Quantum Transport through a Fully Connected Network with Disorder

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Abstract

A matrix method is used to calculate the quantum transport of spinless electrons through a fully connected network with site disorder. The method calculates the transport probability from the time independent Schrödinger equation, for both the leads and a network in the tight binding approximation. The exact solution is a simple formula, and is derived without the use of Green’s functions. An exact solution is also given for the wavefunction on the network sites. A fully connected network with \( n \) sites may have up to \( n - 1 \) points where the transmission goes to zero within the physical range of energies.

Keywords: quantum transmission, Anderson localization

PACS: 72.10.Bg, 72.15.Rn

1. Introduction

One of the standard first problems solved in a quantum mechanics class is that of an incoming (spinless) particle scattering from a potential well in one dimension [1, 2]. The equation to solve is the time independent Schrödinger equation, \( \mathcal{H}|\Psi\rangle = E|\Psi\rangle \). Here \( \mathcal{H} \) is the Hamiltonian of the incoming particle, \( E \) is the energy of the particle, and \( |\Psi\rangle \) is the wavefunction. Let the particle come from \( x = -\infty \), scatter off a potential well located in the vicinity of \( x = 0 \), and be detected at \( x = \pm \infty \). The tight-binding analogue [3] of this scattering problem can be obtained by discretizing space [4, 5]. In the tight-binding analogue there are still an infinite number of discrete points, due to the incoming and outgoing leads. Therefore the time-independent Schrödinger equation to solve is

\[
\mathcal{H}_\infty \tilde{\Psi}_\infty - E \tilde{\Psi}_\infty = 0
\]

where the subscript \( \infty \) serves as a reminder that Eq. (1) is an infinite-dimensional matrix equation. In the tight-binding model every site has an on-site energy, which is taken to be zero in the incoming \( (x \ll 0) \) and in the outgoing \( (x \gg 0) \) lead sites. This sets the zero of energy in the problem. Every nearest-neighbor site has a hopping parameter, from the kinetic energy term of \( \mathcal{H} \), taken to have a magnitude of unity in both leads. This sets the unit for energy in the problem.

Once the tight-binding problem has been set up, any network can be attached to the incoming and outgoing leads and Eq. (1) solved. This is regardless of whether or not the network corresponds to a physically realizable network [6]. Although often the solution is given using a Green’s function method [4, 5], there is an alternative using only matrix algebra to solve Eq. (1) [7]. For scattering from physical lattices, the matrix method of [7] has been used to solve numerically disordered square lattices [8] and honeycomb lattices [9]. For scattering from non-physical lattices, the matrix method has been used to calculate the transport exactly for Bethe networks without disorder [10], Hanoi...
lattices [11], and fully connected lattices [12]. Further details of the matrix method can be found in the Ph.D. thesis of L. Solomon [13].

As Anderson pointed out more than a half century ago [14], disorder can lead to additional physically interesting consequences, such as localization [15, 16]. Unfortunately except for the one-dimensional case, exact solutions to the scattering problem with disorder are extremely difficult. In this paper we derive and present a simple closed-form solution to scattering from a fully connected network with on-site disorder.

2. Model and Method

Assume a fully connected network with \(n\) sites. For simplicity the fully connected network is called a blob. It is assumed that every site in the network has the same hopping energy \(-t_b\) to every other site. The negative sign is inserted so that \(t_b\) is positive after discretizing the Schrödinger equation. Furthermore assume that site \(j\) in the blob has an on-site energy given by \(\epsilon_0 + \epsilon_j\), where \(\epsilon_0\) is the same for all \(n\) sites but the \(\epsilon_j\) may be chosen randomly. Introduce the diagonal matrix \(D_e\) with elements

\[
\langle k | D_e | j \rangle = \delta_{kj} \epsilon_j,
\]

the identity matrix \(I\), a vector \(d\) which has all elements unity, and a matrix \(J\) that has all elements unity. Then the Hamiltonian for the blob of \(n\) sites is a \(n \times n\) matrix given by

\[
\mathcal{H}_n = (\epsilon_0 + t_b) I - t_b J + D_e.
\]

Note that \(J = d d^T\).

Eq. (1) can be reduced to a finite matrix equation [7, 13] of size \((n+2) \times (n+2)\). This is accomplished by making an ansatz for the wavefunctions in the leads. The finite equation to solve is

\[
\begin{pmatrix}
-E + e^{iq} & \bar{\psi}^T \\
\bar{\psi} & \mathcal{H}_n - E I \\
0 & -E + e^{iq}
\end{pmatrix}
\begin{pmatrix}
1 + r \\
\bar{\psi} \\
t_r
\end{pmatrix} =
\begin{pmatrix}
2i \sin(q) \\
0 \\
0
\end{pmatrix}.
\]

Here the wavevector \(q\) is given by \(E = e^{-iq} + e^{iq} = 2 \cos(q)\). The energy scale and zero of energy set in the leads means that the physical range for the energy is \(-2 \leq E \leq 2\). Note that \(\sin(q) = \sqrt{4 - E^2}/2\). In Eq. (4) the blob wavefunction is given by the \(n\)-dimensional vector \(\bar{\psi}\). The incoming lead is connected to the blob by the \(n\)-dimensional vector of hopping parameters \(\bar{\psi}\). Similarly, the outgoing lead is connected to the blob by the \(n\)-dimensional vector of hopping parameters \(u\). The transmission probability is given by

\[
T = |t_r|^2,
\]

where \(t_r\) is in general complex. Furthermore the reflection probability \(R = |r|^2\), and since all scattered particles must leave to \(x = \pm \infty\) one has \(R + T = 1\).

Rather than finding the inverse of the \((n+2) \times (n+2)\) matrix of Eq. (4), the solution can be reduced to finding the inverse of a \(n \times n\) matrix \(L^{-1}\) [10, 11, 13] defined by

\[
L^{-1} = \mathcal{H} - E I - S^* \bar{\psi} \bar{\psi}^T - S^* u u^T.
\]

Here \(S = -E + e^{iq}\), and \(S^{-1} = S^*\). In particular one has that the desired solution is

\[
\frac{1 + r}{\psi^T} = \frac{2i \sin(q)}{S^2}
\begin{pmatrix}
S + \bar{\psi}^T L \bar{\psi} \\
S L \bar{\psi} \\
-\bar{\psi}^T L \bar{\psi}
\end{pmatrix}.
\]

Thus to solve exactly the scattering problem requires that one be able to find the inverse of the symmetric (in general complex) matrix \(L^{-1}\) of Eq. (6).
Although we have derived expressions for other cases, here results are limited to the case where all \( n \) sites of the blob are connected to the input lead by the hopping parameter \(-t_w\) and are all equally connected to the output lead by the hopping parameter \(-t_u\). Explicitly

\[
\vec{w} = -t_w \vec{e} \quad \text{and} \quad \vec{u} = -t_u \vec{e}.
\]

(8)

Consider first the case of a fully connected blob without disorder. Then from Eq. (3) and Eq. (6) one has

\[
\mathcal{H}_n = (\epsilon_0 + t_b) I - t_b J \quad \text{and} \quad L^{-1} = (\epsilon_0 + t_b - E) I - \left( t_b + \frac{t_w^2}{S} + \frac{t_u^2}{S} \right) J.
\]

(9)

Use the properties \( I^2 = I, JJ = JJ, \) and \( J^2 = nJ \) to obtain the general form for the inverse matrix of \( X_I + X_J J \) is

\[
(X_I + X_J J) \left( \frac{1}{X_I} I + Y_J J \right) = I
\]

provided that

\[
Y_J = -\frac{X_J}{X_I (X_I + nX_J)}.
\]

(11)

\( X_I \neq 0, \) and \( X_I + nX_J \neq 0. \) Simplifying results of Eq. (10) on Eq. (9) gives the transmission probability for the pure case

\[
T_{\text{Pure}} = |\tau_T|^2 = \frac{\left( \frac{4 - E^2}{4} \right) t_w^2 t_u^2}{\left( \frac{\epsilon_0 - E - t_b}{n} - t_b + \frac{E}{2} \left( t_w^2 + t_u^2 \right) \right)^2 + \left( \frac{4 - E^2}{4} \right) \left( t_w^2 + t_u^2 \right)^2}.
\]

(12)

Figure 1(a) shows graphically how \( T_{\text{Pure}} \) depends on the energy \( E \) for different numbers of sites \( n \) in the blob without disorder. The results are identical to the solution in reference [12], but are derived here without using a renormalization-group approach. Fig. 1(a) illustrates that the \( n \rightarrow \infty \) limit is approached rather quickly. Note that as required physically \( T \) goes to zero if either \( t_w \) or \( t_u \) are zero, as these correspond to disconnecting either the input or the output lead from the blob.

Next concentrate on the case with on-site disorder in the blob. Consider a matrix of the form

\[
L^{-1} = \tilde{D} - bJ
\]

(13)

Figure 1: The transmission \( T \) is plotted as a function of the energy \( E \) of the incoming electron. The parameters used are \( \epsilon_0 = 1 \) with hopping parameters \( t_w = t_u = t_b = 1. \) (a) Illustrates how quickly with the blob size \( n \) the transmission approaches the \( n \rightarrow \infty \) limit. All curves have \( \epsilon_j = 0. \) (b) Shows the effects of random on-site disorder, here for \( n = 8. \) The zero-disorder curve \( T_{\text{Pure}} \) is shown in black. The other three curves are for different realizations of \( \epsilon_j, \) where in all cases the \( \epsilon_j \) are uniformly distributed in the interval \([-1, 1].\)
with $\tilde{D}$ a diagonal matrix, which here is explicitly $\tilde{D} = (\epsilon_0 + t_b - E) I + D_\epsilon$ with $D_\epsilon$ defined in Eq. (2). Here $b$ is whatever multiplies the matrix $J$ once $L^{-1}$ is constructed, and is explicitly $b = t_b + S^{-1} (t_w^2 + t_b^2)$. The inverse of the matrix of Eq. (13) is

$$L = \tilde{D}^{-1} + \frac{b}{1 - b \sigma} \tilde{D}^{-1} J \tilde{D}^{-1}$$

where $\sigma = \text{Tr}(\tilde{D}^{-1})$. In particular using the Hamiltonian of Eq. (3), introduce the sum

$$\sigma = \sum_{j=1}^{n} \frac{1}{\epsilon_0 + \epsilon_j - E + t_b} = \epsilon^T \left[ (\epsilon_0 - E + t_b) I + D_\epsilon \right]^{-1} \epsilon .$$

The transmission for the case of a $n$-site blob with on-site disorder is given by

$$T = \frac{(4 - E^2) \epsilon^T \epsilon}{\left( \frac{1}{2} - t_b + \frac{E}{2} (t_w^2 + t_b^2) \right)^2 + \left( \frac{4 - E^2}{2} \right) (t_w^2 + t_b^2)^2} .$$

Consider putting all $n$ terms in Eq. (15) over the common denominator and setting specific (real) values for $\epsilon_0$, $\{\epsilon_j\}$, $t_b$, $t_w$, and $t_b$. Then the numerator of $\sigma$ is a $(n - 1)$-order polynomial in $E$, which may have up to $n - 1$ distinct real solutions. Whenever the numerator of $\sigma$ is zero the denominator of Eq. (16) is infinite, and hence the transmission $T$ is zero. Of course the roots of the $(n - 1)$-order polynomial may be complex, repeated, or real but outside the physical range $-2 \leq E \leq 2$. Therefore $T$ will be zero at at most $n - 1$ values of $E$. Results for $n = 8$ are shown in Fig. 1(b). As $n$ increases the curves become even more complex, with $T$ rapidly falling between zero and values near unity. Thus the solution of the fully connected blob with disorder has the same type of transmission as does scattering from a physical network. The advantage is that the exact transmission has a simple functional form given by Eq. (16). With Eq. (7) the wavefunction on the blob sites is

$$\tilde{\psi} = -\frac{2 i t_w \sin(q)}{S - S \epsilon t_b - \sigma t_w^2 - \sigma t_b^2} \left[ (\epsilon_0 + t_b - E) I + D_\epsilon \right]^{-1} \epsilon$$

with $D_\epsilon$ defined in Eq. (2). Therefore the solution for the wavefunction also has a simple form given by Eq. (17).

3. Discussion and Conclusions

A compact exact expression for the transmission of (spinless) electrons through a fully connected network with random site disorder has been presented. The calculation uses only matrix algebra, for a matrix of size the number of sites in the fully connected network, $n$. The exact expression, Eq. (16), illustrates the effect of the disorder, namely the possible $n - 1$ rapid oscillations in the transmission $T$ between values of zero and values near unity. Further work to calculate exactly the transport through other disordered networks is underway.

Acknowledgements

This work is supported in part by NSF grant number DMR 1206233.