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Quantum Transport through a Fully Connected Network with Disorder

M.A. Novotny, L. Solomon, and G. Inkoom

Department of Physics and Astronomy and HPC^2 Center for Computational Sciences, Mississippi State University, Mississippi State, MS 39762-5167 U.S.A.

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.

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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

$$\mathcal{H}_\infty \vec{\Psi}_\infty - E\vec{\Psi}_\infty = \vec{0} \tag{1}$$

where the subscript ∞ 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

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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 ϵ_0 is the same for all n sites but the ϵ_j may be chosen randomly. Introduce the diagonal matrix $\mathbf{D}_\epsilon$ with elements

$$\langle k|\mathbf{D}_\epsilon|j\rangle = \delta_{kj}\epsilon_j \;, \tag{2}$$

the identity matrix $\mathbf{I}$, a vector $\vec{e}$ which has all elements unity, and a matrix $\mathbf{J}$ that has all elements unity. Then the Hamiltonian for the blob of n sites is a $n \times n$ matrix given by

$$\mathcal{H}_n = (\epsilon_0 + t_b)\,\mathbf{I} - t_b\mathbf{J} + \mathbf{D}_\epsilon \;. \tag{3}$$

Note that $\mathbf{J} = \vec{e}\,\vec{e}^{\mathrm{T}}$.

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

$$\begin{pmatrix} -E + e^{iq} & \vec{w}^{\mathrm{T}} & 0 \\ \vec{w} & \mathcal{H}_n - E\mathbf{I} & \vec{u} \\ 0 & \vec{u}^{\mathrm{T}} & -E + e^{iq} \end{pmatrix} \begin{pmatrix} 1 + r \\ \vec{\psi} \\ t_{\mathcal{T}} \end{pmatrix} = \begin{pmatrix} 2i\sin(q) \\ \vec{0} \\ 0 \end{pmatrix} . \tag{4}$$

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 $-2 \le E \le 2$. Note that $\sin(q) = \sqrt{4 - E^2}/2$. In Eq. (4) the blob wavefunction is given by the n-dimensional vector $\vec{\psi}$. The incoming lead is connected to the blob by the n-dimensional vector of hopping parameters $\vec{w}$. Similarly, the outgoing lead is connected to the blob by the n-dimensional vector of hopping parameters $\vec{u}$. The transmission probability is given by

$$\mathcal{T} = |t_{\mathcal{T}}|^2 \;, \tag{5}$$

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

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 $\mathbf{L}^{-1}$ [10, 11, 13] defined by

$$\mathbf{L}^{-1} = \mathcal{H} - E\mathbf{I} - S^*\vec{w}\vec{w}^{\mathrm{T}} - S^*\vec{u}\vec{u}^{\mathrm{T}} \;. \tag{6}$$

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

$$\begin{pmatrix} 1 + r \\ \vec{\psi} \\ t_{\mathcal{T}} \end{pmatrix} = \frac{2i\sin(q)}{S^2} \begin{pmatrix} S + \vec{w}^{\mathrm{T}}\mathbf{L}\vec{w} \\ -S\,\mathbf{L}\vec{w} \\ \vec{u}^{\mathrm{T}}\mathbf{L}\vec{w} \end{pmatrix} . \tag{7}$$

Thus to solve exactly the scattering problem requires that one be able to find the inverse of the symmetric (in general complex) matrix $\mathbf{L}^{-1}$ of Eq. (6).