Phase recovery from phaseless scattering data for discrete Schrödinger operators

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July 2023

Abstract. We consider scattering for the discrete Schrödinger operator on the square lattice $\mathbb{Z}^d$, $d \geq 1$, with compactly supported potential. We give formulas for finding the phased scattering amplitude from phaseless near-field scattering data.

Keywords: discrete Schrödinger operators, monochromatic scattering data, phase retrieval, phaseless inverse scattering

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1. Introduction

We consider the discrete Schrödinger equation

$$-\Delta\psi(x) + v(x)\psi(x) = E\psi(x), \quad x \in \mathbb{Z}^d, d \geq 1. \tag{1}$$

We assume that Δ is the discrete Laplacian defined by

$$\Delta\psi\left(x\right) = \sum_{|x'-x|=1} \psi\left(x'\right), \quad x, x' \in \mathbb{Z}^d, \tag{2}$$

v is a scalar potential such that

$$\operatorname{supp} v \subset \mathcal{D}, \tag{3}$$

where $\mathcal{D}$ is bounded in $\mathbb{Z}^d$, and

$$E \in S := [-2d, 2d] \setminus S_0, \tag{4}$$

where

$$\begin{aligned} S_0 := \{ &\pm 4n \text{ when } d \text{ is even}, \\ &\pm 2(2n+1) \text{ when } d \text{ is odd}, n \in \mathbb{Z} \text{ and } 2n \leq d\}. \end{aligned} \tag{5}$$

The discrete Schrödinger equation (1) appears in the TB (tight-binding) model of the electrons in crystals, as in many cases the electrons of a crystal are strongly attached to the atoms [1, 2] involving a very weak hopping interaction with the neighboring atoms due to quantum tunnelling. The TB model is also closely related to LCAO (linear combination of atomic orbitals) [3]. Moreover, for example when $d = 1$ and $d = 2$, it has played a crucial role in uncovering significant phenomena associated with electrons in crystals [4, 5, 6]. At a different length scale, in the domain of electrical engineering, lattice structures of LC circuits involve similar difference equations where they play an important role in network synthesis and filter design [7]; lately such equations also appear in the lumped circuit models for electromagnetic metamaterials [8]. The same equation also appears, for $d = 1, 2$, in case of of time harmonic lattice waves [9, 10] and reveals structure in simple cases also for $d = 3$. In particular, the case $d = 2$ corresponds to a discrete analogue of anti-plane shear waves in elastic continuum. Examples of forward analysis of such equations, in the case $d = 2$, with an exact solution of scattering of time harmonic lattice waves by atomically sharp crack tips and rigid constraints, can be found in [11, 12, 13, 14, 15, 16, 17, 18]. The physical literature concerning the discrete Schrödinger equation also includes, in particular, [19].

The discrete Schrödinger equation was studied by [20], [21], [22] and [23] from pure mathematical viewpoint.

Let

$$\Gamma(E) = \{k : k \in T^d,\ \phi\left(k\right) = E\}, \quad E \in \left[-2d, 2d\right]. \tag{6}$$

Here $T^d = \mathbb{R}^d / 2\pi\mathbb{Z}^d$ and

$$\phi(k) = 2\sum_{i=1}^{d} \cos k_i. \tag{7}$$

One can fix the orientation of $\Gamma(E)$ with the choice of the (non-normalized) normal vector

$$n := \nabla\phi(k). \tag{8}$$

For Eq. (1) we consider the scattering solutions

$$\psi^+(x,k) = \psi_0^+ + \psi_{sc}^+, \tag{9}$$

where

$$\psi_0^+(x,k) = e^{ik\cdot x}, \quad k \in \Gamma(E), \quad x \in \mathbb{Z}^d, \tag{10}$$

and $\psi_{sc}^+(x,k)$ is the outgoing solution for the non-homogenous equation

$$-\Delta\psi_{sc} - E\psi_{sc} + v\psi_{sc} = -v\psi_0^+, \tag{11}$$

obtained using the limiting absorption principle; see [22]. Strictly speaking, to consider ψ^+ we also assume that v is real-valued or that energy E is not singular for the case of complex v.

Remark 1.1 *For positive E, it is convenient to consider $\Gamma(E)$ to be symmetric with respect to the origin in $\mathbb{R}^d$. For negative E, it may be convenient to consider $\Gamma(E)$ to be symmetric with respect to the point in $\mathbb{R}^d$, where all coordinates are equal to π.*

If

$$2d - 4 < |E| < 2d, \tag{12}$$

then the surface $\Gamma(E)$ is strictly convex with non-zero principal curvatures, and there is a unique point

$$\gamma = \gamma(\omega, E) \in \Gamma(E), \quad \omega \in S^{d-1}, \tag{13}$$

where the normal n, defined by (8), to the surface $\Gamma(E)$ is parallel to and has the same direction as ω.

In this case ψ_{sc}^+ has the asymptotic expansion

$$\psi^+(x,k) = e^{ik\cdot x} + \frac{e^{+i\mu(\omega,E)|x|}}{|x|^{\frac{d-1}{2}}} f^+(k,\omega) + O\left(\frac{1}{|x|^{\frac{d+1}{2}}}\right)$$
$$\text{as } |x| \longrightarrow \infty, \quad \omega = \frac{x}{|x|}, \tag{14}$$

where

$$\mu(\omega, E) = \gamma(\omega, E)\cdot\omega, \tag{15}$$

and the coefficient $f^+(k,\omega)$ is smooth and the remainder can be estimated uniformly in ω [20, 21, 22]. The coefficient f^+ is the scattering amplitude for (1). In many respects, expansion (14) is similar to the related expansion for the case of continuous Schrödinger equation, where

$$\Gamma(E) = S^{d-1}_{\sqrt{E}} = \{k \in \mathbb{R}^d : |k| = \sqrt{E}\}, \quad \mu(\omega, E) = \sqrt{E} > 0; \tag{16}$$

see, for example, [24]. For both discrete and continuous cases, the remainder $O(|x|^{-(d+1)/2}) \equiv 0$ for $d = 1$.

In quantum mechanics, according to the Born principle, the complex values of wave functions ψ^+ and scattering amplitude f^+ do not have direct physical interpretations, whereas the absolute values of these functions admit probabilistic interpretation and can be measured directly in physical experiments. For example, in the problem of electronic transport through interfaces, naturally described in terms of transmission and reflection, following the Landauer-Büttiker approach [25, 26], the scattering amplitudes (the probability amplitude) decide the conductance in the linear response regime; see, for example, [27, 28, 29, 30] for an application to transport in waveguides where the forward problem of discrete Schrödinger equation has been solved exactly.

In the present work, we give explicit asymptotic formulas for finding complex f^+ from $|\psi^+|^2$ measured on $\mathbb{Z}^d \setminus \mathcal{D}$, under assumption (12). In many respects these formulas are similar to the formulas in [31, 32, 33] given for the case of continuous Schrödinger equation. In particular, for equation (1), these formulas can be used in the framework of phaseless inverse scattering from $|\psi^+|^2$, using results on inverse scattering from f^+ with phase information. For equation (1), some results on inverse scattering from f^+, in fact, are given in [19, 21, 23, 34, 35]. In connection with inverse scattering for continuous Schrödinger equation, see, for example, the review article [24] and references therein.

The present article can be considered as the first work on phaseless inverse scattering for the discrete Schrödinger equation (1). In connection with phaseless inverse scattering for the continuous Schrödinger equation and other continuous equations of wave propagation, see, for example, [36, 37, 38, 39, 40, 41, 42, 32, 24, 43, 44] and references therein.

The main results of the present article are given in Section 2 and proved in Sections 3 and 4.

2. Main Results

Let us define

$$a(x,k) = |x|^{\frac{d-1}{2}} (|\psi^+(x,k)|^2 - 1), \quad x \in \mathbb{Z}^d \setminus \{0\}, \quad k \in \Gamma(E), \tag{17}$$

where $\psi^+(x,k)$ is defined as in (9) in introduction.

In particular, we consider $a(x,k)$ at two measurement points

$$x = \mathrm{Int}(s\omega) \text{ and } y = x + \zeta, \quad s > 0, \quad \omega \in S^{d-1}, \quad \zeta \in \mathbb{Z}^d \setminus \{0\}, \tag{18}$$

where

$$\mathrm{Int}(\xi) = \sum_{i=1}^{d} \mathrm{sgn}(\xi_i)\ \lfloor |\xi_i| \rfloor\ \mathbf{e}_i, \quad \xi \in \mathbb{R}^d, \tag{19}$$

and $\lfloor \cdot \rfloor$ denotes the floor function while $\mathbf{e}_i$ are unit basis vectors in $\mathbb{Z}^d$ or in $\mathbb{R}^d$.

In dimension $d \geq 2$, we have, in particular, the following theorem.

Theorem 2.1 *Suppose that assumptions (3) and (12) are satisfied, $d \geq 2$, and definitions (13), (15) hold. Then we have the following formulas:*

$$\begin{aligned} f^+(k,\omega) &= \frac{1}{D}\Big((e^{i(k\cdot y - \mu(\omega,E)|y|)} a(x,k) - e^{i(k\cdot x - \mu(\omega,E)|x|)} a(y,k)) + O(|x|^{-\sigma}) \Big) \\ &\quad \textit{as } s \to +\infty, \\ D &= 2i \sin\left(k\cdot\zeta + \mu(\omega,E)(|x| - |y|)\right), \\ &\quad \sigma = 1/2 \textit{ for } d = 2, \quad \sigma = 1 \textit{ for } d \geq 3, \end{aligned} \tag{20}$$

where $k \in \Gamma(E)$, $\omega \in S^{d-1}$, $a(x,k)$ is defined by (17), and x, y, ζ, s are as in (18).

We consider (20) assuming that $D \neq 0$. In addition, we use the following formula:

$$\begin{aligned} D &= 2i \sin\left((k - \mu(\omega,E)\hat{x})\cdot\zeta + O(|x|^{-1})\right) \\ &= 2i \sin\left((k - \mu(\omega,E)\omega)\cdot\zeta + O(s^{-1})\right) \text{ as } s \to +\infty, \end{aligned} \tag{21}$$

uniformly in ω for fixed ζ, where $\hat{x} = x/|x|$.

For fixed k and ζ, in view of formula (21), formula (20) can be used for finding f^+ under the condition that $\omega \in S^{d-1} \setminus \mathcal{E}_{k,\zeta}$ with

$$\mathcal{E}_{k,\zeta} = \{\omega \in S^{d-1} : (k - \mu(\omega,E)\omega)\cdot\zeta = 0 \pmod{\pi}\}. \tag{22}$$

In addition,

$$\mathrm{Meas}\ \mathcal{E}_{k,\zeta} = 0 \text{ in } S^{d-1}, \tag{23}$$

at least under assumption (12).

Theorem 2.1 and formulas (21) and (23) are proved in Section 3.

Remark 2.2 *In many respects, Theorem 2.1 is similar to Theorem 3.1 in [32] given for the continuous case. However, in Theorem 2.1, the direction $\hat{y}$ is typically different from $\hat{x}$ in view of definitions (18), although, asymptotically these directions become equal to ω, as $s \to +\infty$. We recall that $\hat{y} = \hat{x}$ in Theorem 3.1 in [32].*

Remark 2.3 *Formulas (20)–(23) can be also considered for the continuous case, assuming (16) and assuming that $\zeta \in \mathbb{R}^d \setminus \{0\}$ in (18). These formulas are new for the continuous case if $\hat{\zeta} \neq \hat{x}$.*

Note that, for $d = 1$,

$$\Gamma(E) = \{-\arccos\frac{E}{2}, \arccos\frac{E}{2}\}, \quad \mu(E) = \arccos\frac{E}{2}, \tag{24}$$

where $\arccos(\kappa) \in [0, \pi]$ for $\kappa \in [-1, 1]$. In this case, we consider $\Gamma(E)$ to be symmetric with respect to the origin in $\mathbb{R}$ even for negative E inspite of Remark 1.1.

In dimension $d = 1$, we have, in particular, the following propositions.

Proposition 2.4 *Suppose that assumption (3) holds, $|E| < 2, d = 1$, and $k = \arccos(E/2)$. Let $x, y \in (\mathbb{Z} \setminus \mathcal{D}) \cap \mathbb{R}^-, x \neq y \mod (\pi/(2k))$. Then*

$$\begin{aligned} s_{21} &:= f^+(k, -1) \\ &= \frac{1}{D}\Big(e^{2iky}a(x, k) - e^{2ikx}a(y, k) + |s_{21}|^2(e^{2ikx} - e^{2iky})\Big), \\ D &= 2i\sin(2k(y - x)). \end{aligned} \tag{25}$$

Proposition 2.5 *Suppose that assumption (3) holds, $|E| < 2, d = 1$, and $k = \arccos(E/2)$. Let $x_1, x_2, x_3 \in (\mathbb{Z} \setminus \mathcal{D}) \cap \mathbb{R}^-$, and $x_i \neq x_j \mod (\pi/k)$. Then*

$$\begin{aligned} s_{21} &= \frac{1}{D}\Big((e^{2ikx_3} - e^{2ikx_1})(a(x_2, k) - a(x_1, k)) \\ &\qquad + (e^{2ikx_1} - e^{2ikx_2})(a(x_3, k) - a(x_1, k))\Big), \\ D &= 16i(\sin(k(x_2 - x_3))\sin(k(x_2 - x_1))\sin(k(x_1 - x_3))). \end{aligned} \tag{26}$$

In these propositions, $a(x, k)$ is defined by (17) for $d = 1$.

Propositions 2.4 and 2.5 are proved in Section 4.

Formulas similar to (25), (26) can be also given for $s_{12} := f^+(k, 1)$, where $k = -\arccos(E/2)$.

Remark 2.6 *In fact, propositions 2.4 and 2.5 are completely similar to theorems 2.1 and 2.2 in the arXiv preprint of [33] given for the continuous case.*

Remark 2.7 *A natural open question concerns finding analogues of Theorem 2.1 in the case when the condition (12) is not fulfilled, i.e. when $|E| < 2d - 4$. The generalization of asymptotic formula (14), in this case, is given in [22] and involves several scattered waves with different scattering amplitudes. We expect that, for approximately finding these scattering amplitudes, $|\psi^+(x, k)|^2$ should be measured at several points x and not just two points as in Theorem 2.1.*

Remark 2.8 *To our knowledge, open question also includes establishing the full Atkinson-type expansion for function $\psi^+(x, k)$ even under conditions (3), (12). Proceeding from this full expansion, one could develop Theorem 2.1 in multi-points' style as, for example, in [45].*

Remark 2.9 *Open questions also include extending Theorem 2.1 and formulas (21), (23) to the case of Schrödinger operators on more complicated lattices, for example, as in [46].*

3. Proofs of Theorem 2.1 and formulas (21) and (23)

Due to (14), we have

$$|\psi^+|^2 = 1 + e^{-ik\cdot x}\frac{e^{+i\mu(\omega,E)|x|}}{|x|^{\frac{d-1}{2}}}f^+ + e^{+ik\cdot x}\frac{e^{-i\mu(\omega,E)|x|}}{|x|^{\frac{d-1}{2}}}\overline{f^+}$$
$$+ \frac{1}{|x|^{d-1}}\overline{f^+}f^+ + O\left(\frac{1}{|x|^{\frac{d+1}{2}}}\right) \quad \text{as } |x|\to\infty. \tag{27}$$

Using (17) and (27), we obtain

$$e^{-ik\cdot x}e^{+i\mu(\omega,E)|x|}f^+(k,\omega) + e^{+ik\cdot x}e^{-i\mu(\omega,E)|x|}\overline{f^+}(k,\omega) = a(x,k) + O(|x|^{-\sigma})$$
$$\text{as } |x|\to\infty, \tag{28}$$
$$e^{-ik\cdot y}e^{+i\mu(\omega,E)|y|}f^+(k,\omega) + e^{+ik\cdot y}e^{-i\mu(\omega,E)|y|}\overline{f^+}(k,\omega) = a(y,k) + O(|y|^{-\sigma})$$
$$\text{as } |y|\to\infty, \tag{29}$$

where x and y are defined by (18) and σ is as in (20). We consider (28) and (29) as a linear system for finding f^+ and $\overline{f^+}$, approximately, in terms of $a(x,k)$ and $a(y,k)$. As a result, we get (20), where D is the determinant of the 2×2 coefficient matrix.

In order to obtain formula (21), we use the definitions (18), the definition of D in (20), and the formulas

$$|y| = |x+\zeta| = \sqrt{|x|^2 + 2x\cdot\zeta + |\zeta|^2}$$
$$= |x| + \hat{x}\cdot\zeta + O(|x|^{-1}) \text{ as } |x|\to\infty, \tag{30}$$
$$\hat{x} = \omega + O(s^{-1}) \text{ as } s\to+\infty. \tag{31}$$

Under assumption (12), formula (23) follows from the statements:
(i) The function $\alpha(\omega) := (k - \mu(\omega,E)\omega)\cdot\zeta$ is real-analytic in $\omega\in S^{d-1}$ for fixed k and ζ.
(ii) $\alpha(\omega)$ is not identically constant.
(iii) Meas $\mathcal{E} = 0$ in S^{d-1} if $\mathcal{E}$ is the set of zeroes of a non-zero real-analytic function u on S^{d-1}.

Statement (i) follows from definition of μ by (15) and the real-analyticity of γ in formula (13). The latter analyticity of γ follows from analyticity, strict convexity, and non-zero principal curvatures of $\Gamma(E)$. Alternatively, one can use explicit formulas, relating ω and γ, mentioned in the Proof of Lemma 3 in [22] (where γ is denoted as k and E is denoted as λ).

Statement (ii) follows from the property that $\mu(\omega,E)\omega\cdot\zeta$ is not identically constant, for example, it is not identically zero but the set of its zeroes is non-empty in S^{d-1}. The latter property follows from the observation that $\mu(\omega,E)$ has no zeroes in view of strict convexity of $\Gamma(E)$, whereas $\omega \cdot \zeta$ is not identically zero on S^{d-1} but the set of its zeros is non-empty.

Statements of type statement (iii) are well-known in analysis; see, for example, [47] and references therein.

Actually, formula (22) follows from statement (iii) used for $u = \alpha - n\pi$ for several integer n.

4. Proofs of Propositions 2.4 and 2.5

Due to (14), with $O\left(|x|^{-\frac{d+1}{2}}\right) \equiv 0$ for $d = 1$, we have

$$s_{21}e^{-2ikx} + \overline{s_{21}}e^{2ikx} + |s_{21}|^2 = a(x,k). \tag{32}$$

To prove Proposition 2.4, we use (32) and also (32) with x replaced by y, i.e.,

$$s_{21}e^{-2iky} + \overline{s_{21}}e^{2iky} + |s_{21}|^2 = a(y,k). \tag{33}$$

As a result we consider (32) and (33) as a linear system for finding s_{21} and $\overline{s_{21}}$ from $a(x,k) - |s_{21}|^2$ and $a(y,k) - |s_{21}|^2$. Solving this system, we get formula (25).

To prove Proposition 2.5, we consider formula (32) with $x = x_1, x_2, x_3$. Subtracting equality (32) for $x = x_1$ from equality (32) for $x = x_2$ and from equality (32) for $x = x_3$, we obtain the system

$$s_{21}(e^{-2ikx_2} - e^{-2ikx_1}) + \overline{s_{21}}(e^{2ikx_2} - e^{2ikx_1}) = a(x_2,k) - a(x_1,k), \tag{34}$$

$$s_{21}(e^{-2ikx_3} - e^{-2ikx_1}) + \overline{s_{21}}(e^{2ikx_3} - e^{2ikx_1}) = a(x_3,k) - a(x_1,k), \tag{35}$$

for finding s_{21} and $\overline{s_{21}}$. One can see that

$$D = 2i\Big(\sin(2k(x_3 - x_2)) + \sin(2k(x_2 - x_1)) + \sin(2k(x_1 - x_3))\Big), \tag{36}$$

where D is the determinant of the system (34), (35). This determinant can be also re-written in the form of D in (26); see (3.7) in the arXiv preprint of [33]. Solving (34), (35) we get formula (26). Due to our assumption that $x_i \neq x_j$ mod (π/k), we have that $D \neq 0$ in (26).

Acknowledgments

This work was started during the stay (in May 2023) of both authors at the Isaac Newton Institute (INI) for Mathematical Sciences, Cambridge. The authors would like to thank INI for support and hospitality during the programmes – 'Mathematical theory and applications of multiple wave scattering' (MWS) and 'Rich and Nonlinear Tomography - a multidisciplinary approach' (RNT) – where work on this paper was undertaken. This work was supported by EPSRC grant no EP/R014604/1. A part of the work of BLS, for the same visit to INI during January-June 2023 and participation in MWS, was partially supported by a grant from the Simons Foundation.

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