma) = E_H(\Gamma)\mathcal{H}_{ac}(H)$*.*

*Proof of Theorem 3.1.3.* It remains to prove $W^{\pm}_J(\Gamma) = W'^{,\pm}_s(\Gamma) W'^{,\pm}_{J,\ell}(\Gamma)$. For $u \in \mathcal{H}$, it follows from Lemma 3.2.1 that

$$\begin{aligned} e^{itH} J e^{-itH_0} E_{H_0}(\Gamma) u =& e^{itH} J e^{-itH'_0} E_{H'_0}(\Gamma) u \\ =& e^{itH} e^{-itH'_\ell} \cdot e^{itH'_\ell} J e^{-itH'_0} E_{H'_0}(\Gamma) u. \end{aligned}$$

Note that by Theorem 3.3.1 there exist $T_\pm > 0$ such that for $\pm t > T_\pm$, $e^{itH'_\ell} J e^{-itH'_0} E_{H'_0}(\Gamma) u = W'^{,\pm}_{J,\ell}(\Gamma) u + r_\pm(t)$ and $\|r_\pm(t)\|_{\mathcal{H}} \to 0$ as $t \to \pm\infty$. Thus we have for $\pm t > T_\pm$

$$\begin{aligned} &\|e^{itH} J e^{-itH_0} E_{H_0}(\Gamma) u - W'^{,\pm}_s(\Gamma) W'^{,\pm}_{J,\ell}(\Gamma) u\|_{\mathcal{H}} \\ \leq& \left\| \left(e^{itH} e^{-itH'_\ell} - W'^{,\pm}_s(\Gamma)\right) W'^{,\pm}_{J,\ell}(\Gamma) u \right\|_{\mathcal{H}} + \|r_\pm(t))\|_{\mathcal{H}}. \end{aligned} \tag{3.3.4}$$

Since $W'^{,\pm}_{J,\ell}(\Gamma) u \in \operatorname{Ran} W'^{,\pm}_{J,\ell}(\Gamma) = E_{H'_\ell}(\Gamma)\mathcal{H}_{ac}(H'_\ell)$, Theorem 3.3.2 implies that (3.3.4) tends to 0 as $t \to \pm\infty$. □

In the following, we prove Theorems 3.3.1 and 3.3.2.

### 3.3.1 Proof of Theorem 3.3.1

We reduce a long-range scattering problem on $\mathcal{H} = \ell^2(\mathbb{Z}^2; \mathbb{C}^2)$ into that on $\ell^2(\mathbb{Z}^2)$, which is considered in the last chapter.

The existence and completeness of (3.3.2) are equivalent to those of

$$\tilde{W}'^{,\pm}_{\tilde{J},\ell}(\Gamma) := \operatorname*{s-lim}_{t\to\pm\infty} e^{it\tilde{H}'_\ell} \tilde{J} e^{-it\tilde{H}'_0} E_{\tilde{H}'_0}(\Gamma), \tag{3.3.5}$$

where $\tilde{J} = (U')^* JU'$ and

$$\tilde{H}'_\ell := \left(U'\right)^* H'_\ell U' = \tilde{H}'_0 + V_\ell. \tag{3.3.6}$$

Indeed, a direct calculus implies

$$W'^{,\pm}_{J,\ell}(\Gamma) = U' \tilde{W}'^{,\pm}_{\tilde{J},\ell}(\Gamma) \left(U'\right)^*. \tag{3.3.7}$$

Set $\tilde{J} = \begin{pmatrix} \tilde{J}_+ & 0 \\ 0 & \tilde{J}_- \end{pmatrix}$, $\tilde{J}_\pm \in \mathcal{B}(\ell^2(\mathbb{Z}^2))$. Then the scattering problem of operators on $\mathcal{H}$ is reduced to that on $\ell^2(\mathbb{Z}^2)$:

$$\begin{aligned} &\tilde{W}^{\pm}_{\tilde{J},\ell}(\Gamma) \\ =& \operatorname*{s-lim}_{t\to\pm\infty} \begin{pmatrix} e^{it(\lambda_+ + V_\ell)} \tilde{J}_+ e^{-it\lambda_+} E_{\lambda_+}(\Gamma) & 0 \\ 0 & e^{it(\lambda_- + V_\ell)} \tilde{J}_- e^{-it\lambda_-} E_{\lambda_-}(\Gamma) \end{pmatrix}. \end{aligned} \tag{3.3.8}$$

Therefore we obtain the following theorem by Theorem 2.1.5.

**Theorem 3.3.3.** *There exist Fredholm operators $\tilde{J}_\#$, $\# \in \{+,-\}$, of the form*

$$\tilde{J}_\# v[x] = (2\pi)^{-1} \int_{\mathbb{T}^2} e^{i\varphi_\#(x,\xi)} Fv(\xi) d\xi, \quad v \in \ell^2(\mathbb{Z}^2), \tag{3.3.9}$$

*such that the modified wave operators*

$$W^{\pm}_{\ell,\#}(\Gamma) := \operatorname*{s-lim}_{t\to\pm\infty} e^{it(\lambda_\# + V_\ell)} \tilde{J}_\# e^{-it\lambda_\#} E_{\lambda_\#}(\Gamma) \tag{3.3.10}$$

*exist and they are partial isometries from $E_{\lambda_\#}(\Gamma)\mathcal{H}_{ac}(\lambda_\#)$ onto $E_{\lambda_\#}(\Gamma)\mathcal{H}_{ac}(\lambda_\#)$.*

Note that each $\varphi_\#(x,\xi)$ in (3.3.9) is constructed as a smooth function on $\mathbb{R}^2 \times \mathbb{T}^2$ which solves the eikonal equation

$$\lambda_\#(\nabla_x \varphi_\#(x,\xi)) + \tilde{V}_\ell(x) = \lambda_\#(\xi) \tag{3.3.11}$$

on the outgoing and incoming regions, where $\tilde{V}_\ell \in C^\infty(\mathbb{R}^2)$ is an extension of $V_\ell$ as in Assumption 2.1.3. For detailed properties of $J_\pm$ and $\varphi_\pm$, see the last chapter.

Let $J := U' \tilde{J} (U')^*$, $\tilde{J} := \begin{pmatrix} \tilde{J}_+ & 0 \\ 0 & \tilde{J}_- \end{pmatrix}$. Then using Theorem 3.3.3 and (3.3.7), we obtain Theorem 3.3.1. □

### 3.3.2 Proof of Theorem 3.3.2

Theorem 3.3.2 is proved by Proposition 3.3.4 and the Cook-Kuroda method. The proof of the next proposition is given in Appendix 3.4.

**Proposition 3.3.4.** *i) $H$ and $H'_\ell$ have at most finite discrete eigenvalues in $\Gamma$ with counting their multiplicities.*
*ii) Let $s > \frac{1}{2}$ and $\chi \in C_c^\infty(\Gamma\backslash\sigma_{pp}(H))$ (resp. $\chi \in C_c^\infty(\Gamma\backslash\sigma_{pp}(H'_\ell))$). Then $\langle x\rangle^{-s}\chi(H)$ (resp. $\langle x\rangle^{-s}\chi(H'_\ell)$) is $H$(resp. $H'_\ell$)-smooth.*

According to Proposition 3.3.4 i) and a density argument, it suffices to show the existence of wave operators

$$\lim_{t\to\pm\infty} e^{itH}e^{-itH'_\ell}u, \tag{3.3.12}$$

$$\lim_{t\to\pm\infty} e^{itH'_\ell}e^{-itH}v \tag{3.3.13}$$

for $u \in \mathcal{H}_{\mathrm{ac}}(H'_\ell)$ and $v \in \mathcal{H}_{\mathrm{ac}}(H)$ such that

$$\chi(H'_\ell)u = u, \quad \psi(H)v = v \tag{3.3.14}$$

with $\chi \in C_c^\infty(\Gamma\backslash\sigma_{\mathrm{pp}}(H'_\ell))$ and $\psi \in C_c^\infty(\Gamma\backslash\sigma_{\mathrm{pp}}(H))$. We prove the existence of (3.3.12) as $t \to \infty$ only. The other cases are proved similarly.

By (3.3.14), we have

$$\begin{aligned} e^{itH}e^{-itH'_\ell}u =& e^{itH}\chi(H'_\ell)^3e^{-itH'_\ell}u \\ =& e^{itH}\chi(H)\chi(H'_0)\chi(H'_\ell)e^{-itH'_\ell}u \\ &+ e^{itH}\left(\chi(H'_\ell)^2 - \chi(H)\chi(H'_0)\right)\chi(H'_\ell)e^{-itH'_\ell}u. \end{aligned} \tag{3.3.15}$$

Since $H - H_0 = V_\ell$ and $H'_\ell - H'_0 = (U')^*\, V_\ell U'$ are compact operators, the Helffer-Sjöstrand formula implies that $\chi(H) - \chi(H_0) = \chi(H) - \chi(H'_0)$ and $\chi(H'_\ell) - \chi(H'_0)$ are compact. Thus $\chi(H'_\ell)^2 - \chi(H)\chi(H'_0)$ is also a compact operator. Note that $u \in \mathcal{H}_{ac}(H'_\ell)$ implies $e^{-itH'_\ell}u \to 0$ weakly as $t \to \infty$. Thus the last term of (3.3.15) converges to 0 as $t \to \infty$, and it suffices to prove the existence of the limit

$$\lim_{t\to\infty} e^{itH}\chi(H)\chi(H'_0)\chi(H'_\ell)e^{-itH'_\ell}u.$$

Now we use the Cook-Kuroda method. First note that

$$\begin{aligned} &e^{itH}\chi(H)\chi(H'_0)\chi(H'_\ell)e^{-itH'_\ell}u - e^{it'H}\chi(H)\chi(H'_0)\chi(H'_\ell)e^{-it'H'_\ell}u \\ &= \int_{t'}^{t} \frac{d}{ds}(e^{isH}\chi(H)\chi(H'_0)\chi(H'_\ell)e^{-isH'_\ell}u)ds. \end{aligned}$$

A direct calculus implies

$$\begin{aligned}
&\frac{d}{dt}\left(e^{itH}\chi(H)\chi(H_0')\chi(H_\ell')e^{-itH_\ell'}u\right)\\
&= ie^{itH}\chi(H)\left(H\chi(H_0') - \chi(H_0')H_\ell'\right)\chi(H_\ell')e^{-itH_\ell'}u\\
&= ie^{itH}\chi(H)\left(V_s\chi(H_0') + V_\ell\chi(H_0') - \chi(H_0')\left(U'\right)^* V_\ell U'\right)\chi(H_\ell')e^{-itH_\ell'}u\\
&= ie^{itH}\chi(H)\left(V_s\chi(H_0') + [V_\ell, \chi(H_0')\left(U'\right)^*]U'\right)\chi(H_\ell')e^{-itH_\ell'}u\\
&= ie^{itH}(A_1^*B_1 + A_2^*B_2)e^{-itH_\ell'}u,
\end{aligned}$$

where $\gamma := \frac{1+\rho}{2}$ and

$$\begin{aligned}
A_1 &:= \langle x\rangle^{\gamma}V_s\chi(H), \quad B_1 := \langle x\rangle^{-\gamma}\chi(H_0')\chi(H_\ell'),\\
A_2 &:= \langle x\rangle^{-\gamma}\chi(H), \quad B_2 := \langle x\rangle^{\gamma}[V_\ell, \chi(H_0')\left(U'\right)^*]U'\chi(H_\ell').
\end{aligned}$$

Then by a standard argument of short-range scattering theory (see, e.g., [15]), it suffices to prove that each $A_j(B_j)$ is $H(H_\ell')$-smooth, respectively. The $H$-smoothness of $A_1$ and $A_2$ is a direct consequence of Proposition 3.3.4. For the $H_\ell'$-smoothness of $B_1$ and $B_2$, note that

$$\begin{aligned}
B_1 &= \langle x\rangle^{-\gamma}\chi(H_0')\langle x\rangle^{\gamma}\cdot\langle x\rangle^{-\gamma}\chi(H_\ell'),\\
B_2 &= \langle x\rangle^{\gamma}[V_\ell, \chi(H_0')\left(U'\right)^*]U'\langle x\rangle^{\gamma}\cdot\langle x\rangle^{-\gamma}\chi(H_\ell').
\end{aligned}$$

Then it follows from Lemma 3.2.2 and Assumption 3.1.1 that $\langle x\rangle^{-\gamma}\chi(H_0')\langle x\rangle^{\gamma}$ and $\langle x\rangle^{\gamma}[V_\ell, \chi(H_0')(U')^*]U'\langle x\rangle^{\gamma}$ are bounded. Combining this and Proposition 3.3.4, we obtain the $H_\ell'$-smoothness of $B_1$ and $B_2$. $\square$

## 3.4 Appendix: Mourre theory for $H$ and $H_\ell'$, and the proof of Proposition 3.3.4

In this appendix, we review the Mourre theory, the limiting absorption principle and Kato's smooth perturbation theory. Let $\Gamma \Subset \sigma(H_0)\backslash\mathcal{T}$ be an open interval as in Theorem 3.1.3. For a selfadjoint operator $A$ and $n \in \mathbb{N}$, let

$$C^n(A) = \{S \in \mathcal{B}(\mathcal{H}) \mid \mathbb{R} \to \mathcal{B}(\mathcal{H}), t \mapsto e^{-itA}Se^{itA} \text{ is strongly of class } C^n\},$$

and $C^\infty(A) := \cap_{n\in\mathbb{N}}C^n(A)$. We denote by $\mathcal{C}^{1,1}(A)$ the set of the operators satisfying

$$\int_0^1 \|e^{-itA}Se^{itA} + e^{itA}Se^{-itA} - 2S\|\frac{dt}{t^2} < \infty. \tag{3.4.1}$$

Note that $C^2(A) \subset \mathcal{C}^{1,1}(A) \subset C^1(A)$. We denote by $B$ the Besov space $(\mathcal{D}(A), \mathcal{H})_{\frac{1}{2},1}$ obtained by real interpolation. We also denote by $B^*$ its dual. The definition of real interpolation is found in [1, Section 2.3].

We recall the characterization of Kato smoothness; for a selfadjoint operator $H$ and an $H$-bounded operator $G$, we say that $G$ is $H$-smooth if

$$C_1 := \frac{1}{2\pi} \sup_{u \in D(H), \|u\|=1} \int_{\mathbb{R}} \left\| G e^{-itH} u \right\| dt < \infty. \tag{3.4.2}$$

It is known that there are other characterizations of $H$-smoothness and one of them is

$$C_2 := \sup_{\lambda \in \mathbb{R}, \varepsilon > 0} \|G \delta(\lambda, \varepsilon) G^*\| < \infty, \tag{3.4.3}$$

moreover $C_1 = C_2$, where $\delta(\lambda, \varepsilon) := \frac{1}{2\pi i} \left( (H - \lambda - i\varepsilon)^{-1} - (H - \lambda + i\varepsilon)^{-1} \right)$. For other characterizations, see [9].

In order to prove Proposition 3.3.4, we apply the two operators $H$ and $H'_\ell$ to Theorem 3.4.1 described below with $I \Subset \Gamma$ and a suitable conjugate operator $A$. The following theorem is a standard result of the Mourre theory and is due to [1, Proposition 7.1.3, Corollary 7.2.11, Theorem 7.3.1].

**Theorem 3.4.1.** *Let $S \in \mathcal{C}^{1,1}(A)$ and $I \subset \mathbb{R}$ be an open interval. Suppose that there exist a constant $c > 0$ and a compact operator $K$ on $\mathcal{H}$ such that*

$$E_S(I)[S, iA]E_S(I) \geq cE_S(I) + K. \tag{3.4.4}$$

*Then*
*i) $S$ has at most a finite number of eigenvalues in $I$ and each eigenvalues in $I$ has finite multiplicity.*
*ii) For any $\lambda \in I \backslash \sigma_{pp}(S)$, there exist the weak-* limits in $\mathcal{B}(B, B^*)$*

$$\text{w*-}\lim_{\varepsilon \to +0} (S - \lambda \mp i\varepsilon)^{-1}, \tag{3.4.5}$$

*and the convergence is locally uniform in $I \backslash \sigma_{pp}(S)$. In particular, for any $I' \Subset I \backslash \sigma_{pp}(S)$, $S$ is purely absolutely continuous in $I'$ and*

$$\sup_{\lambda \in I', \varepsilon > 0} \|(S - \lambda \mp i\varepsilon)^{-1}\|_{\mathcal{B}(B, B^*)} < \infty. \tag{3.4.6}$$

We define the conjugate operator $A$ by

$$A := U' \circ \tilde{A} \circ (U')^* \tag{3.4.7}$$

$$\tilde{A} := \begin{pmatrix} \tilde{A}_+ & 0 \\ 0 & \tilde{A}_- \end{pmatrix}, \tag{3.4.8}$$

$$\tilde{A}_\pm := \frac{1}{2}\sum_{j=1}^{2} \left( F^*(\partial_{\xi_j}\lambda_\pm)F \cdot x_j + x_j \cdot F^*(\partial_{\xi_j}\lambda_\pm)F \right), \tag{3.4.9}$$

where $U'$ and $\lambda_\pm(\xi) \in C^\infty(\mathbb{T}^2)$ are given by (3.2.2), (3.2.3), (3.2.5), (3.2.6). Then Nelson's commutator theorem with the positive selfadjoint operator $\langle x \rangle$ implies that $A$ is essentially selfadjoint on the Schwarz space on $\mathbb{Z}^2$ defined by $\mathcal{S}(\mathbb{Z}^2) = \{u : \mathbb{Z}^2 \to \mathbb{C}^2 \mid \sup_{x\in\mathbb{Z}^2} \langle x \rangle^N |u[x]| < \infty \text{ for any } N \in \mathbb{N}\}$.

First we verify a relation between $A$ and the unperturbed operators $H_0$ and $H_0'$.

**Lemma 3.4.2.** *Both $H_0$ and $H_0'$ belong to $C^\infty(A)$. Moreover, let*

$$c := \min\left\{ \inf_{\xi\in\lambda_+^{-1}(\Gamma)} |\nabla_\xi \lambda_+(\xi)|^2, \inf_{\xi\in\lambda_-^{-1}(\Gamma)} |\nabla_\xi \lambda_-(\xi)|^2 \right\}.$$

*Then, $c > 0$ and*

$$E_{H_0}(\Gamma)[H_0, iA]E_{H_0}(\Gamma) \geq cE_{H_0}(\Gamma), \tag{3.4.10}$$

$$E_{H_0'}(\Gamma)[H_0', iA]E_{H_0'}(\Gamma) \geq cE_{H_0'}(\Gamma). \tag{3.4.11}$$

*Proof.* Note that the LHS (resp. RHS) of (3.4.10) equals to the LHS (resp. RHS) of (3.4.11) by the construction of $H_0'$.

Since $\mathcal{F}^*H_0\mathcal{F}$ and $\mathcal{F}^*H_0'\mathcal{F}$ are multipliers with smooth symbols on $\mathbb{T}^2$ and $\mathcal{F}^*A\mathcal{F}$ is a differential operator of degree 1 on $\mathbb{T}^2$, $\mathcal{F}^*[H_0, iA]\mathcal{F}$ and $\mathcal{F}^*[H_0', iA]\mathcal{F}$ are also multipliers with smooth symbols. Inductively we see that $H_0, H_0' \in C^\infty(A)$.

For the proof of (3.4.11), a direct calculus implies

$$\begin{aligned} (U')^*[H_0', iA]U &= [\tilde{H}_0', i\tilde{A}] \\ &= \begin{pmatrix} |\nabla_\xi \lambda_+(D_x)|^2 & 0 \\ 0 & |\nabla_\xi \lambda_-(D_x)|^2 \end{pmatrix}, \\ (U')^*E_{H_0'}(\Gamma)U' &= E_{\tilde{H}_0'}(\Gamma) \\ &= \begin{pmatrix} \chi_{\lambda_+^{-1}(\Gamma)}(D_x) & 0 \\ 0 & \chi_{\lambda_-^{-1}(\Gamma)}(D_x) \end{pmatrix}, \end{aligned}$$

where $\chi_{\lambda_\pm^{-1}(\Gamma)}$ denote the characteristic function of $\lambda_\pm^{-1}(\Gamma)$. Therefore we obtain

$$\begin{aligned}
&E_{H_0'}(\Gamma)[H_0', iA]E_{H_0'}(\Gamma) \\
=&U'E_{\tilde{H}_0'}(\Gamma)[\tilde{H}_0', i\tilde{A}]E_{\tilde{H}_0'}(\Gamma)(U')^* \\
=&U'\begin{pmatrix} |\nabla_\xi\lambda_+(D_x)|^2\chi_{\lambda_+^{-1}(\Gamma)}(D_x) & 0 \\ 0 & |\nabla_\xi\lambda_-(D_x)|^2\chi_{\lambda_-^{-1}(\Gamma)}(D_x) \end{pmatrix}(U')^* \\
\geq&U'cE_{\tilde{H}_0'}(\Gamma)(U')^* \\
=&cE_{H_0'}(\Gamma).
\end{aligned}$$

□

We consider commutators of the perturbations $V_s$, $V_\ell$ and $U'V_\ell\,(U')^*$, and the conjugate operator $A$. The next lemma claims that the commutators are small in the sense of the Mourre theory, i.e., compact.

**Lemma 3.4.3.** *Let $V_s$ and $V_\ell$ satisfy the condition in Assumption 3.1.1 with $\rho > 0$. Then, for $W = V_s$, $V_\ell$ and $U'V_\ell\,(U')^*$,*

$$\langle x\rangle^\rho[W, iA] \in \mathcal{B}(\mathcal{H}). \tag{3.4.12}$$

*Proof.* First note that

$$(U')^*\,[U'V_\ell\,(U')^*, iA]U' = [V_\ell, i\tilde{A}] = \begin{pmatrix} [V_\ell, i\tilde{A}_+] & 0 \\ 0 & [V_\ell, i\tilde{A}_-] \end{pmatrix}. \tag{3.4.13}$$

Since $\tilde{A}_\pm = \mathrm{Op}(\tilde{a}_\pm)$ with some functions $\tilde{a}_\pm$ on $\mathbb{T}^2\times\mathbb{Z}^2$ satisfying the condition of Lemma 3.2.2 with $m_1 = 1$, it follows that $\langle x\rangle^{1+\rho}[V_\ell, i\tilde{A}_\pm]$ are bounded on $\ell^2(\mathbb{Z}^2)$. Since

$$[U'V_\ell\,(U')^*, iA] = U'[V_\ell, i\tilde{A}]\,(U')^*,$$

using Lemma 3.2.2 again shows (3.4.12) for $W = U'V_\ell\,(U')^*$. In order to show (3.4.12) for $W = V_\ell$ or $V_s$, note that $A$ has the representation

$$A = \begin{pmatrix} \mathrm{Op}(a_{11}) & \mathrm{Op}(a_{12}) \\ \mathrm{Op}(a_{21}) & \mathrm{Op}(a_{22}) \end{pmatrix},$$

where each $a_{ij}$ satisfies the condition of Lemma 3.2.2 with $m_1 = 1$. Then (3.4.12) for $W = V_\ell$ is a direct result of Lemma 3.2.2. The last case is also proved since $\langle x\rangle^\rho V_sA$ and $\langle x\rangle^\rho AV_s$ are bounded operators by Lemma 3.2.2.
□

Using the above lemma, we see that the perturbations are of the class of $\mathcal{C}^{1,1}(A)$.

**Lemma 3.4.4.** *Let $V_s$ and $V_\ell$ satisfy the condition in Assumption 3.1.1 with $\rho > 0$. Then $V_s$, $V_\ell$ and $U'V_\ell(U')^*$ belong to $\mathcal{C}^{1,1}(A)$.*

*Proof.* The proof is motivated by [14, Lemma 6.2]. First we remark that the operator $\Lambda u[x] := \langle x\rangle u[x]$ satisfies the condition of [5, Theorem 6.1]; the first condition is attained by the unitarity of $e^{-it\Lambda}$, $t \in \mathbb{R}$, on $\mathcal{H}$, and the second one that $A^N\Lambda^{-N}$ is a bounded operator on $\mathcal{H}$ for some integer $N \geq 1$, follows from Lemma 3.2.2. Thus it suffices to show

$$\int_1^\infty \frac{d\lambda}{\lambda}\left\|\theta\left(\frac{\Lambda}{\lambda}\right)[W, iA]\right\|_{\mathcal{B}(\mathcal{H})} < \infty \tag{3.4.14}$$

for $W = V_s$, $V_\ell$ and $U'V_\ell(U')^*$ and some $\theta \in C_c^\infty((0,\infty))$ not identically zero. However this follows from Lemma 3.4.3 and

$$\begin{aligned}\left\|\theta\left(\frac{\Lambda}{\lambda}\right)[W, iA]\right\|_{\mathcal{B}(\mathcal{H})} &\leq \left\|\theta\left(\frac{\Lambda}{\lambda}\right)\Lambda^{-\rho}\right\|_{\mathcal{B}(\mathcal{H})}\|\Lambda^\rho[W, iA]\|_{\mathcal{B}(\mathcal{H})}\\ &\leq C\langle\lambda\rangle^{-\rho}\|\Lambda^\rho[W, iA]\|_{\mathcal{B}(\mathcal{H})}.\end{aligned}$$

□

We have confirmed that Theorem 3.4.1 is applicable to $S = H$ or $H'_\ell$ and $A$ defined by (3.4.7), (3.4.8) and (3.4.9). Therefore we obtain the limiting absorption principle for $H'_\ell$ and $H$.

**Theorem 3.4.5.** *i) $H$ and $H'_\ell$ have finitely many eigenvalues with counting multiplicity in $\Gamma$.*
*ii) For any $I \Subset \Gamma\backslash\sigma_{pp}(H)$, $I' \Subset \Gamma\backslash\sigma_{pp}(H'_\ell)$ and $s > \frac{1}{2}$,*

$$\sup_{\lambda\in I,\ \varepsilon>0}\left\|\langle x\rangle^{-s}(H - \lambda \mp i\varepsilon)^{-1}\langle x\rangle^{-s}\right\|_{\mathcal{B}(\mathcal{H})} < \infty,$$
$$\sup_{\lambda'\in I',\ \varepsilon>0}\left\|\langle x\rangle^{-s}(H'_\ell - \lambda' \mp i\varepsilon)^{-1}\langle x\rangle^{-s}\right\|_{\mathcal{B}(\mathcal{H})} < \infty.$$

*Proof.* It remains to prove that $\mathcal{H}_s := \langle x\rangle^{-s}\mathcal{H} \subset B$ if $s > \frac{1}{2}$. However it is shown if we remark that $\mathcal{H}_1 \subset \mathcal{D}(A)$ and hence $\mathcal{H}_s \subset (\mathcal{H}_1, \mathcal{H})_{\frac{1}{2},1} \subset (\mathcal{D}(A), \mathcal{H})_{\frac{1}{2},1} = B$. □

*Proof of Proposition 3.3.4.* It suffices to show (3.4.3) for $G = \langle x\rangle^{-s}\chi(H)$ and $\langle x\rangle^{-s}\chi(H'_\ell)$. However this is proved by Theorem 3.4.5 and the condition of $\operatorname{supp}\chi$. □

*Remark* 3.4.6. Theorem 3.4.5 may look like a direct consequence of [14]. However the above assertion is more concrete in that the set $\mathcal{T} = \{0, \pm 1, \pm 3\}$ of threshold energies is explicitly determined.

*Remark* 3.4.7. For any $\lambda \in \Gamma \backslash \sigma_{\mathrm{pp}}(H)$, $\lambda' \in \Gamma \backslash \sigma_{\mathrm{pp}}(\hat{H}_\ell)$ and $s > \frac{1}{2}$, there exist the norm limits

$$\lim_{\varepsilon \downarrow 0} \langle x \rangle^{-s} (H - \lambda \mp i\varepsilon)^{-1} \langle x \rangle^{-s},$$
$$\lim_{\varepsilon \downarrow 0} \langle x \rangle^{-s} (\hat{H}_\ell - \lambda' \mp i\varepsilon)^{-1} \langle x \rangle^{-s}.$$

For the proof, see e.g. [3] and [13].

## 3.5 Appendix: Proof of Lemma 3.2.2

First we observe that

$$\mathrm{Op}(a)u[x] = (2\pi)^{-d} \sum_{y \in \mathbb{Z}^d} A[x, y]u[y], \quad u \in \mathcal{S}(\mathbb{Z}^d),$$

where

$$A[x, y] := \int_{\mathbb{T}^d} e^{i(x-y)\cdot\xi} a(\xi, y) d\xi.$$

A direct calculus implies

$$(\langle \cdot \rangle^p [\mathrm{Op}(b), \mathrm{Op}(a)] \langle \cdot \rangle^q) u[x] = (2\pi)^{-d} \sum_{y \in \mathbb{Z}^d} K[x, y]u[y],$$

where

$$K[x, y] := \langle x \rangle^p \langle y \rangle^q (W[x] - W[y]) A[x, y].$$

According to Young's inequality, the boundedness of the operator follows from the inequalities

$$\sup_{y \in \mathbb{Z}^d} \sum_{x \in \mathbb{Z}^d} K[x, y] < \infty, \tag{3.5.1}$$
$$\sup_{x \in \mathbb{Z}^d} \sum_{y \in \mathbb{Z}^d} K[x, y] < \infty. \tag{3.5.2}$$

Let $z := x - y$, $k := \sum_{j=1}^{d} |z_j|$, and $z^0 = 0, z^1, \dots, z^k = z$ be a path from 0 to $z$ in $\mathbb{Z}^d$ such that $|z^i - z^{i-1}| = 1$ for $i = 1, 2, \dots, k$. Then we learn

$$
\begin{aligned}
|W[x] - W[y]| &\le \sum_{i=1}^{k} |W[z^i + y] - W[z^{i-1} + y]| \\
&\le C \sum_{i=1}^{k} \langle z^i + y \rangle^{-m_2} \\
&= C \sum_{i=1}^{k} \langle z^i + y \rangle^{-p} \langle z^i + y \rangle^{-q+m_1} \\
&\le C' \sum_{i=1}^{k} \langle x - y - z^i \rangle^{|p|} \langle x \rangle^{-p} \langle z^i \rangle^{|q-m_1|} \langle y \rangle^{-q+m_1} \\
&\le C'' \langle x - y \rangle^{M} \langle x \rangle^{-p} \langle y \rangle^{-q+m_1},
\end{aligned}
$$

where $M := |p| + |q - m_2|$. Note that the second last inequality follows from

$$
\begin{aligned}
\langle x + y \rangle &\le C_d \langle x \rangle \langle y \rangle, \\
\langle x + y \rangle^{-1} &\le C_d \langle x \rangle \langle y \rangle^{-1}
\end{aligned}
$$

for $x, y \in \mathbb{R}^d$. In order to estimate $A[x, y]$, we observe for $\alpha \in \mathbb{Z}_+^d$

$$
|(x - y)^{\alpha} A[x, y]| = \left| i^{|\alpha|} \int_{\mathbb{T}^d} e^{i(x-y)\cdot\xi} \partial_{\xi}^{\alpha} a(\xi, y) d\xi \right| \le C_{\alpha} \langle y \rangle^{-m_1}.
$$

Thus we have

$$
|K[x, y]| \le C'' \langle x - y \rangle^{M} \langle y \rangle^{m_1} |A[x, y]| \le C_{M,d} \langle x - y \rangle^{-d-1}.
$$

Hence we obtain (3.5.1) and (3.5.2). $\square$

# Bibliography


[1] W. Amrein, A. Boutet de Monvel, V. Georgescu: $C_0$-groups, commutator methods and spectral theory of $N$-body Hamiltonians. Progress in Mathematics, 135. Birkhäuser Verlag, Basel, 1996.

[2] K. Ando: Inverse scattering theory for discrete Schrödinger operators on the hexagonal lattice. Ann. Henri Poincaré **14** (2013), no. 2, 347–383.

[3] K. Ando, H. Isozaki, H. Morioka: Spectral properties of Schrödinger operators on perturbed lattices. Ann. Henri Poincaré **17** (2016), no. 8, 2103–2171.

[4] K. Ando, H. Isozaki, H. Morioka: Inverse Scattering for Schrödinger Operators on Perturbed Lattices. Ann. Henri Poincaré **19** (2018), 3397–3455.

[5] A. Boutet de Monvel, J. Sahbani: On the spectral properties of discrete Schrödinger operators: (The multi-dimensional case). Rev. Math. Phys. **11** (1999), 1061-1078.

[6] J. Dereziński, C. Gérard: Scattering Theory of Classical and Quantum $N$-Particle Systems. Springer Verlag, 1997.

[7] H. Isozaki, H. Kitada: Modified wave operators with time-independent modifiers. J. Fac. Sci. Uni. Tokyo Sect. IA Math. **32** (1985), no. 1, 77-104.

[8] H. Isozaki, I. Korotyaev: Inverse Problems, Trace Formulae for Discrete Schorödinger Operators. Ann. Henri Poincaré **13** (2012), 751-788.

[9] T. Kato: Wave operators and similarity for some non-selfadjoint operators. Math. Ann. **162** (1965/1966), 258–279. 47.48

[10] H. Kitada: Scattering theory for Schrödinger equations with time-dependent potentials of long-range type. J. Fac. Sci. Univ. Tokyo Sect. IA Math. **29** (1982), 353-369.

[11] W. Liu: Criteria for embedded eigenvalues for discrete Schrödinger operators. Preprint, arXiv:1805.02817, 2018.

[12] S. Nakamura: Modified wave operators for discrete Schrödinger operators with long-range perturbations. J. Math. Phys. **55** (2014), 112101 (8 pages).

[13] S. Nakamura: Microlocal properties of scattering matrices. Comm. Partial Differential Equations **41** (2016), no. 6, 894–912.

[14] D. Parra, S. Richard: Spectral and scattering theory for Schrödinger operators on perturbed topological crystals. Rev. Math. Phys. **30** (2018), 1850009-1 – 1850009-39.

[15] M. Reed, B. Simon: The Methods of Modern Mathematical Physics, Volume III, Scattering Theory, Academic Press, 1979.

[16] M. Ruzhansky, V. Turunen: Pseudo-Differential Operators and Symmetries: Background Analysis and Advanced Topics, Pseudo-Differential Operators, Theory and Applications **2**, Springer Basel AG, 2009.

[17] Y. Tadano: Long-range scattering for discrete Schrödinger operators. To appear in Ann. Henri Poincaré (preprint, arXiv:1605.02466).

[18] D. R. Yafaev: Mathematical scattering theory. Analytic theory. Mathematical Surveys and Monographs, 158. American Mathematical Society, Providence, RI, 2010.

# Chapter 4

# On a continuum limit of discrete Schrödinger operators on square lattice

## 4.1 Introduction

Let $d \geq 1$, $V(x)$ be a real-valued function on $\mathbb{R}^d$ and $H$ be the Schrödinger operator perturbed with $V$:

$$H = H_0 + V = -\Delta + V(x) \tag{4.1.1}$$

on $\mathcal{H} = L^2(\mathbb{R}^d)$.

We consider the discretized operators $H_{0,h}$, $V_h$ and $H_h$ on the $d$-dimensional square lattice $h\mathbb{Z}^d$ with width $h > 0$. In particular, we call $H_h$ the discrete Schrödinger operators. The above operators are defined on $\mathcal{H}_h = \ell^2(h\mathbb{Z}^d)$ with norm $\|v\|_{\mathcal{H}_h} = h^{\frac{d}{2}} \left(\sum_{z \in h\mathbb{Z}^d} |v(z)|^2\right)^{\frac{1}{2}}$:

$$H_{0,h}v(z) = h^{-2} \sum_{j=1}^{d} \left(2v(z) - v(z + he_j) - v(z - he_j)\right), \tag{4.1.2}$$

$$V_h v(z) = V(z)v(z), \tag{4.1.3}$$

$$H_h = H_{0,h} + V_h \tag{4.1.4}$$

for $z \in h\mathbb{Z}^d$, where $\{e_j\}_{j=1}^d \subset \mathbb{Z}^d$ denotes the canonical basis of $\mathbb{R}^d$. Note that $H_{0,h}$ denotes the negative of the difference Laplacian on $h\mathbb{Z}^d$ and is obtained by a formal calculus of the Taylor expansion

$$v(x \pm he_j) = v(x) \pm h\partial_{x_j} v(x) + \frac{h^2}{2}\partial_{x_j}^2 v(x) + O(h^3).$$

There are studies concerning continuum limits of NLS equations, in many cases, in the view point of numerical analysis. For the case where the space is discretized and the time is not, see Bambusi and Penati [2], Hong and Yang [4] and references therein. For linear discrete Schrödinger operators, Rabinovich [8] has studied the relation between the essential and discrete spectra of the discrete and continuum Schrödinger operators, provided $V$ is bounded and uniformly continuous.

The goal of this chapter is to give a meaning of $H_h \to H$ as the width $h$ of the lattice tends to zero in the spectral theoretical point of view. More precisely, we establish a continuum limit of discrete Schrödinger operators $H_h$ defined on $\mathcal{H}_h$ with respect of the operator norm topology, and as a corollary, we observe the asymptotics of the spectrum $\sigma(H_h)$.

In order to make a relationship between $\mathcal{H}$ and $\mathcal{H}_h$, we need some notations. We set $\varphi \in L^2(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ such that

$$\sup_{x\in[0,1]^d} \sum_{n\in\mathbb{Z}^d} |\varphi(x-n)| < \infty, \tag{4.1.5}$$

and we set

$$\varphi_{h,z}(x) := \varphi(h^{-1}(x-z)), \quad h>0,\ z\in h\mathbb{Z}^d. \tag{4.1.6}$$

Let $P_h = P_{h,\varphi} : \mathcal{H} \to \mathcal{H}_h$ be defined by

$$P_h u(z) := h^{-d}\int_{\mathbb{R}^d} \overline{\varphi_{h,z}(x)} u(x)dx, \quad h>0,\ z\in h\mathbb{Z}^d. \tag{4.1.7}$$

Then it follows that $P_h$ is bounded by Young's inequality and its adjoint is

$$P_h^* v(x) = \sum_{z\in h\mathbb{Z}^d} \varphi_{h,z}(x)v(z), \quad h>0,\ v\in\mathcal{H}_h. \tag{4.1.8}$$

We prepare a lemma for $P_h$.

**Lemma 4.1.1.** *Let $\varphi \in L^2(\mathbb{R}^d)\cap L^1(\mathbb{R}^d)$ satisfy (4.1.5). Then, the following are equivalent.*

*(1) $P_h^*$ is isometric.*

*(2)* $\operatorname{Ran} P_h = \mathcal{H}_h$.

*(3)* $\int_{\mathbb{R}^d} \varphi(x)\overline{\varphi(x-n)}dx = \delta_{n,0}$ *for* $n \in \mathbb{Z}^d$.

*(4)* $\sum_{n\in\mathbb{Z}^d} |\hat{\varphi}(\xi + 2\pi n)|^2 = 1$ *for* $\xi \in \mathbb{R}^d$, *where* $\hat{\varphi}(\xi) := \int_{\mathbb{R}^d} e^{-ix\cdot\xi}\varphi(x)dx$.

*Proof.* (1) and (2) are equivalent by the standard properties of adjoint operators. Since (2) implies the orthonormality of the basis $\{h^{-\frac{d}{2}}\varphi_{h,z}\}_{z\in h\mathbb{Z}^d}$, we learn

$$\int_{\mathbb{R}^d} \varphi(x)\overline{\varphi(x-n)}dx = h^d \int_{\mathbb{R}^d} \varphi_{h,0}(x)\overline{\varphi_{h,hn}(x)}dx = \delta_{0,n},$$

which implies (3). For the equivalence of (3) and (4), we learn by Parseval's identity

$$\begin{aligned}
\int_{\mathbb{R}^d} \varphi(x)\overline{\varphi(x-n)}dx =&(2\pi)^{-d} \int_{\mathbb{R}^d} \hat{\varphi}(\xi)\overline{e^{-in\cdot\xi}\hat{\varphi}(\xi)}d\xi \\
=&(2\pi)^{-d} \int_{\mathbb{R}^d} e^{in\cdot\xi}|\hat{\varphi}(\xi)|^2 d\xi \\
=&(2\pi)^{-d} \int_{\mathbb{T}^d} \sum_{m\in\mathbb{Z}^d} e^{in\cdot(\xi+2\pi m)}|\hat{\varphi}(\xi+2\pi m)|^2 d\xi \\
=&(2\pi)^{-d} \int_{\mathbb{T}^d} e^{in\cdot\xi} \sum_{m\in\mathbb{Z}^d} |\hat{\varphi}(\xi+2\pi m)|^2 d\xi,
\end{aligned}$$

where $\mathbb{T}^d := [-\pi,\pi)^d$. Since $\{(2\pi)^{-\frac{d}{2}}e^{in\cdot\xi}\}_{n\in\mathbb{Z}^d}$ is a complete orthonormal basis of $L^2(\mathbb{T}^d)$, we conclude that (3) is equivalent to (4). $\square$

The next theorem is our main result concerning the asymptotic behavior of $P_h^*(H_h-\mu)^{-1}P_h$ as $h \to 0$, where $\mu \in \mathbb{C}\backslash\mathbb{R}$.

**Theorem 4.1.2.** *Suppose that* $\varphi$ *satisfies one of the conditions in Lemma 4.1.1, and* $\hat{\varphi} \in C_c^\infty\left((-2\pi,2\pi)^d\right)$. *Assume that* $V$ *is a bounded function from below such that the following hold: Let* $M := \inf_{x\in\mathbb{R}^d} V(x) - 1$. *Then* $(V(x)-M)^{-1}$ *is uniformly continuous and for sufficiently small* $\varepsilon > 0$ *and* $C_1, C_2 > 0$,

$$C_1(V(x)-M) \le V(y) - M \le C_2(V(x)-M) \quad \text{if} \quad |x-y| < \varepsilon. \tag{4.1.9}$$

*Then, for any* $\mu \in \mathbb{C}\backslash\mathbb{R}$,

$$\|P_h^*(H_h-\mu)^{-1}P_h - (H-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H})} \to 0, \ h \to 0. \tag{4.1.10}$$

*Furthermore,*

$$\|P_h^*(H_{h,0}-\mu)^{-1}P_h-(H_0-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H})}\le C_\mu h^2, \tag{4.1.11}$$
$$\|P_h^*(H_h-\mu)^{-1}P_h-(H-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H})}\le C_\mu h^\beta \tag{4.1.12}$$

*for* $0<\beta<\alpha\le 1$, *provided in addition that* $(V(x)-M)^{-1}\in C^{0,\alpha}(\mathbb{R}^d)$.

*Remark* 4.1.3. It does not holds that $P_h^*H_hP_h\to H$ as $h\to 0$ in the norm resolvent sense, i.e.

$$\|(P_h^*H_hP_h-\mu)^{-1}-(H-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H})}\to 0,\ h\to 0.$$

In fact, the above statement is equivalent to the following assertion: For any $\chi\in C(\mathbb{R})$ decaying at $\pm\infty$,

$$\chi(P_h^*H_hP_h)\to\chi(H),\ h\to 0 \tag{4.1.13}$$

in the operator norm topology. Since a direct calculus implies $\chi(P_h^*H_hP_h)=P_h^*\chi(H_h)P_h+\chi(0)(1-P_h^*P_h)$, (4.1.13) holds if and only if $\chi(0)=0$.

*Remark* 4.1.4. When we consider the strong resolvent convergence, the condition for $\varphi$ will be relaxed. In particular, for $\varphi$ satisfying the condition of Lemma 4.1.1, $(P_h^*H_{0,h}P_h-\mu)^{-1}$ converges strongly to $(H_0-\mu)^{-1}$ if and only if $|\hat{\varphi}(0)|=1$.

As a corollary of the above theorem, we obtain the asymptotic behavior of the spectrum of $H_h$.

**Corollary 4.1.5.** *Under the assumption of Theorem 4.1.2, the following hold:*

*(1) Let* $a,b\in\mathbb{R}$, $a<b$ *be not in* $\sigma(H)$. *Then* $a,b\notin\sigma(H_h)$ *for sufficiently small* $h$ *and*

$$\|P_h^*E_{H_h}((a,b))P_h-E_H((a,b))\|_{\mathcal{B}(\mathcal{H})}\to 0,\quad h\to 0. \tag{4.1.14}$$

*(2) Let* $d_H(X,Y)=\max\left\{\sup_{x\in X}d(x,Y),\sup_{y\in Y}d(y,X)\right\}$ *denote the Hausdorff distance. Then*

$$d_H\left(\sigma((H_h-M)^{-1}),\sigma((H-M)^{-1})\right)\to 0,\quad h\to 0. \tag{4.1.15}$$

*Proof.* (1) The proof is similar to that of [9, Theorem VIII.23 (b)].

(2) We set $X_h:=\sigma((H_h-M)^{-1})$ and $X:=\sigma((H-M)^{-1})$ for simplicity. Then we have

$$\begin{aligned}d_{\mathrm{H}}\left(X_h,X\right)\le& d_{\mathrm{H}}\left(X_h,X_h\cup\{0\}\right)+d_{\mathrm{H}}\left(X_h\cup\{0\},X\right)\\=&d\left(0,X_h\right)+d_{\mathrm{H}}\left(X_h\cup\{0\},X\right).\end{aligned}$$

Note that $d(0, X_h) \le Ch^2$ if $V$ is bounded and $d(0, X_h) = 0$ otherwise. Since $X_h \cup \{0\} = \sigma(P_h^*(H_h - M)^{-1}P_h)$, it suffices to show for $A, B \in \mathcal{B}(\mathcal{H})$

$$d_{\mathrm{H}}(\sigma(A), \sigma(B)) \le \|A - B\|_{\mathcal{B}(\mathcal{H})}. \tag{4.1.16}$$

Equivalently, it suffices to show that $d(\mu, \sigma(B)) > \|A-B\|$ implies $\mu \in \rho(A)$. However this is easy to prove since $\|(A - B)(B - \mu)^{-1}\| < 1$ and

$$\begin{aligned}
&(A-\mu)^{-1} = (B - \mu + A - B)^{-1} \\
=&(B-\mu)^{-1}(1 + (A-B)(B-\mu)^{-1})^{-1} \\
=&(B-\mu)^{-1}\sum_{n=0}^{\infty}(-1)^n\left((A-B)(B-\mu)^{-1}\right)^n.
\end{aligned}$$

□

*Examples* 4.1.6. (1) The assumption of Theorem 4.1.2 is satisfied if $V$ is a uniformly continuous bounded function.

(2) One of the most interesting examples is $V(x) = C|x|^\alpha$, $C, \alpha > 0$. In particular, the harmonic potential $V(x) = |x|^2$ is suggestive; if $a, b \in \mathbb{R}$, $a < b$, are not in the spectrum $\sigma(H) = \{d, d+2, d+4, \dots\}$, then

$$d_{\mathrm{H}}(\sigma(H_h) \cap (a, b), \sigma(H) \cap (a, b)) \le C_{a,b}h.$$

Moreover, we can see that for any eigenfunction $u$ of $H$ there exists the corresponding eigenfunction $v_h$ of $H_h$ such that $\|P_h^* v_h - u\|_{\mathcal{H}} \le C_u h^{1-\varepsilon}$ for any $\varepsilon > 0$. Note that, for $d = 1$, each eigenfunction $v$ of $H_h$ corresponds to the periodic solution to Mathieu's differential equation

$$-g''(x) + 2h^{-2}(1 - \cos hx)g(x) = \lambda g(x), \quad x \in h^{-1}\mathbb{T}, \tag{4.1.17}$$

and $\lambda \in \sigma(H_h)$ if and only if there exists a periodic solution to (4.1.17).

(3) Theorem 4.1.2 can treat exponentially increasing potentials $V(x) = Ce^{\alpha|x|}$. On the other hand, super-exponentially increasing potentials are not under the assumption.

(4) A constant electric field $V(x) = x_1$ is not treated by Theorem 4.1.2 due to its unboundedness from below.

We describe the outline of this chapter. Sections 4.2 and 4.3 are devoted to the preparation of lemmas and notations for the proof of Theorem 4.1.2 given in Section 4.4. In Section 4.2, we show that $H_0$ (resp. $H_{0,h}$) is $H$-(resp. $H_h$-)bounded and the relative bound of $H_{0,h}$ is uniform in $h > 0$ by their form boundedness and a commutator calculus. In Section 4.3, we introduce the continuum and discrete Fourier transforms $F$, $F_h$ and define $Q_h = F_h P_h F^*$ for the proofs of Lemmas 4.4.1 and 4.4.2.

## 4.2 Relative boundedness

In this section, we prove the relative boundedness of $H$ and $H_h$ with respect to $H_0$ and $H_{0,h}$, respectively. The assertion is the following.

**Proposition 4.2.1.** *Suppose that $V$ is bounded from below and (4.1.9) holds for some $\varepsilon > 0$ and $C_1, C_2 > 0$. Then*

$$\|H_0(H+i)^{-1}\| < \infty, \tag{4.2.1}$$

$$\|V(H+i)^{-1}\| < \infty, \tag{4.2.2}$$

$$\sup_{h\in(0,1)} \|H_{0,h}(H_h+i)^{-1}\| < \infty, \tag{4.2.3}$$

$$\sup_{h\in(0,1)} \|V_h(H_h+i)^{-1}\| < \infty. \tag{4.2.4}$$

Note that (4.2.1) (resp. (4.2.3)) is equivalent to (4.2.2) (resp. (4.2.4)). Since (4.1.9) for some $\varepsilon > 0$ implies (4.1.9) for any $\varepsilon > 0$, we may assume $\varepsilon = 1$. In order to prove Proposition 4.2.1, we first prepare the claim on the form boundedness.

**Lemma 4.2.2.** *If $V$ is bounded from below,*

$$\|(H_0+1)^{\frac{1}{2}}(H-M)^{-\frac{1}{2}}\| < \infty, \tag{4.2.5}$$

$$\|(V-M)^{\frac{1}{2}}(H-M)^{-\frac{1}{2}}\| < \infty, \tag{4.2.6}$$

$$\sup_{h\in(0,1)} \|(H_{0,h}+1)^{\frac{1}{2}}(H_h-M)^{-\frac{1}{2}}\| < \infty, \tag{4.2.7}$$

$$\sup_{h\in(0,1)} \|(V_h-M)^{\frac{1}{2}}(H_h-M)^{-\frac{1}{2}}\| < \infty. \tag{4.2.8}$$

*Proof.* It is proved by the positivity of $V - M$ and $V_h - M$:

$$\begin{aligned}(u, Hu) &\geq \max\left\{(u, H_0 u) + M\|u\|^2, (u, Vu)\right\},\\ (v, H_h v) &\geq \max\left\{(v, H_{0,h} v) + M\|v\|^2, (v, V_h v)\right\}\end{aligned}$$

for $u \in \mathcal{H}$ and $v \in \mathcal{H}_h$. □

We also prepare the mollified potential $\tilde{V}$ with a suitable differential condition.

**Lemma 4.2.3.** *Under the assumption of Proposition 4.2.1, there exists* $\tilde{V} \in C^\infty(\mathbb{R}^d)$ *such that* $\tilde{V}(x) \geq \inf_{x\in\mathbb{R}^d} V(x)$ *and*

$$c(V(x) - M) \leq \tilde{V}(x) - M \leq C(V(x) - M),\ x \in \mathbb{R}^d, \tag{4.2.9}$$

$$c(\tilde{V}(x) - M) \leq \tilde{V}(y) - M \leq C(\tilde{V}(x) - M),\ |x - y| < 1, \tag{4.2.10}$$

$$\frac{|\partial_x^\alpha \tilde{V}(x)|}{\tilde{V}(x) - M} \leq C_\alpha, \quad x \in \mathbb{R}^d, \alpha \in \mathbb{Z}_+^d = \{0, 1, \dots\}^d \tag{4.2.11}$$

*for some* $C, c, C_\alpha > 0$.

*Proof.* We set $\psi \in C_c^\infty(\{|x| < 1\})$ so that $\int_{\mathbb{R}^d} \psi(x)dx = 1$, and let

$$\tilde{V}(x) := V * \psi(x) = \int_{\mathbb{R}^d} V(x - y)\psi(y)dy.$$

Since the assumption of $V$ implies that $C_1(V(x) - M) \leq V(x - y) - M \leq C_2(V(x) - M)$ for $y \in \operatorname{supp}\psi$, we obtain (4.2.9). We can prove (4.2.10) by (4.2.9) and the assumption of $V$. If $\alpha \neq 0$, we have by (4.2.9) and (4.2.10)

$$\begin{aligned}
|\partial_x^\alpha \tilde{V}(x)| =& |\partial_x^\alpha (\tilde{V}(x) - M)| \\
=& \left| \int_{\mathbb{R}^d} (V(x - y) - M)\partial_x^\alpha \psi(y)dy \right| \\
\leq& \int_{\mathbb{R}^d} C_2(V(x) - M)|\partial_x^\alpha \psi(y)|dy \\
\leq& C_\alpha(V(x) - M) \\
\leq& C'_\alpha(\tilde{V}(x) - M).
\end{aligned}$$

□

*Proof of Proposition 4.2.1.* Since (4.2.9) implies $(\tilde{V} - M)(V - M)^{-1} \in \mathcal{B}(\mathcal{H})$ and $\sup_{h>0} \|(\tilde{V}_h - M)(V_h - M)^{-1}\|_{\mathcal{B}(\mathcal{H}_h)} < \infty$, it suffices to prove the (uniform) boundedness of $(\tilde{V} - M)(H - M)^{-1}$ and $(\tilde{V}_h - M)(H_h - M)^{-1}$. In the following, we write $W = \tilde{V} - M$ and $W_h = \tilde{V}_h - M$ for simplicity.

We observe

$$W(H - M)^{-1} = W^{\frac{1}{2}}(H - M)^{-1}W^{\frac{1}{2}} + W^{\frac{1}{2}}[W^{\frac{1}{2}}, (H - M)^{-1}].$$

The first term is bounded by (4.2.6) and (4.2.9). The second term is calculated as

$$
\begin{aligned}
&W^{\frac{1}{2}}[W^{\frac{1}{2}},(H-M)^{-1}] \qquad (4.2.12)\\
=&W^{\frac{1}{2}}(H-M)^{-1}[W^{\frac{1}{2}},H_0](H-M)^{-1}\\
=&W^{\frac{1}{2}}(H-M)^{-1}\sum_{j=1}^{d}\left((\partial_{x_j}W^{\frac{1}{2}})\partial_{x_j}+(\partial_{x_j}^2W^{\frac{1}{2}})\right)(H-M)^{-1}.
\end{aligned}
$$

Since a simple calculation implies

$$
\begin{aligned}
&\partial_{x_j}W^{\frac{1}{2}}(x)=\frac{1}{2}W^{-\frac{1}{2}}(x)\partial_{x_j}W(x),\\
&\partial_{x_j}^2W^{\frac{1}{2}}(x)=-\frac{1}{4}W^{-\frac{3}{2}}(x)(\partial_{x_j}W(x))^2+\frac{1}{2}W^{-\frac{1}{2}}(x)\partial_{x_j}^2W(x),
\end{aligned}
$$

each term of (4.2.12) is bounded by (4.2.5), (4.2.6), (4.2.9) and (4.2.11). Thus we obtain (4.2.2).

For the proof of (4.2.4), we calculate

$$
W_h(H_h-M)^{-1}=W_h^{\frac{1}{2}}(H_h-M)^{-1}W_h^{\frac{1}{2}}+W_h^{\frac{1}{2}}[W_h^{\frac{1}{2}},(H_h-M)^{-1}].
$$

It follows from (4.2.8) that the first term is bounded. For the second term, note that $H_{0,h}=\sum_{j=1}^{d}\nabla_j^*\nabla_j$, where

$$
\nabla_j v(z):=\frac{1}{h}\left(v(z+he_j)-v(z)\right),\ v\in\mathcal{H}_h.
$$

Then we learn

$$
\begin{aligned}
&W_h^{\frac{1}{2}}[W_h^{\frac{1}{2}},(H_h-M)^{-1}] \qquad (4.2.13)\\
=&W_h^{\frac{1}{2}}(H_h-M)^{-1}[W_h^{\frac{1}{2}},H_{0,h}](H_h-M)^{-1}\\
=&\sum_{j=1}^{d}W_h^{\frac{1}{2}}(H_h-M)^{-1}\left([W_h^{\frac{1}{2}},\nabla_j^*]\nabla_j+\nabla_j^*[W_h^{\frac{1}{2}},\nabla_j]\right)(H_h-M)^{-1}.
\end{aligned}
$$

Since

$$
\begin{aligned}
[W_h^{\frac{1}{2}},\nabla_j]v(z)=&h^{-1}\left(W^{\frac{1}{2}}(z+he_j)-W^{\frac{1}{2}}(z)\right)v(z+he_j),\\
W^{\frac{1}{2}}(z+he_j)-W^{\frac{1}{2}}(z)=&h\int_0^1\partial_{x_j}\left(W^{\frac{1}{2}}\right)(z+h\theta e_j)d\theta\\
=&\frac{1}{2}h\int_0^1W^{-\frac{1}{2}}(z+h\theta e_j)\partial_{x_j}W(z+h\theta e_j)d\theta,
\end{aligned}
$$

the uniform boundedness of (4.2.13) follows from (4.2.7), (4.2.8), (4.2.10) and (4.2.11). This completes the proof of (4.2.4). □

## 4.3 continuum and discrete Fourier transforms

We denote by $F$ the continuum Fourier transform from $\mathcal{H}$ onto $\hat{\mathcal{H}} = L^2(\mathbb{R}^d)$:

$$Fu(\xi) = (2\pi)^{-\frac{d}{2}}\hat{u}(\xi) = (2\pi)^{-\frac{d}{2}}\int_{\mathbb{R}^d} e^{-ix\cdot\xi}u(x)dx. \tag{4.3.1}$$

We set the discrete Fourier transform $F_h$ from $\mathcal{H}_h$ onto $\hat{\mathcal{H}}_h = L^2(h^{-1}\mathbb{T}^d)$, $\mathbb{T}^d = [-\pi, \pi)^d$, by

$$F_h v(\zeta) = (2\pi)^{-\frac{d}{2}}h^d \sum_{z\in h\mathbb{Z}^d} e^{-iz\cdot\zeta}v(z), \quad \zeta \in h^{-1}\mathbb{T}^d. \tag{4.3.2}$$

Then $F_h$ is a unitary operator and

$$F_h^* g(z) = (2\pi)^{-\frac{d}{2}}\int_{h^{-1}\mathbb{T}^d} e^{iz\cdot\zeta}g(\zeta)d\zeta, \quad z \in h\mathbb{Z}^d. \tag{4.3.3}$$

Furthermore we have

$$H_{0,h}v(z) = F_h^*\left(H_{0,h}(\cdot)F_h v(\cdot)\right)(z), \tag{4.3.4}$$

where

$$H_{0,h}(\zeta) = 2h^{-2}\sum_{j=1}^{d}(1-\cos h\zeta_j), \quad \zeta \in h^{-1}\mathbb{T}^d. \tag{4.3.5}$$

In order to prove Theorem 4.1.2, we prepare a convenient notation. We set

$$Q_h := F_h P_h F^* : \hat{\mathcal{H}} \to \hat{\mathcal{H}}_h. \tag{4.3.6}$$

Then we see that for $f \in \mathcal{S}(\mathbb{R}^d)$,

$$
\begin{aligned}
&Q_h f(\zeta) \qquad\qquad (4.3.7)\\
=&(2\pi)^{-\frac{d}{2}} h^d \sum_{z \in h\mathbb{Z}^d} e^{-iz\cdot\zeta} \left( h^{-d} \int_{\mathbb{R}^d} \overline{\varphi_{h,z}(x)} (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{ix\cdot\xi} f(\xi) d\xi dx \right)\\
=&(2\pi)^{-d} \sum_{z \in h\mathbb{Z}^d} e^{-iz\cdot\zeta} \int_{\mathbb{R}^d} \overline{\varphi_{h,z}(x)} \int_{\mathbb{R}^d} e^{ix\cdot\xi} f(\xi) d\xi dx\\
=&(2\pi)^{-d} h^d \sum_{z \in h\mathbb{Z}^d} \int_{\mathbb{R}^d} e^{iz\cdot(\xi-\zeta)} \overline{\hat{\varphi}(h\xi)} f(\xi) d\xi\\
=&(2\pi)^{-d} h^d \sum_{z \in h\mathbb{Z}^d} \sum_{n \in \mathbb{Z}^d} \int_{h^{-1}(\mathbb{T}^d + 2\pi n)} e^{iz\cdot(\xi-\zeta)} \overline{\hat{\varphi}(h\xi)} f(\xi) d\xi\\
=&(2\pi)^{-d} h^d \sum_{z \in h\mathbb{Z}^d} \sum_{n \in \mathbb{Z}^d} \int_{h^{-1}\mathbb{T}^d} e^{iz\cdot(\xi + 2\pi h^{-1} n - \zeta)} \overline{\hat{\varphi}(h\xi + 2\pi n)} f(\xi + 2\pi h^{-1} n) d\xi\\
=&(2\pi)^{-d} h^d \sum_{z \in h\mathbb{Z}^d} \sum_{n \in \mathbb{Z}^d} \int_{h^{-1}\mathbb{T}^d} e^{iz\cdot(\xi-\zeta)} \overline{\hat{\varphi}(h\xi + 2\pi n)} f(\xi + 2\pi h^{-1} n) d\xi\\
=&(2\pi)^{-d} h^d \sum_{z \in h\mathbb{Z}^d} \int_{h^{-1}\mathbb{T}^d} e^{iz\cdot(\xi-\zeta)} \sum_{n \in \mathbb{Z}^d} \overline{\hat{\varphi}(h\xi + 2\pi n)} f(\xi + 2\pi h^{-1} n) d\xi\\
=&\sum_{n \in \mathbb{Z}^d} \overline{\hat{\varphi}(h\zeta + 2\pi n)} f(\zeta + 2\pi h^{-1} n).
\end{aligned}
$$

Note that, for $g \in \hat{\mathcal{H}}_h$,

$$Q_h^* g(\xi) = \hat{\varphi}(h\xi)\tilde{g}(\xi), \quad \xi \in \mathbb{R}^d,$$

where $\tilde{g}$ is the function of $g$ extended periodically from $h^{-1}\mathbb{T}^d$ onto $\mathbb{R}^d$.

## 4.4 Proof of Theorem 4.1.2

Let $V$ and $\varphi$ be as in Theorem 4.1.2. Then we learn

$$
\begin{aligned}
&P_h^*(H_h - \mu)^{-1} P_h - (H - \mu)^{-1} \qquad\qquad (4.4.1)\\
=&P_h^*(H_h - \mu)^{-1} P_h - P_h^* P_h (H - \mu)^{-1} - (1 - P_h^* P_h)(H - \mu)^{-1}\\
=&P_h^* \left( (H_h - \mu)^{-1} P_h - P_h (H - \mu)^{-1} \right) - (1 - P_h^* P_h)(H - \mu)^{-1}\\
=&P_h^*(H_h - \mu)^{-1}(P_h H - H_h P_h)(H - \mu)^{-1} - (1 - P_h^* P_h)(H - \mu)^{-1}.
\end{aligned}
$$

We see by Lemma 4.4.1 and Proposition 4.2.1 that the last term of (4.4.1) is negligible.

**Lemma 4.4.1.** $\|(1 - P_h^* P_h)(H_0 - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H})} \le Ch^2$.

*Proof.* Note that

$$\|(1 - P_h^* P_h)(H_0 - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H})} = \|(1 - Q_h^* Q_h)(|\xi|^2 - \mu)^{-1}\|_{\mathcal{B}(\hat{\mathcal{H}})},$$

where $Q_h$ is defined by (4.3.6). Let $f \in \hat{\mathcal{H}}$ and $g = (|\xi|^2 - \mu)^{-1} f$. Then we have

$$\begin{aligned}(1 - Q_h^* Q_h) g(\xi) =& (1 - |\hat{\varphi}(h\xi)|^2) g(\xi) \\ & - \hat{\varphi}(h\xi) \sum_{n \ne 0} \overline{\hat{\varphi}(h\xi + 2\pi n)} g(\xi + 2\pi h^{-1} n).\end{aligned}$$

For the first term, we observe by the assumption of $\varphi$ that $|\hat{\varphi}(h\xi)| = 1$ if $|\xi| \le h^{-1}\delta$ for some small $\delta > 0$. Then it follows that

$$\|(1 - |\hat{\varphi}(h\xi)|^2) g(\xi)\|_{\hat{\mathcal{H}}} \le \sup_{|\xi| > h^{-1}\delta} \left| |\xi|^2 - \mu \right|^{-1} \|f\|_{\hat{\mathcal{H}}} \le Ch^2 \|f\|_{\hat{\mathcal{H}}}.$$

For the second term, we note that the summation on $\mathbb{Z}^d \setminus \{0\}$ equals to that on $\{1, 0, -1\}^d \setminus \{0\}^d$ by the support condition of $\hat{\varphi}$. Using the support condition of $\hat{\varphi}$ again, we learn that $\hat{\varphi}(h\xi)\overline{\hat{\varphi}(h\xi + 2\pi n)} = 0$ if $|\xi| \le h^{-1}\delta$ for some small $\delta > 0$. Thus the same argument as the first term implies that the second term is bounded by $Ch^2$. □

The first term of (4.4.1) is estimated by Proposition 4.2.1 as

$$\begin{aligned}& \|(H_h - \mu)^{-1}(P_h H - H_h P_h)(H - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \\ \le& \|(H_h - \mu)^{-1}(P_h H_0 - H_{0,h} P_h)(H - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \\ & \quad + \|(H_h - \mu)^{-1}(P_h V - V_h P_h)(H - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \\ \le& C\|(H_{0,h} - \mu)^{-1}(P_h H_0 - H_{0,h} P_h)(H_0 - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \\ & \quad + C\|(V_h - \mu)^{-1}(P_h V - V_h P_h)(V - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \\ =& C\|(H_{0,h} - \mu)^{-1} P_h - P_h (H_0 - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \\ & \quad + C\|(V_h - \mu)^{-1} P_h - P_h (V - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)}.\end{aligned}$$

Then the two lemmas below complete the proof of Theorem 4.1.2.

**Lemma 4.4.2.** $\|(H_{0,h} - \mu)^{-1} P_h - P_h (H_0 - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_h)} \le Ch^2$.

*Proof.* Note that

$$\begin{aligned}&\|(H_{0,h}-\mu)^{-1}P_h - P_h(H_0-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_h)}\\=&\|(H_{0,h}(\zeta)-\mu)^{-1}Q_h - Q_h(|\xi|^2-\mu)^{-1}\|_{\mathcal{B}(\hat{\mathcal{H}},\hat{\mathcal{H}}_h)}.\end{aligned}$$

Then we learn

$$\begin{aligned}&\left((H_{0,h}(\cdot)-\mu)^{-1}Q_h - Q_h(|\xi|^2-\mu)^{-1}\right) f(\zeta)\\=&\sum_{n\in\mathbb{Z}^d} A(\zeta,n;h) f(\zeta+2\pi h^{-1}n),\end{aligned}\tag{4.4.2}$$

where

$$A(\zeta,n;h) := \overline{\hat{\varphi}(h\zeta+2\pi n)}\left((H_{0,h}(\zeta)-\mu)^{-1} - (|\zeta+2\pi h^{-1}n|^2-\mu)^{-1}\right).$$

Similarly to Lemma 4.4.1, the summation on $\mathbb{Z}^d$ equals to that on $\{1,0,-1\}^d$. Since $H_{0,h}(\zeta) = H_{0,h}(\zeta+2\pi h^{-1}n)$, it suffices to consider the bound of

$$B(\zeta;h) := \overline{\hat{\varphi}(h\zeta)}\left((H_{0,h}(\zeta)-\mu)^{-1} - (|\zeta|^2-\mu)^{-1}\right).$$

If we use the formula

$$\begin{aligned}H_{0,h}(\zeta) =&2h^{-2}\sum_{j=1}^d(1-\cos h\zeta_j)\\=&2h^{-2}\sum_{j=1}^d\left(\frac{1}{2}(h\zeta_j)^2 - \frac{1}{4!}\int_0^{h\zeta_j}(h\zeta_j-y)^3\cos y dy\right),\end{aligned}$$

we learn

$$\begin{aligned}|H_{0,h}(\zeta)-|\zeta|^2| =&\left|-12^{-1}h^{-2}\sum_{j=1}^d\int_0^{h\zeta_j}(h\zeta_j-y)^3\cos y dy\right|\\\le&48^{-1}h^2\sum_{j=1}^d|\zeta_j|^4.\end{aligned}$$

We also learn for $\zeta\in h^{-1}(-2\pi+\varepsilon, 2\pi-\varepsilon)^d$ with $\varepsilon>0$,

$$H_{0,h}(\zeta) = 4h^{-2}\sum_{j=1}^d\sin^2\frac{h}{2}\zeta_j \ge c_\varepsilon|\zeta|^2$$

for some $c_\varepsilon > 0$. Since $\operatorname{supp}\hat{\varphi}(\cdot) \subset (-2\pi+\varepsilon, 2\pi-\varepsilon)^d$ for a small $\varepsilon > 0$, we obtain

$$\begin{aligned}|B(\zeta;h)| \leq & \sup_{\zeta\in\operatorname{supp}\hat{\varphi}(h\cdot)} \left|(H_{0,h}(\zeta)-\mu)^{-1} - (|\zeta|^2-\mu)^{-1}\right| \\ \leq & \sup_{\zeta\in\operatorname{supp}\hat{\varphi}(h\cdot)} |H_{0,h}(\zeta)-\mu|^{-1} C h^2 |\zeta|^4 \left||\zeta|^2-\mu\right|^{-1} \\ \leq & Ch^2.\end{aligned}$$

□

**Lemma 4.4.3.** *If $(V(x)-\mu)^{-1}$ is a uniformly continuous bounded function,*

$$\|(V_h-\mu)^{-1}P_h - P_h(V-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_h)} \to 0, \quad h\to 0.$$

*If, in addition, $(V(x)-\mu)^{-1} \in C^{0,\alpha}(\mathbb{R}^d)$, $\alpha\in(0,1]$,*

$$\|(V_h-\mu)^{-1}P_h - P_h(V-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_h)} \leq Ch^{\alpha-\varepsilon}$$

*for any $\varepsilon > 0$.*

*Proof.* A direct calculus implies

$$\left((V_h-\mu)^{-1}P_h - P_h(V-\mu)^{-1}\right)u(z) = \int_{\mathbb{R}^d} K(x,z;h)u(x)dx, \tag{4.4.3}$$

where

$$K(x,z;h) := h^{-d}\left((V(z)-\mu)^{-1} - (V(x)-\mu)^{-1}\right)\overline{\varphi(h^{-1}(x-z))}.$$

By Young's inequality, it suffices to show

$$\sup_{z\in h\mathbb{Z}^d}\int_{\mathbb{R}^d}|K(x,z)|dx \to 0, \tag{4.4.4}$$

$$\sup_{x\in\mathbb{R}^d} h^d \sum_{z\in h\mathbb{Z}^d}|K(x,z)| \to 0 \tag{4.4.5}$$

as $h\to 0$. Let

$$R(\delta) := \sup_{x,y\in\mathbb{R}^d, |x-y|<\delta}\left|(V(x)-\mu)^{-1} - (V(y)-\mu)^{-1}\right|.$$

Then, since $\varphi\in\mathcal{S}(\mathbb{R}^d)$, we have for any $n\geq 0$

$$|K(x,z)| \leq C_n h^{-d} R(|x-z|)\langle h^{-1}(x-z)\rangle^{-n}.$$

Thus we obtain for $n > d$

$$\begin{aligned}\int_{\mathbb{R}^d} |K(x,z)|dx =& \int_{|x-z|<\delta} |K(x,z)|dx + \int_{|x-z|\geq\delta} |K(x,z)|dx \\ \leq& CR(\delta) \int_{|y|<h^{-1}\delta} \langle y\rangle^{-n} dy + C \int_{|y|\geq h^{-1}\delta} \langle y\rangle^{-n} dy \\ \leq& CR(\delta) + C\langle h^{-1}\delta\rangle^{-\frac{n-d}{2}}.\end{aligned}$$

Similarly, we have for $n > d$,

$$\begin{aligned}& h^d \sum_{z\in h\mathbb{Z}^d} |K(x,z)| \\ =& h^d \sum_{|x-z|<\delta} |K(x,z)| + h^d \sum_{|x-z|\geq\delta} |K(x,z)| \\ \leq& CR(\delta)h^d \sum_{|x-z|<\delta} \langle h^{-1}(x-z)\rangle^{-n} + Ch^d \sum_{|x-z|\geq\delta} \langle h^{-1}(x-z)\rangle^{-n} \\ \leq& CR(\delta) + C\langle h^{-1}\delta\rangle^{-\frac{n-d}{2}}.\end{aligned}$$

Since $R(\delta) \to 0$ as $\delta \to 0$, (4.4.4) and (4.4.5) are proved. If $(V(x) - \mu)^{-1} \in C^{0,\alpha}(\mathbb{R}^d)$, then $R(\delta) \leq C\delta^\alpha$ for small $\delta > 0$. Thus substituting $\delta = h^{1-\varepsilon}$, $\varepsilon > 0$, we obtain $\|(V_h - \mu)^{-1}P_h - P_h(V-\mu)^{-1}\| \leq Ch^{(1-\varepsilon)\alpha}$.

□

# Bibliography


[1] K. Ando, H. Isozaki, H. Morioka: Spectral properties of Schrödinger operators on perturbed lattices. Ann. Henri Poincaré **17** (2016), 2103–2171.

[2] D. Bambusi, T. Penati: Continuous approximation of breathers in one- and two-dimensional DNLS lattices. Nonlinearity **23** (2010), 143–157.

[3] A. Boutet de Monvel, J. Sahbani: On the spectral properties of discrete Schrödinger operators: (The multi-dimensional case). Rev. Math. Phys. **11** (1999), 1061–1078.

[4] Younghun Hong, Changhun Yang: Strong Convergence for Discrete Nonlinear Schrödinger equations in the Continuum Limit. arXiv:1806.07542.

[5] H. Isozaki, I. Korotyaev: Inverse Problems, Trace Formulae for Discrete Schorödinger Operators. Ann. Henri Poincaré **13** (2012), 751–788.

[6] S. Nakamura: Modified wave operators for discrete Schrödinger operators with long-range perturbations. J. Math. Phys. **55** (2014), 112101 (8 pages).

[7] D. Parra, S. Richard: Spectral and scattering theory for Schrödinger operators on perturbed topological crystals. Rev. Math. Phys. **30** (2018), 1850009-1 – 1850009-39.

[8] V. Rabinovich: Wiener algebra of operators on the lattice $(\mu\mathbb{Z})^n$ depending on the small parameter $\mu > 0$. Complex Variables and Elliptic Equations **58** (2013), No. 6, 751–766.

[9] M. Reed, B. Simon: The Methods of Modern Mathematical Physics, Volume I, Functional Analysis, Academic Press, 1979.