Long-range scattering theory of discrete Schrödinger operators and its application to quantum walks

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1. Introduction

We consider generalized form of discrete Schrödinger operators defined on $\mathcal{H} = \ell^2(\mathbb{Z}^d; \mathbb{C}^n)$, d, $n \geq 1$. We let

$$Hu(x) = H_0 u(x) + V(x)u(x), \tag{1.1}$$

where H_0 is a convolution operator

$$H_0 u = \begin{pmatrix} H_{0,11} & H_{0,12} & \cdots & H_{0,1n} \\ H_{0,21} & H_{0,22} & \cdots & H_{0,2n} \\ \vdots & \vdots & \ddots & \vdots \\ H_{0,n1} & H_{0,n2} & \cdots & H_{0,nn} \end{pmatrix} u, \quad u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \in \mathcal{H}, \tag{1.2}$$

$$H_{0,jk} u_k(x) = \sum_{y \in \mathbb{Z}^d} f_{jk}(x-y) u_k(y), \quad u_k \in \ell^2(\mathbb{Z}^d), \tag{1.3}$$

and $V(x) = {}^t\left(V_1(x), \ldots, V_n(x)\right)$ is an $\mathbb{R}^n$-valued function on $\mathbb{Z}^d$.

The above operator H is derived from discrete Schrödinger operators on periodic lattices, which are considered as tight binding Hamiltonians of an electron moving in a crystal in the field of solid-state physics.

Example 1.1. Discrete Schrödinger operator on square lattice. For $u \in \ell^2(\mathbb{Z}^d)$, we set

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

Example 1.2. Triangular lattice. For $u \in \ell^2(\mathbb{Z}^2)$ and $V : \mathbb{Z}^2 \to \mathbb{R}$, we set

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

where $n_1 = (1,0)$, $n_2 = (-1,0)$, $n_3 = (0,1)$, $n_4 = (0,-1)$, $n_5 = (1,-1)$ and $n_6 = (-1,1)$.

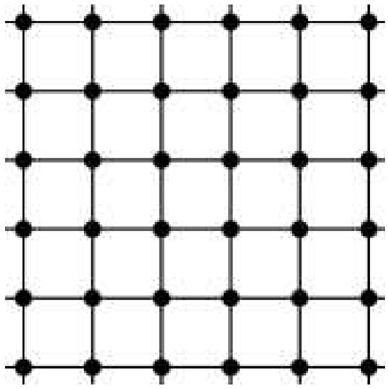

FIGURE 1. Square lattice.

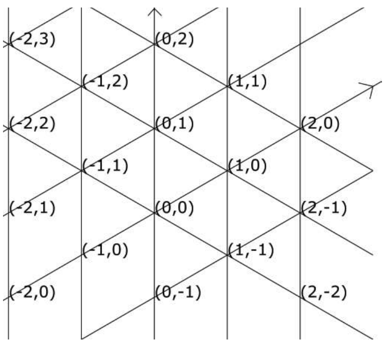

FIGURE 2. Trianular lattice

EXAMPLE 1.3. Hexagonal lattice (graphene). For $u = {}^t(u_1, u_2) \in \ell^2(\mathbb{Z}^2) \oplus \ell^2(\mathbb{Z}^2) = \ell^2(\mathbb{Z}^2; \mathbb{C}^2)$ and $V : \mathbb{Z}^2 \to \mathbb{R}^2$, we set

$$\begin{aligned} H_{\mathrm{he}}u(x) &= H_{\mathrm{he},0}u(x) + Vu(x) \\ &= -\frac{1}{3}\begin{pmatrix} u_2(x_1,x_2) + u_2(x_1-1,x_2) + u_2(x_1,x_2-1) \\ u_1(x_1,x_2) + u_1(x_1+1,x_2) + u_1(x_1,x_2+1) \end{pmatrix} \\ &\quad + \begin{pmatrix} V_1(x_1,x_2)u_1(x_1,x_2) \\ V_2(x_1,x_2)u_2(x_1,x_2) \end{pmatrix}, \quad x = (x_1,x_2) \in \mathbb{Z}^2. \end{aligned}$$

Note that hexagonal lattice $\cong \mathbb{Z}^2 \times \{0,1\}$ ($\ncong \mathbb{Z}^2$) with considering the canonical $\mathbb{Z}^2$-action.

More examples of lattices, such as Kagome lattice, diamond lattice and graphite, are found in [**1**].

In this note we develop a scattering theory for the pair of operators H_0 and H of the form (1.1) with V of long-range type, and we see that as an application we can construct a long-range scattering theory of quantum walks on $\mathbb{Z}^d$.

We note that if $f = (f_{jk}) \neq 0$ has a finite support and

$$\overline{f_{jk}(-x)} = f_{kj}(x), \quad x \in \mathbb{Z}^d,\ 1 \le j,k \le n, \tag{1.4}$$

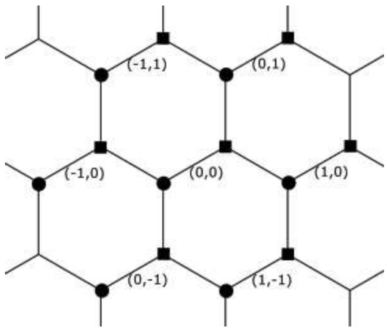

FIGURE 3. Hexagonal lattice. Circles and squares correspond to the first and second entries, respectively.

and if V is short-range, i.e. $|V(x)| \le C\langle x\rangle^{-\rho}$ with $\rho > 1$, then the wave operators

$$W^{\pm} = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH}e^{-itH_0}P_{\mathrm{ac}}(H_0)$$

exist and are complete $\mathrm{Ran}\, W^{\pm} = \mathcal{H}_{\mathrm{ac}}(H)$ (see [**2**], [**1**] and [**6**]). Here $\mathcal{H}_{\mathrm{ac}}(A)$ denotes the absolutely continuous subspace of A and $P_{\mathrm{ac}}(A)$ denotes the orthogonal projection onto $\mathcal{H}_{\mathrm{ac}}(A)$ for an selfadjoint operator A.

2. Main theorem

We denote the Fourier transform $\mathcal{F}$ by

$$\mathcal{F}u(\xi) = \begin{pmatrix} Fu_1(\xi) \\ Fu_2(\xi) \\ \vdots \\ Fu_n(\xi) \end{pmatrix}, \quad \xi \in \mathbb{T}^d := [-\pi, \pi)^d, \tag{2.1}$$

$$Fu_j(\xi) = (2\pi)^{-\frac{d}{2}} \sum_{x\in\mathbb{Z}^d} e^{-ix\cdot\xi}u_j(x). \tag{2.2}$$

Then $\mathcal{F}$ is a unitary operator from $\mathcal{H}$ onto $\hat{\mathcal{H}} = L^2(\mathbb{T}^d; \mathbb{C}^n)$. We easily see that $\mathcal{F} \circ H_0 \circ \mathcal{F}^*$ is a multiplication operator on $\mathbb{T}^d$ by the matrix-valued function

$$H_0(\xi) = \begin{pmatrix} h_{11}(\xi) & h_{12}(\xi) & \cdots & h_{1n}(\xi) \\ h_{21}(\xi) & h_{22}(\xi) & \cdots & h_{2n}(\xi) \\ \vdots & \vdots & \ddots & \vdots \\ h_{n1}(\xi) & h_{n2}(\xi) & \cdots & h_{nn}(\xi) \end{pmatrix}, \tag{2.3}$$

where

$$h_{jk}(\xi) := \sum_{x\in\mathbb{Z}^d} e^{-ix\cdot\xi} f_{jk}(x). \tag{2.4}$$

In this note we assume that h_{jk}'s are smooth functions on $\mathbb{T}^d$, equivalently f_{jk}'s are rapidly decreasing:

$$\sup_{x\in\mathbb{Z}^d} \langle x\rangle^m |f_{jk}(x)| < \infty$$

for any $m \in \mathbb{N}$, where $\langle x\rangle = (1+|x|^2)^{\frac{1}{2}}$.

Note that $\sigma(H_0) = \{\lambda \mid \det(H_0(\xi)-\lambda) = 0 \text{ for some } \xi \in \mathbb{T}^d\}$ and H_0 is a self-adjoint operator if and only if $H_0(\xi)$ is a symmetric matrix for any $\xi \in \mathbb{T}^d$, equivalently, (1.4).

We assume the selfadjointness of H_0 and a long-range condition of V.

Assumption 2.1. (1) f_{jk}'s are rapidly decreasing functions satisfying (1.4).

(2) $V = {}^t(V_1, \cdots, V_n)$ has the following representation

$$V = V_L + V_S,$$

where each entry of V_L is the same, i.e., $V_L = {}^t(V_\ell, \cdots, V_\ell)$ with some $V_\ell : \mathbb{Z}^d \to \mathbb{R}$. Furthermore, there exist $\rho > 0$ and $C, C_\alpha > 0$ such that

$$|\tilde{\partial}_x^\alpha V_\ell(x)| \le C_\alpha \langle x\rangle^{-\rho-|\alpha|}, \tag{2.5}$$

$$|V_S(x)| \le C\langle x\rangle^{-1-\rho} \tag{2.6}$$

for any $x \in \mathbb{Z}^d$ and $\alpha \in \mathbb{Z}_+^d$. Here $\tilde{\partial}_x^\alpha = \tilde{\partial}_{x_1}^{\alpha_1} \cdots \tilde{\partial}_{x_d}^{\alpha_d}$, $\tilde{\partial}_{x_j} V(x) = V(x) - V(x-e_j)$ is the difference operator with respect to the j-th variable.

We denote the set of Fermi surfaces corresponding to the energies in $\Gamma \subset \mathbb{R}$ by

$$\begin{aligned} \mathrm{Ferm}(\Gamma) :=& \{p = (\xi,\lambda) \in \mathbb{T}^d \times \Gamma \mid \lambda \text{ is an eigenvalue of } H_0(\xi)\} \\ =& \{p = (\xi,\lambda) \in \mathbb{T}^d \times \Gamma \mid \det(H_0(\xi)-\lambda) = 0\}. \end{aligned} \tag{2.7}$$

Definition 2.2. $\lambda_0 \in \sigma(H_0)$ is said to be *a non-threshold energy of* H_0 if the following properties hold:

(1) For any $\xi_0 \in \mathbb{T}^d$ such that $\det(H_0(\xi_0)-\lambda_0) = 0$, there exists an open neighborhood $G \subset \mathbb{T}^d \times \mathbb{R}$ of $p = (\xi_0, \lambda_0)$ such that $\mathrm{Ferm}(\mathbb{R}) \cap G$ has a graph representation, i.e.

$$\mathrm{Ferm}(\mathbb{R}) \cap G = \{(\xi, \lambda(\xi)) \mid \xi \in U\} \tag{2.8}$$

with some $U \ni \xi_0$ and $\lambda \in C^\infty(U)$.

(2) Let ξ_0 be arbitrarily fixed so that $\det(H_0(\xi_0)-\lambda_0) = 0$ holds, and let $\lambda(\xi)$ be as in (2.8). Then $\nabla_\xi \lambda(\xi_0) \ne 0$ holds (note that $\lambda_p(\xi)$ is smooth function on U_{ξ_0} by the smoothness of $H_0(\xi)$).

Let $\Gamma(H_0)$ be the set of non-threshold energies of H_0. Then H_0 has purely absolutely continuous spectrum on $\Gamma(H_0)$, i.e., $\sigma_{pp}(H_0) \cap \Gamma(H_0) = \sigma_{sc}(H_0) \cap \Gamma(H_0) = \phi$.

THEOREM 2.3 ([**10**]). *Suppose Assumption 2.1 and* $\Gamma \Subset \Gamma(H_0)$. *Then one can construct Isozaki-Kitada modifiers* $J_\pm = J_{\pm,\Gamma}$ *such that the modified wave operators exist:*

$$W_{IK}^{\pm}(\Gamma) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} J_\pm e^{-itH_0} E_{H_0}(\Gamma), \tag{2.9}$$

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

i) Intertwining property: $HW_{IK}^{\pm}(\Gamma) = W_{IK}^{\pm}(\Gamma)H_0$.

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

iii) Completeness: $\operatorname{Ran} W_{IK}^{\pm}(\Gamma) = E_H(\Gamma)\mathcal{H}_{ac}(H)$.

The case of $n = 1$, e.g. discrete Schrödinger operators on square and triangular lattices, is considered by Nakamura [**5**] and the author [**8**]. Moreover, Theorem 2.3 includes the result by the author [**9**], where a long-range scattering theory for discrete Schrödinger operators on the hexagonal lattice is studied. See also [**3**], [**4**], [**7**], [**12**] and references therein for scattering theory of Schrödinger operators on $\mathbb{R}^d$.

3. Formal proof

For $n = 1$, modified wave operators are constructed as follows: Let $\varphi_\pm : \mathbb{R}^d \times \mathbb{T}^d \to \mathbb{R}$ and

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

The phase functions $\varphi_\pm \sim x \cdot \xi$ are solutions to the eikonal equation

$$H_0(\nabla_x \varphi_\pm(x,\xi)) + \tilde{V}_\ell(x) = H_0(\xi),$$

where $\tilde{V}_\ell$ is a smooth extension of V_ℓ onto $\mathbb{R}^d$.

The proof of existence of (2.9) is given by the stationary phase method. Let $W(t)u = e^{itH}e^{-itH_0}u$. Then we have for $\pm t$, $\pm s \geq 0$

$$W(t)u - W(s)u = \int_s^t e^{i\tau H}(HJ_\pm - J_\pm H_0)e^{-i\tau H_0} u d\tau.$$

It follows that

$$(HJ_\pm - J_\pm H_0)e^{-itH_0}u(x) = \int_{\mathbb{T}^d} e^{i(\varphi_\pm(x,\xi) - tH_0(\xi))} a_\pm(x,\xi)\mathcal{F}u(\xi) d\xi,$$

where

$$\begin{aligned} a_\pm(x,\xi) =& H_0(\nabla_x\varphi_\pm(x,\xi)) + \tilde{V}_\ell(x) - H_0(\xi) + O(\langle x\rangle^{-\rho-1}) \\ =& O(\langle x\rangle^{-\rho-1}). \end{aligned}$$

The stationary points are determined by $\nabla_\xi \varphi_\pm(x,\xi) - t\nabla_\xi H_0(\xi) = 0$, approximately

$$x \simeq t\nabla_\xi H_0(\xi) \neq 0$$

by the nonthreshold condition in Definition 2.2. Thus we obtain $\|(HJ_\pm - J_\pm H_0)e^{-itH_0}u\| = O(\langle t\rangle^{-1-\rho})$ and $W(t)u$ is a Cauchy sequence. We omit the proof of completeness. For a rigorous proof, see [**8**] and [**10**].

If $n \geq 2$, one of the reasonable proofs is to diagonalize $H_0(\xi)$. We choose a unitary matrix $U(\xi)$ such that

$$U(\xi)^* H_0(\xi) U(\xi) = \operatorname{diag}(\lambda_j(\xi)) \text{ if } E_{H_0(\xi)}(\Gamma) \neq 0.$$

Let $J_{\pm,j}$ be the corresponding modifier to $\lambda_j(D_x)$. Then

$$J_\pm = U(D_x) \operatorname{diag}(J_{\pm,j}) U(D_x)^*$$

satisfy the claim of Theorem 2.3. The above argument works in the hexagonal lattice case (see [**9**]). However there is a case where $U(\xi)$ cannot be taken globally, e.g. $\begin{pmatrix} \xi_1 & \xi_2 + i\xi_3 \\ \xi_2 - i\xi_3 & -\xi_1 \end{pmatrix}$ on $|\xi| = 1$. For a rigorous proof, we consider orthogonal projections onto $\operatorname{Ker}(H_0(\xi) - \lambda_j(\xi))$ instead. For details, see [**10**].

4. Application to quantum walks

Let $\mathcal{H} = \ell^2(\mathbb{Z}; \mathbb{C}^2)$. For $\Psi \in \mathcal{H}$, we use the notation

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}, \quad \Psi_j \in \ell^2(\mathbb{Z}) = \ell^2(\mathbb{Z}; \mathbb{C}).$$

We consider quantum walks

$$U := SC \text{ and } U_0 := SC_0$$

defined as unitary operators on $\mathcal{H}$, where

$$S\Psi(x) = \begin{pmatrix} \Psi_1(x+1) \\ \Psi_2(x-1) \end{pmatrix},$$
$$C_0 : \ 2 \times 2 \text{ unitary matrix},$$

and

$$C = C(x) : \ 2 \times 2 \text{ unitary matrix-valued function on } \mathbb{Z}.$$

Then $\mathcal{F} \circ U_0 \circ \mathcal{F}^*$ is a multiplication operator on $\mathbb{T}$ by

$$U_0(\xi) = S(\xi) C_0,$$

where

$$S(\xi) := \begin{pmatrix} e^{i\xi} & 0 \\ 0 & e^{-i\xi} \end{pmatrix}.$$

Note that

$$\sigma(U_0) = \{\lambda \mid \det(U_0(\xi) - \lambda) = 0 \text{ for some } \xi \in \mathbb{T}\} \subset S^1.$$

We set

$$\operatorname{Ferm}(\Gamma) := \{p = (\xi, \lambda) \in \mathbb{T} \times \Gamma \mid \lambda : \text{eigenvalue of } U_0(\xi)\}$$

for $\Gamma \subset S^1$.

Definition 4.1. $\lambda_0 \in \sigma(U_0) \subset S^1$ is said to be *a non-threshold energy of* U_0 if

$$\frac{d}{d\xi}\det(U_0(\xi) - \lambda_0) \neq 0 \quad \text{for any } \xi \text{ s.t. } \det(U_0(\xi) - \lambda_0) = 0.$$

Let $\Gamma(U_0)$ be the set of non-threshold energies of U_0.

In this case, the long-range condition for perturbation is the following.

Assumption 4.2. Let $B(x) := C_0^{-1}C(x)$. Then

$$B(x) = e^{iV_\ell} Id + B_S(x),$$

where

$$|\tilde{\partial}_x^\alpha V_\ell(x)| \le C_\alpha \langle x \rangle^{-\rho-|\alpha|},$$
$$|B_S(x)| \le C\langle x \rangle^{-1-\rho}$$

for $x \in \mathbb{Z}^d$ and $\alpha \in \mathbb{Z}_+^d$ with some $\rho > 0$.

Theorem 4.3. *Suppose Assumption 4.2 and* $\Gamma \Subset \Gamma(U_0)$. *Then one can construct Isozaki-Kitada modifiers* $J_\pm = J_{\pm,\Gamma}$ *such that the modified wave operators exist:*

$$W_{IK}^{\pm}(\Gamma) = \operatorname*{s-lim}_{t\to\pm\infty} e^{-tU} J_\pm e^{tU_0} E_{U_0}(\Gamma), \tag{4.1}$$

where E_{U_0} *denotes the spectral measure of* U_0. *Moreover, they are partially isometric from* $\operatorname{Ran} E_{U_0}(\Gamma)$ *onto* $E_H(\Gamma)\mathcal{H}_{ac}(H)$.

Remark 4.4. Wada [**11**] has already studied a long-range scattering theory, however the method from discrete Schrödinger operators can cover any dimensional case. Note also that the long-range condition by [**11**] is different with that of this note.

The construction of $J_\pm$ is as follows. Let $\lambda(\xi)$ be arbitrary branch of eigenvalues with $\operatorname{Ran}\lambda \Subset \Gamma$, and $\varphi_\pm(x,\xi)$ be such that

$$\lambda(\partial_x \varphi_\pm(x,\xi)) + \tilde{V}_\ell(x) = \lambda(\xi).$$

Then we define $J_\pm$ by the same manner. The proof is given similarly to [**10**].

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