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

Yukihide TADANO
Department of Mathematics, Tokyo University of Science

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

$$Hu(x) = H_0u(x) + V(x)u(x), \tag{1.1}$$

where H_0 is a convolution operator

$$H_0u = \begin{pmatrix} H_{0,11} & H_{0,12} & \cdots & H_{0,1n} \\ H_{0,21} & H_{0,22} & \cdots & H_{0,2n} \\ \vdots & \vdots & \ddots & \vdots \\ H_{0,n1} & H_{0,n2} & \cdots & H_{0,nn} \end{pmatrix} u, \quad u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \in \mathcal{H}, \tag{1.2}$$

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

and $V(x) = {}^t(V_1(x), \dots, V_n(x))$ 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 $n_6 = (-1,1)$.

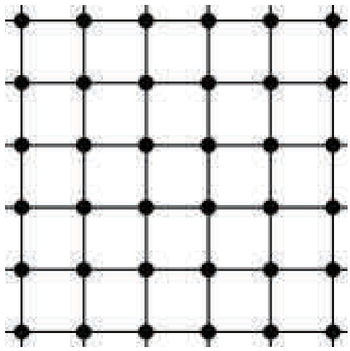

FIGURE 1. Square lattice.

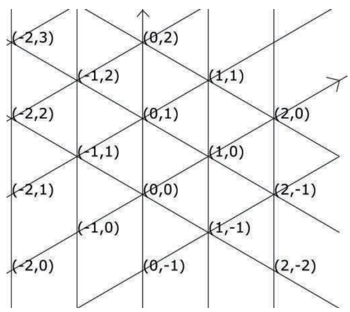

FIGURE 2. Trianular lattice

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

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

Note that hexagonal lattice $\cong \mathbb{Z}^2 \times \{0, 1\}$ ($\not\cong \mathbb{Z}^2$) 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

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

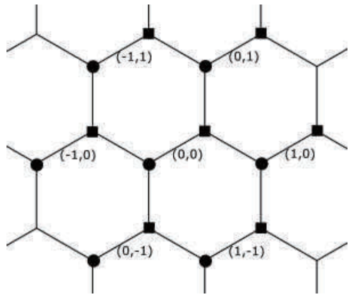

FIGURE 3. Hexagonal lattice. Circles and squares correspond to the first and second entries, respectively.

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

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

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

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

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 $\text{Ferm}(\mathbb{R}) \cap G$ has a graph representation, i.e.

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

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

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

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

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

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 $\mathrm{Ker}(H_0(\xi) - \lambda_j(\xi))$ 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

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

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

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

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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Department of Mathematics, Tokyo University of Science, 1-3, Kagurazaka, Shinjuku, Tokyo 162-8601, Japan

Email address: `y.tadano@rs.tus.ac.jp`