

Hidden symmetries of electronic transport in a disordered one-dimensional lattice

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Correlated, or extended, impurities play an important role in the transport properties of dirty metals. Here, we examine, in the framework of a tight-binding lattice, the transmission of a single electron through an array of correlated impurities. In particular we show that particles transmit through an impurity array in identical fashion, regardless of the direction of traversal. The demonstration of this fact is straightforward in the continuum limit, but requires a detailed proof for the discrete lattice. We also briefly demonstrate and discuss the time evolution of these scattering states, to delineate regions (in time and space) where the aforementioned symmetry is violated.

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I. INTRODUCTION

In a one-dimensional lattice, correlated impurities or defects may give rise to extended electronic states for particular energy levels.¹⁻³ Various disordered systems with correlation have been investigated, such as the random dimer,^{1,3} the random trimer,⁴ nonsymmetric dimers,⁵ the random trimer-dimer,⁶ the Thue-Morse lattice,⁷ the random polymer chain,⁸ the Fibonacci chain,^{9,10} and other systems.¹¹⁻¹³

A built-in internal structure of the impurity configuration is important^{1,3} even if an internal symmetry is not necessary.⁵ In the context of electronic transport, the transmission resonance for a certain energy value implies the disordered system behaves like an ordered lattice for the corresponding electronic state, which is extended throughout the entire lattice. In this respect, it is possible to understand the increase in the conductivity for a conducting polymer² and to apply to a quasiperiodic chain.¹⁴

One may, in fact, envision many other impurity configurations that give rise to extended states for various energy values. For example, let us consider a pair of impurities with a potential V with respect to the lattice potential (taken to be zero). We assume that the spacing between the two impurities is always $n_d a$, where a is the lattice constant and n_d is a positive integer. This is then a “dimer,” whose length can be any value. If we adopt a tight-binding model, so that energies are given by $E = -2t_0 \cos(ka)$, where t_0 is the nearest-neighbor hopping amplitude, then one can obtain the transmission probability $|T|^2$ for this state. It is

$$|T|^2 = \frac{\sin^2(k)}{\sin^2(k) + V^2 \left[\cos(kn_d) + \frac{V \sin(kn_d)}{2 \sin(k)} \right]^2}. \quad (1)$$

where t_0 and a have been set to unity for simplicity. Inspection of Eq. (1) reveals a critical strength of the impurity potential $V_c/t_0 = \pm 2/n_d$ for repulsive and attractive interactions, respectively, which determines how many states are extended, i.e., have unit transmission. A graphical construction readily shows that, for $V > 2/n_d$, there are $n_d - 1$ extended states while for $V \leq 2/n_d$, there are n_d extended states.

As in the nearest-neighbor dimer case, consideration of one dimer helps us to understand electronic transport in a lattice with many dimers, following the analysis of Ref. 1. In Fig. 1, we show $|T|^2$ as a function of E for randomly distributed 50 impurity dimers (blue) and 500 dimers (green) in comparison with a single dimer (red). The inner spacing of a pair $n_d = 3$ and the potential $V = 1/2$. Note that in this instance $V < V_c = 2/3$. The transmission probability is calculated to be an ensemble average over 50 impurity configurations. Remarkably, the transmission remains unity at the three energies for which a single dimer has unit transmission, and the “width” of the resonance narrows as the number of impurities increases.

This specific example is given by way of introduction to more general considerations of impurity potentials on a lat-

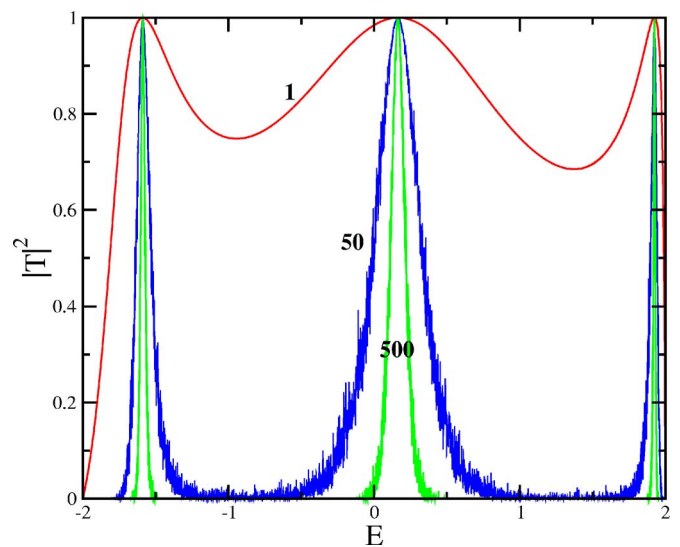


FIG. 1. (Color online) Transmission probability as a function of E for randomly distributed 50 impurity dimers (blue) and 500 dimers (green) in comparison with a single dimer (red). The inner spacing of a pair $n_d = 3$ and the potential $V = 1/2$ while the critical value $V_0 = 2/3$. The transmission probability is calculated as an ensemble average over 50 impurity configurations.

tice. In this paper we will show there exist hidden symmetries underlying the physics of electronic transport in a one-dimensional lattice with an arbitrary impurity configuration, using the transfer matrix formalism. We will also demonstrate the time evolution of a wave packet by direct diagonalization of the Hamiltonian since the transfer matrix formalism does not produce the dynamics of a wave function. While the dynamics can be insightful, we are also hopeful that present-day technology can spatially and temporally resolve some of the interesting dynamics that result from our (and future) work.

Perhaps the most general correlated impurity configuration is the following. Suppose there are N impurities $A_1 A_2 \cdots A_N$ embedded at the sites 1 through N in a host lattice. The corresponding impurity potentials are given by (U_1, U_2, \dots, U_N) , where $U_i (i=1, \dots, N)$ can be positive, zero, or negative. Our main result is that the transmission amplitude T for this impurity configuration is identical to T for its reverse configuration; namely, $T(U_1, U_2, \dots, U_N) = T(U_N, U_{N-1}, \dots, U_1)$. Given this then obviously the equality holds for the transmission $|T|^2$ and reflection $|R|^2$ probabilities. In other words, $|T|^2$ and $|R|^2$ are independent of the direction of the incoming wave. This symmetry is striking because the impurity configuration is assumed arbitrary without possessing any parity. For example, it has been shown that the chains of ABBABAAB \cdots and BAABABBA \cdots contribute identically for electronic transport.⁷ This is a simple example of the general symmetry we describe. Note that an exchange of any two impurity potentials does not show this symmetry; for example, $T(U_1, U_2, U_3, U_4) \neq T(U_2, U_1, U_3, U_4)$.¹⁵

We should emphasize now that this symmetry does *not* hold in the impurity region (as perhaps one would expect), but this can only be determined by solving the time-dependent Schrödinger equation (see below). We also explain another symmetry associated with a particular momentum $k = \pi/(2a)$, where a is the lattice constant: $|T(U_1, U_2, \dots, U_N)|^2 = |T(-U_1, -U_2, \dots, -U_N)|^2$. This equality indicates a potential barrier or well produces identical transmission and reflection probabilities for the electronic state with $k = \pi/(2a)$. This is unrelated to the other remarkable feature of wave packets on a one-dimensional lattice with nearest-neighbor hopping and $k = \pi/(2a)$: They do not diffuse as a function of time, because they lack group velocity dispersion. One can show that no matter what the range of the hopping is, there will be a wave vector for which the wave packet retains its initial width. In fact, this symmetry is a particular example of a general case; $|T(U_1, U_2, \dots, U_N)|^2$ with E is identical to $|T(-U_1, -U_2, \dots, -U_N)|^2$ with $-E$.

II. FORMALISM

We start with a tight-binding Hamiltonian for a one-dimensional lattice with N impurities:

$$H = -t_0 \sum_i [c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i] + \sum_{i \in \mathcal{I}} U_i c_i^\dagger c_i \quad (2)$$

where the hopping amplitude t_0 will be set to be unity, c_i^\dagger creates an electron at a site i , and \mathcal{I} represents an impurity

configuration. The Schrödinger equation is $H|\psi\rangle = E|\psi\rangle$ with $|\psi\rangle = \sum_j \psi_j c_j^\dagger |0\rangle$; this becomes

$$-[\psi_{j+1} + \psi_{j-1}] + U_j \psi_j = E \psi_j \quad (3)$$

where ψ_j is an amplitude to find an electron at site j . In order to use the transfer matrix formalism we write Eq. (3) in a matrix form as follows:

$$\begin{pmatrix} \psi_{j+1} \\ \psi_j \end{pmatrix} = \begin{pmatrix} U_j - E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_j \\ \psi_{j-1} \end{pmatrix} \equiv M_j \begin{pmatrix} \psi_j \\ \psi_{j-1} \end{pmatrix}. \quad (4)$$

Note that M_i is a unimodular matrix, i.e., $\det(M_i) = 1$. The wave functions ψ_L (for $i < 1$) and ψ_R (for $i > N$) are $\psi_L = e^{ikx_i} + R e^{-ikx_i}$ and $\psi_R = T e^{ikx_i}$, where $x_i = a \cdot i$. Using the transfer matrix formalism, one can express the coefficients R and T in terms of k , U_i , and E as follows:

$$\begin{pmatrix} T \\ iT \end{pmatrix} = P \begin{pmatrix} 1 + R \\ i(1 - R) \end{pmatrix}, \quad (5)$$

where $P = S^{-1} M S$ with $S = \begin{pmatrix} \cos(k) & \sin(k) \\ 1 & 0 \end{pmatrix}$, and $M = M_N M_{N-1} \cdots M_1$. It is misleading to express $M = \prod_{i=1}^N M_i$ because M_i and $M_j (i \neq j)$ do not commute with each other. Solving Eq. (5), one can obtain¹⁶

$$T = \frac{2i}{i(P_{11} + P_{22}) + P_{12} - P_{21}} \quad (6)$$

$$R = \frac{P_{12} + P_{21} - i(P_{11} - P_{22})}{i(P_{11} + P_{22}) + P_{12} - P_{21}}. \quad (7)$$

Consequently, the transmission probability $|T|^2 = 4 / [\text{tr}(P\tilde{P}) + 2]$ and the reflection probability $|R|^2 = [\text{tr}(P\tilde{P}) - 2] / [\text{tr}(P\tilde{P}) + 2]$, where $\text{tr}(P)$ means the trace of P , and \tilde{P} is the transpose of P . Note that Eq. (1) is readily obtained with this formalism by using $M' = M_V M_0^{n_d-1} M_V$, where $M_V = M_1 (U_1 = V)$ and $M_0 = M_1 (U_1 = 0)$, and n_d is the inner spacing of the impurity pair.

One of the symmetries we introduced earlier is $T(U_1, U_2, \dots, U_N) = T(U_N, U_{N-1}, \dots, U_1)$. In order to show this equality, let us introduce $Q = S^{-1} M' S$ where $M' = M_1 M_2 \cdots M_N$. Notice the order of the matrix multiplication because M_i and $M_j (i \neq j)$ do not commute with each other. Since the desired equality implies that $T[P] = T[Q]$, we need to show $P_{11} + P_{22} = Q_{11} + Q_{22}$ and $P_{12} - P_{21} = Q_{12} - Q_{21}$. On the other hand, from the definitions of $P = S^{-1} M S$ and $Q = S^{-1} M' S$, this equality in turn implies that $M_{11} = M'_{11}$, $M_{22} = M'_{22}$, and $M_{12} - M_{21} = M'_{12} - M'_{21}$. Note, however, that in general $M \neq M'$, as we will show later.

For simplicity, we define $U_i = U_i - E$. We also introduce 2×2 matrices α and β such as $\alpha = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ to have $M_i = U_i \alpha + \beta$. Note that $\alpha^2 = \alpha$, $\beta^2 = -1$, $\alpha\beta + \beta\alpha = \beta$, and $\alpha\beta\alpha = 0$. Since $M = M_N M_{N-1} \cdots M_1$, we obtain

$$M = (\mathcal{U}_N \alpha + \beta)(\mathcal{U}_{N-1} \alpha + \beta) \cdots (\mathcal{U}_1 \alpha + \beta) = \beta^N + \sum_n \sum_{\{j_n\}} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) \beta^{N-j_n} \alpha \beta^{j_n-j_{n-1}-1} \alpha \cdots \alpha \beta^{j_2-j_1-1} \alpha \beta^{j_1-1}, \quad (8)$$

where $\{j_n\}$ means $j_1, j_2, \dots, j_n = 1, 2, \dots, N$ with $j_1 < j_2 < \dots < j_n$. Since $\alpha\beta\alpha=0$ and $\beta^2=-1$, nonvanishing terms should have $j_l - j_{l-1} - 1 = \text{even}$, where $l=2, 3, \dots, n$ for a given n . Therefore, we obtain

$$M = \beta^N + \sum_n \sum_{\{j_n\}} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(j_n-j_1-n+1)} \beta^{N-j_n} \alpha \beta^{j_1-1}, \quad (9)$$

where $\{\{j_n\}\}$ means $\{j_n\}$ with $j_l - j_{l-1} - 1 = \text{even}$. Since $\alpha = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $\alpha\beta = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}$, $\beta\alpha = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, and $\beta\alpha\beta = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}$, we use these as the basis matrices to expand M :

$$M = c_1 \alpha + c_2 \alpha \beta + c_3 \beta \alpha + c_4 \beta \alpha \beta = \begin{pmatrix} c_1 & -c_2 \\ c_3 & -c_4 \end{pmatrix}. \quad (10)$$

As we mentioned, the equality of the transmission amplitude, $T[P]=T[Q]$, is associated with some particular relations among the components of the two matrices $M = M_1 M_2 \cdots M_N$ and $M' = M_N M_{N-1} \cdots M_1$. Following the same way as for M , we expand M' in terms of $\mathcal{U}_i (i=1, 2, \dots, N)$, α , and β to obtain

$$M' = (\mathcal{U}_1 \alpha + \beta)(\mathcal{U}_2 \alpha + \beta) \cdots (\mathcal{U}_N \alpha + \beta) = \beta^N + \sum_n \sum_{\{j_n\}} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) \beta^{j_1-1} \alpha \beta^{j_2-j_1-1} \alpha \cdots \alpha \beta^{j_n-j_{n-1}-1} \times \alpha \beta^{N-j_n}. \quad (11)$$

It is also true for M' that non-vanishing terms have $j_l - j_{l-1} - 1 = \text{even}$ because $\alpha\beta\alpha=0$. Therefore,

$$M' = \beta^N + \sum_n \sum_{\{j_n\}} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) \times (-1)^{1/2(j_n-j_1-n+1)} \beta^{j_1-1} \alpha \beta^{N-j_n}. \quad (12)$$

Expanding M' , again, in terms of the basis matrices, we know

$$M' = c'_1 \alpha + c'_2 \alpha \beta + c'_3 \beta \alpha + c'_4 \beta \alpha \beta = \begin{pmatrix} c'_1 & -c'_2 \\ c'_3 & -c'_4 \end{pmatrix}. \quad (13)$$

Comparing Eqs. (10) and (13), the equalities $M_{11}=M'_{11}$, $M_{22}=M'_{22}$, and $M_{12}-M_{21}=M'_{12}-M'_{21}$ are equivalent to the equalities $c_1=c'_1$, $c_4=c'_4$, and $c_2+c_3=c'_2+c'_3$. Since β^N does not depend on \mathcal{U}_i and $\beta^N = (-1)^{N/2}$ or $(-1)^{(N-1)/2} \beta$ for even (or odd) N , we can ignore β^N for the purpose of showing these equalities, or, alternatively, we can redefine M as $M - \beta^N$ and M' as $M' - \beta^N$. To obtain (i) c_1 of M , we should have $j_1 - 1 = \text{even}$ and $N - j_n = \text{even}$. Similarly, (ii) for c_2 , $j_1 - 1 = \text{odd}$ and $N - j_n = \text{even}$, (iii) for c_3 , $j_1 - 1 = \text{even}$ and $N - j_n = \text{odd}$, and (iv) for c_4 , $j_1 - 1 = \text{odd}$ and $N - j_n = \text{odd}$. In terms of \mathcal{U}_i , we obtain

$$c_1 = \sum_n \sum_{\{j_n\}_1} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n)}$$

$$c_2 = \sum_n \sum_{\{j_n\}_2} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n-1)}$$

$$c_3 = \sum_n \sum_{\{j_n\}_3} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n-1)}$$

$$c_4 = \sum_n \sum_{\{j_n\}_4} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n-2)}$$

where $\{\{j_n\}\}_1$ means $\{\{j_n\}\}$ with $(j_1 - 1, N - j_n) = (\text{even}, \text{even})$. Similarly, $\{\{j_n\}\}_2 = \{\{j_n\}\}$ with (odd, even), $\{\{j_n\}\}_3 = \{\{j_n\}\}$ with (even, odd), and $\{\{j_n\}\}_4 = \{\{j_n\}\}$ with (odd, odd).

For c'_1 , c'_2 , c'_3 , and c'_4 of Eq. (13), we should have $(j_1 - 1, N - j_n) = (\text{even}, \text{even})$, (even, odd), (odd, even), and (odd, odd), respectively. Note that we need (even, odd) for c'_2 while (odd, even) for c_2 . On the other hand, we need (odd, even) for c'_3 while (even, odd) for c_3 . Therefore, we obtain

$$c'_1 = \sum_n \sum_{\{j_n\}_1} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n)}$$

$$c'_2 = \sum_n \sum_{\{j_n\}_3} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n-1)}$$

$$c'_3 = \sum_n \sum_{\{j_n\}_2} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n-1)}$$

$$c'_4 = \sum_n \sum_{\{j_n\}_4} (\mathcal{U}_{j_1} \mathcal{U}_{j_2} \cdots \mathcal{U}_{j_n}) (-1)^{1/2(N-n-2)}$$

Consequently, we have $c_1=c'_1$, $c_4=c'_4$, and $c_2+c_3=c'_2+c'_3$; in other words, $T[P]=T[Q]$, or equivalently, $T(U_1, U_2, \dots, U_N) = T(U_N, U_{N-1}, \dots, U_1)$. In fact, $M_{12} = -M'_{21}$ and $M_{21} = -M'_{12}$. Note, however, that in general $M \neq M'$.

One may anticipate a similar symmetry in the continuum limit.¹⁷ Consider a time-dependent Schrödinger equation: $i\partial_t \psi(t, x) = H(x) \psi(t, x)$, where the Hamiltonian $H(x)$ includes an impurity potential $V(x)$ for $|x| \leq l$. The wave function for $|x| > l$ can be represented as $\psi(|x| > l) = [e^{ikx} + R e^{-ikx}] \Theta(-x - l) + T e^{ikx} \Theta(x - l)$, where $\Theta(x)$ is the step function. Let us introduce another time-dependent Schrödinger equation: $i\partial_t \psi'(t, x) = H(-x) \psi'(t, x)$, where $\psi(|x| > l) = [e^{ikx} + R' e^{-ikx}] \times \Theta(-x - l) + T' e^{ikx} \Theta(x - l)$. Invoking both space inversion and time reversal, one can see that $\psi(t, -x)$ and $\psi^*(-t, -x)$ satisfy the same equation as $\psi'(t, x)$ does. Equating $a_1 \psi(t, -x) + a_2 \psi^*(-t, -x) = \psi'(t, x)$ for $|x| > l$ leads to $T' = T$ and $R' T^* + R^* T = 0$. The first relation corresponds to $T[P] = T[Q]$ in a lattice. The second relation, however, does not hold in a lattice. Instead, we found in a lattice

$$\frac{T^*[P](R[Q] - R[P])}{T[P](R^*[Q] - R^*[P])} = e^{2ik}. \quad (14)$$

Nevertheless, we can still define $R[Q] = e^{i\delta}R[P]$. The phase δ is determined by $e^{i\delta} = -e^{2ik}R^*T/(RT^*)$ in a lattice while $e^{i\delta} = -R^*T/(RT^*)$ in the continuum limit.

We also found another symmetry associated with electronic transport in a one-dimensional lattice; in this case there is no applicability in the continuum limit. Suppose $k = \pi/2$; then $S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and $S = \tilde{S} = S^{-1}$. Note that for a symmetric (2×2) matrix X such that $X = \tilde{X}$, M_i satisfies $M_i X \tilde{M}_i = \tilde{M}_i X M_i$ with $U_i \rightarrow -U_i$. Now let us consider $\text{tr}(P\tilde{P})$:

$$\begin{aligned} \text{tr}(P\tilde{P}) &= \text{tr}(M_N \cdots M_1 \tilde{M}_1 \cdots \tilde{M}_N) \\ &= \text{tr}(\tilde{M}_N \cdots \tilde{M}_1 M_1 \cdots M_N)_{U \rightarrow -U} = \text{tr}(\tilde{Q}Q)_{-U} = \text{tr}(Q\tilde{Q})_{-U} \end{aligned} \quad (15)$$

This symmetry indicates that for $k = \pi/2$, $|T|^2$ and $|R|^2$ depend only on $|U_i|$. If $E = -2 \cos(k)$, then $U_i = U_i$. In this instance, $|T(U_1, \dots, U_N)|^2 = |T(-U_N, \dots, -U_1)|^2$. Since $|T(U_1, \dots, U_N)|^2 = |T(U_N, \dots, U_1)|^2$ from a general derivation, $|T(U_1, \dots, U_N)|^2 = |T(-U_1, \dots, -U_N)|^2$. Consequently, a potential barrier and a potential well give identical transmission and reflection probabilities for $k = \pi/2$ and $E = -2 \cos(k)$. In fact we found a general symmetry to which this case belongs as an example. Since $\cos(k) = -E/2$ and $\sin(k) = \sqrt{1 - E^2/4}$ for $0 \leq k \leq \pi$, one can show that $S(E)\tilde{S}(E) = (1 - E^2/4)\tilde{S}^{-1}(-E)S^{-1}(-E)$ and $S(-E)\tilde{S}(-E) = (1 - E^2/4)\tilde{S}^{-1}(E)S^{-1}(E)$. Then, a similar procedure will show that $|T(U_1, \dots, U_N)|^2$ with E is identical to $|T(U_1, \dots, U_N)|^2 = |T(-U_1, \dots, -U_N)|^2$ with $-E$.

III. TIME EVOLUTION OF A WAVE PACKET

So far we have been using the transfer matrix formalism. Since, however, the transfer matrix formalism is based on the time-independent Schrödinger equation, we cannot see the time evolution of a wave function, which may indicate the significance of the symmetries we have shown. Let us consider a wave packet with average position x_0 and average momentum k_0 at time $t=0$: $|\Psi(0)\rangle = \sum_i \varphi(x_i, 0) c_i^\dagger |0\rangle$, where

$$\varphi(x_i, 0) = \frac{1}{(2\pi\alpha^2)^{1/4}} e^{ik_0(x_i - x_0)} e^{-\frac{1}{4}(x_i - x_0)^2/\alpha^2}. \quad (16)$$

We introduced the initial uncertainty α associated with position. We wish to propagate (in real time) this wave packet towards the potentials. To do this we first diagonalize the Hamiltonian, which is an $(L \times L)$ matrix, where L is the total number of lattice sites under consideration. We thus obtain the eigenstates $|n\rangle$ and the corresponding eigenvalues ϵ_n such that $H|n\rangle = \epsilon_n|n\rangle$. An eigenstate is a column vector with L components which describes the probability of finding an electron at a particular site in the lattice. With eigenstates in hand, the time evolution of the wave packet is given by

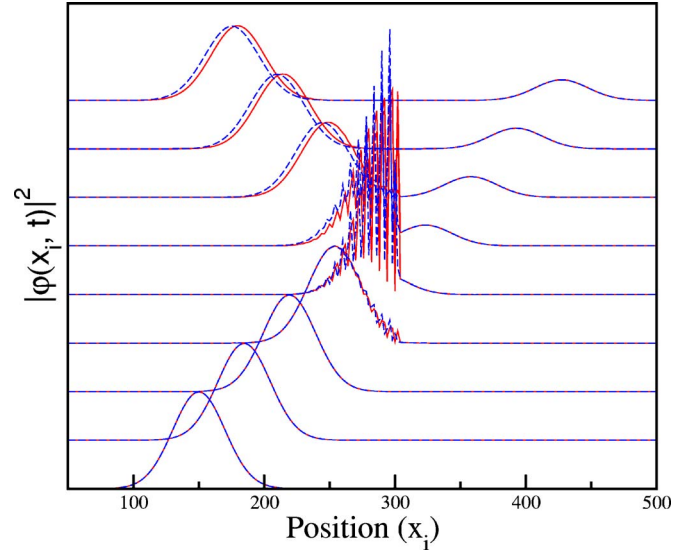


FIG. 2. (Color online) Time evolution of a wave packet in two impurity configurations [I] (red solid) and [II] (blue dashed curve). Each configuration has five impurities: For [I] the potential is $(-0.5, 0, 0.5, 1.5, 1)$ while for [II] its reverse holds.

$$|\Psi(t)\rangle = \sum_{n=1}^L |n\rangle \langle n | \Psi(0)\rangle e^{-i\epsilon_n t}. \quad (17)$$

As time goes on, the wave packet initially at x_0 moves to the potential region and scatters off the potential. A part of the wave packet is reflected and the other part is transmitted. Mathematically we can define the reflection and the transmission as $|R|^2 = \sum_{left} |\varphi(x_i, t)|^2$ and $|T|^2 = \sum_{right} |\varphi(x_i, t)|^2$, respectively, as $t \rightarrow \infty$, where $\sum_{left(right)}$ means the summation includes only the left(right) side of the impurity region.

Figure 2 shows the time evolution of a wave packet impinging on five impurities located at sites 300–304. The parameters of the wave packet are given as follows: $x_0 = 150$, $\alpha = 20$, and $k_0 = \pi/3$. Note we choose $\alpha = 20$ so that the size of the wave packet is much greater than the size of the impurity region. This means that we can consider the wave packet as a plane wave in this case. In fact, the numerical results of the transmission and reflection probabilities are in close agreement with those obtained through the transfer matrix analysis. The impurity configuration is determined by five impurity potentials: $(U_1, U_2, U_3, U_4, U_5)$. For [I] (red solid), we have $(-0.5, 0, 0.5, 1.5, 1)$ while for [II] (blue dashed curve), we have the reverse order. As clearly shown in Fig. 2, the time evolution of the wave packet is different depending on the impurity configurations. In particular, the scattering completely differentiates [I] from [II], as indicated by the very differently behaved red and blue curves in the scattering region. Nonetheless the probability that emerges (either in transmission or reflection) is identical for both, in agreement with the symmetry we just proved. Note that the transmitted wave packets are identical in all other respects as well whereas the reflected wave packets have identical shape, but are phase-shifted with respect to one another. In fact, one can show that the phase shift originates from the phase δ in

$R[Q]=e^{i\delta}R[P]$. The shift measured by the difference between the two reflected wave packets for [I] and [II] at their half width is determined by $\partial\delta(k)/\partial k|_{k_0}$.

IV. CONCLUSIONS

We have determined the transmission and reflection characteristics for various impurity configurations on a one dimensional lattice. In particular we proved that the transmission of a particle through an array of impurities is independent of the direction of travel. This theorem may help understand, among other things, weak localization, where time-reversed paths play an important role. Some important differences arise because of the lattice: First, it becomes clear that the group velocity is most important (in the continuum limit the energy is usually emphasized). Secondly, other symmetries exist on a lattice. As far as the transmission prob-

ability concerns, for a given impurity configuration with (U_i, E) there always exists an equivalent configuration with $(-U_i, -E)$. Naturally these symmetries do not hold in the actual scattering region. While we have no specific proposals at present, we hope this work motivates experimentalists to look for these violations in the vicinity of particular impurity configurations. Further work is in progress with trimer impurity configurations, more general band structures, and higher dimensionality.

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