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Electronic transport of a large scale system studied by renormalized transfer matrix method: Application to armchair graphene nanoribbons between quantum wires

Miao Gao, Gui-Ping Zhang*, Zhong-Yi Lu

Department of Physics, Renmin University of China, Beijing 100872, China

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ABSTRACT

Study on the electronic transport of a large scale two dimensional system by the transfer matrix method (TMM) based on the Schrödinger equation suffers from numerical instability. To address this problem, we propose a renormalized transfer matrix method (RTMM) by setting up a set of linear equations from U times of multiplication of traditional transfer matrix ($U = \frac{N}{S}$ with N and S respectively being the atom number of length and the transfer steps), and smaller S is required for a wider system. Then we solve the above linear equations by Gaussian elimination method and further optimize to reduce the computational complexity from $O(U^3M^3)$ to $O(UM^3)$, in which M is the atom number of the width. Applying the RTMM, we study transport properties of large scale pure and long-range correlated disordered armchair graphene nanoribbons (AGR) (carbon atoms up to 10^6 for pure cases) between quantum wire contacts. For a pure AGR, the conductance is superlinear with the Fermi energy, and linear with the width while independent of the length, showing characteristics of ballistic transport. For a disordered AGR with long-range correlation, there is a metal–insulator transition induced by the correlation strength of disorder. It is straightforward to extend the RTMM to investigate the electronic transports of large scale systems with various structures.

1. Introduction

Transfer matrix method (TMM) based on the Schrödinger equation is a widely used numerical approach to investigate the electronic transport, such as in disordered systems [1–3] or in the presence of electron–phonon interaction [4,5]. However, when the spacial dimension is higher than 1, the size of a system investigated by TMM is very limited due to the numerical instability [1]. This numerical instability originates from such an issue that the smallest eigen-mode in a considered system will be lost in computation when its ratio to the largest is less than the accuracy of our computer, represented by floating point numbers. Thus it more readily occurs for a wider two-dimensional system that has more eigen-modes and then larger difference between the smallest and largest eigen-modes [6,7], especially their ratio dramatically decreasing exponentially with n after n times recursive multiplication of the matrix transfer. To deal with such a numerical instability and realize a large scale calculation, a number of schemes have been proposed, for example, by introducing extra auxiliary parameters that are determined together with reflection coefficients [8], or by diagonalizing the transfer matrix of a conductor using eigenstates of leads [9]. So far these schemes only made certain improvement and cannot handle inhomogeneous systems yet.

In this article, we propose a renormalized transfer matrix method (RTMM) to calculate the conductance of a large system, meanwhile readily incorporating disorders and/or impurities. We sketch it as follows. Conventionally one recursively multiplies the transfer matrix in a scattering region from one lead side into the other lead side to directly resolve the reflection and transmission coefficients. Here we first divide the scattering region into U subregions, similar to the idea proposed in Ref. [10]. In all the subregions, we respectively take the recursive multiplications of the corresponding transfer matrices without the numerical instability, and then lump them into a set of linear equations containing the wavefunction values at all the interfaces between the subregions as the unknowns, among which the reflection and transmission coefficients are related to wavefunction values at the left and right lead-scattering interfaces respectively. We then solve this set of linear equations by using a modified Gaussian elimination method, which has been elaborately optimized by us to reduce the computational complexity from $O(U^3M^3)$ (M being the site number of the width) to $O(UM^3)$ loop executions so that a system with a million of lattice sites can be calculated on a standard desktop computer. For a wider system, clearly a larger U is required to avoid the numerical instability. We will illustrate the method by using it to study the electronic transport of graphene in this article.

* Corresponding author. Tel.: +86 1062517887.
E-mail addresses: bugubird_zhang@hotmail.com (G.-P. Zhang), zlu@ruc.edu.cn (Z.-Y. Lu).

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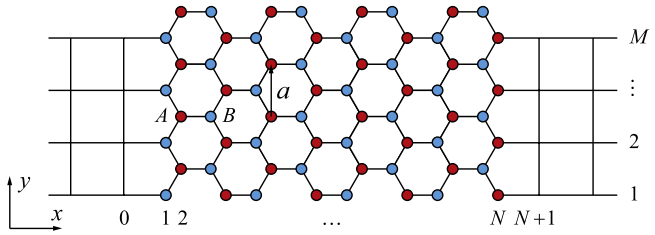

Fig. 1. (Color online) Schematic of armchair graphene ribbon (AGR) with N and M atoms in x and y direction, as connected to square-lattice leads simulating normal metal leads. Here the length of the samples are $(3N-4)\sqrt{3}a/12$ and the width $(M-1/2)a$, where a is the lattice parameter of graphene. Red and blue colors donate different sublattices A and B, respectively.

The discovery of graphene in 2004 [11], a single atomic layer of graphite with carbon atoms sitting at a honeycomb lattice, has aroused widespread interest both theoretically and experimentally, due to its distinctive electronic structure, whose low energy excitations can be interpreted in analogy to the massless Dirac relativistic fermion model, and its great potential on practical applications [12–14]. Among various graphene-based materials, armchair graphene nanoribbon (AGR) attracts intensive attention since there is an energy gap opened [15]. Here we choose AGR as a model system to study.

In most theoretical and numerical studies on the electronic transport of AGR, the leads were made of doped graphene [16,17], however, experimentally the leads were usually made of normal metals such as gold [11,12,18,19]. Similar to Ref. [20], here we employ two semi-infinite square lattice quantum wires as leads to simulate normal metal leads, as shown in Fig. 1. Actually we had previously calculated the transport properties of graphene nanoribbons between such quantum wire leads by the conventional transfer matrix method [21–24], which however would be better to be further examined by large scale graphene calculations, especially considering the effect of long-range correlated disorder and/or impurities that has an important impact on the formation of electron–hole puddles observed in graphene [25], as discussed in Ref. [24]. In addition, large scale system calculations are also required to determine whether or not the existence of Anderson localization [26] in low dimensional disordered system. Meanwhile, the renormalized transfer matrix method can be readily extended to investigate the electronic transports in large scale graphene systems with various structures.

In this article we mainly present the renormalized transfer matrix method. We organize the paper as follows. In Section 2, we present the renormalized transfer matrix method in conjugation with a tight binding model to describe graphene; in Section 3, we introduce optimized Gaussian elimination algorithm; in Section 4, we apply the renormalized transfer matrix scheme to investigate the transport properties of pure armchair graphene nanoribbons and long-range correlated disordered armchair graphene nanoribbons, respectively; and in Section 5, we make a summary.

2. Tight-binding model and renormalized transfer matrix method

Graphene takes a honeycomb lattice with two sites per unit cell, namely consisting of two sublattices A and B. The tight-binding Hamiltonian considering that π electrons hop between the nearest-neighbor atoms in graphene reads as follows,

$$H = -\sum_{\langle ij,i'j'\rangle} t_{ij,i'j'} C_{ij}^{\dagger} C_{i'j'} + \mu \sum_{ij} C_{ij}^{\dagger} C_{ij}, \tag{1}$$

whereas $C_{ij}^{\dagger}$ (C_{ij}) is the operator of creating (annihilating) one electron at a lattice site with site coordinates being x_i and y_j respectively, $\langle , \rangle$ denotes the nearest-neighbors, $t_{ij,i'j'}$ is the nearest-neighbor hopping integral, and μ is the chemical potential, i.e. the Fermi level, which can be adjusted by an effective gate voltage directly applied on the graphene ribbon.

Fig. 1 schematically shows an armchair-shaped graphene ribbon (AGR), connected with two semi-infinite square-lattice quantum wires described also by a tight binding Hamiltonian with only the nearest-neighbor hopping. There are N(length)$\times M$(width) lattice sites in the AGR. For simplicity, the nearest-neighbor hopping integral $t_{ij,i'j'}$ in the AGR sets to t_0, adopted as an energy unit in this article. We further assume the hopping integrals in both the left and right leads and the interface hopping integrals between the leads and AGR all being t_0. We use the natural open boundary condition in the calculations, which means that there are no longer dangling bonds along the boundaries, equivalent to the saturation by hydrogens in experiments.

For the Schrödinger equation $\hat{H}\psi(E) = E\psi(E)$ of the considered system (Fig. 1), any wavefunction $\psi(E)$ at a given energy E can be expressed by a linear combination of localized Wannier bases $|ij\rangle = C_{ij}^{\dagger}|vacuum\rangle$, that is, $\psi(E) = \sum_{ij} \alpha_{ij}|ij\rangle$ with the complex coefficients α_{ij} to be determined. In other words, a set of $\{\alpha_{ij}\}$ is the site representation of the wave function. In the left or right lead, α_{ij} is further denoted as α_{ij}^{L} or α_{ij}^{R}.

In the AGR, by applying the Hamiltonian (1) on $\psi(E) = \sum_{ij} \alpha_{ij}|ij\rangle$ we obtain the following equation regarding the wavefunction in the scattering region for a given energy E,

$$E\alpha_{ij} = -t_0 \sum_{\rho,\delta} \alpha_{i+\rho,j+\delta} + \mu\alpha_{ij}, \tag{2}$$

where ρ and δ denote the nearest neighbors along x and y directions respectively.

We now define a column vector $\hat{\alpha}_i$ which consists of all the M α-coefficients with the same x-axis index i,

$$\hat{\alpha}_i = \begin{pmatrix} \alpha_{i1} \\ \alpha_{i2} \\ \vdots \\ \alpha_{iM} \end{pmatrix}. \tag{3}$$

After rearranging, we can then rewrite Eq. (2) in a more compact form as

$$\begin{pmatrix} \hat{\alpha}_{i-1} \\ \hat{\alpha}_i \end{pmatrix} = \hat{\chi}_i \begin{pmatrix} \hat{\alpha}_i \\ \hat{\alpha}_{i+1} \end{pmatrix}. \tag{4}$$

Here $\hat{\chi}_i$ is the so-called ith transfer matrix which elements consist of E, t_0, and μ. As its name means, $\hat{\chi}_i$ connects M α-coefficients of any slice i with M α-coefficients of its two neighbor slices $i-1$ and $i+1$. There are totally N transfer matrices in the AGR (Fig. 1).

In each lead, there are M right-traveling waves (channels) and M left-traveling waves (channels) for a given energy E, respectively. Each channel is defined by the corresponding transverse wave vector k_y^n determined by the open boundary condition, namely forming standing waves, $k_y^n = \frac{n\pi}{M+1}$ with n being an integer from 1 to M and the lattice constant a being assumed as a length unity. Physically when an unity-amplitude right-traveling wave in the nth channel is scattered into the n'th channel, the wavefunction in the left and right semi-infinite leads can be expressed respectively [27] as

$$\begin{cases} \alpha_{n,ij}^{L} = & \sum_{n'} \left(\delta_{n'n} e^{ik_x x_i} + r_{n',n} e^{-ik_x' x_i}\right) \sin(k_y^{n'} y_j), \\ \alpha_{n,ij}^{R} = & \sum_{n'} t_{n',n} e^{ik_x' x_i} \sin(k_y^{n'} y_j), \end{cases} \tag{5}$$

where $r_{n',n}$ and $t_{n',n}$ are the reflection and transmission coefficients from the nth to the n'th channel respectively, and the continuous