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Analytical study of electronic quantum transport in carbon-based nanomaterials

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ABSTRACT

We introduce a new method based on the tight-binding model and mode space (MS) renormalization approach to the study of quantum transport properties of carbon-based nanomaterials (CBNs) such as carbon nanotubes (CNTs), graphene nanoribbons (GNRs), superlattice structures and conducting polymers. The calculations are based on the Green's function method, in which the electrical conductance, density of states (DOS) and localization length of the systems are calculated, analytically. Our model and simple formulas are useful to study the impact of slice-like defects, to distinguish different regimes and reduce the computation time. The efficiency of our method in reducing the CPU time is tested in electrical conductance, where the computation time is reduced by up to a factor of 40 depending on the parameters of the problem. We demonstrate the power of this approach by studying the electronic transport in partially unzipped carbon nanotubes (UCNTs).

1. Introduction

For the last decades, silicon-based electronics has ruled the semiconductor technology. However, silicon technology has reached its upper limits of design complexity, processing, memory, etc. [1,2]. The potential applications of carbon-based nanosystems such as carbon nanotubes [3], graphene nanoribbons [4–12] and conducting polymers [13] lie in the field of electronic devices (namely, Schottky rectifiers, field-effect transistors, light-emitting diodes and solar cells), electromagnetic interference shielding and microwave absorbing materials, rechargeable batteries and supercapacitors, electrochromic devices, sensors (for instance gas, chemical and biochemical sensors) and artificial muscles. Experimental measurements and theoretical studies are necessary procedures to understand the transport mechanism of nanosystems. The standard transfer matrix and Green's function methods in the tight-binding model have become widely used and powerful tools in the theoretical description of the electronic transport in nanosystems [14–18]. The standard Green's function method will be our concern in this paper. Even for small size systems, we need many numerical calculations because of working with the Green's functions of very large sparse Hamiltonian matrices. So the numerical calculation time greatly increases. For many physical nanosystems (quasi-one dimensional systems), we can reduce the calculation time with introducing the analytical and mode space methods.

In Ref. [19], we used the mode space method [20–22] for studying electronic transport in pure and superlattice-like disordered carbon nanotubes. This model reduces the numerical calculation time and enables us to use the transfer matrix method to investigate transport in a carbon nanotube. Also, in Ref. [23], we combined the mode space method with the renormalization approach [24] and investigated the transport properties of superlattice-carbon nanotubes. In Ref. [25], the renormalization method has been used to study electronic transport of conjugated polymer junctions in real space. In addition to the mentioned methods, we can reduce the calculation time with an analytical approach. The analytical solutions finally enhance our deep understanding of the physics of the systems.

In this paper, by combining the mode space method with the renormalization technique, we present a general analytical formulation to study the electronic transport in carbon-based nanosystems.

First, we map the nanosystems from the real space into the mode space and convert them to diatomic chains with the devices consisting of two effective atoms by the renormalization technique. Second, we derive the analytical formulas for the transport subject. Our model and simple formulas are useful to study the impact of slice-like defects, to distinguish different regimes and reduce the computation time.

After testing our approach, as an application example, we study the electronic transport in partially unzipped carbon nanotubes. In 2009, three experimental groups announced simultaneously a promising way to produce narrow graphene nanoribbons using carbon nanotubes [26–28]. They propose to longitudinally unzip carbon nanotubes to make nanoribbons, by chemical attack, plasma etching and lithium intercalation followed by exfoliation. Unzipping carbon nanotubes appears as a promising way to produce narrow nanoribbons needed for nanoelectronic applications [29,30].

Our calculations are based on the tight-binding model and the Green's function method within the nearest-neighbor approximation.

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Our results can serve as a basis for developments in designing nanoelectronic devices.

The paper is organized as follows: after a brief overview of the electronic transport in nanosystems (Section 1), we will describe our model and derive exact analytical formulas for the transmission coefficient, the density of states and localization length, briefly, in Section 2. In Section 3, we present our numerical results for the illustrative examples which consist of ordered CNTs, GNRs, CNT–GNR junctions and the UCNTs. Finally, in Section 4 we give some conclusions and remarks.

2. Description of the model and method

In this section, we study analytically the electronic quantum transport in a quasi-one-dimensional structure, a nanoribbon (nanotube) formed of N slices (rings) connected to two semi-infinite metallic leads. The carbon slices (rings) of the leads are assumed to comprise between $(-\infty,0]\cup[N+1,+\infty)$. The sandwiched spacer is known as a carbon-based device (CBD). We consider that the CBD consists of two types of carbon and defect slices with slice energies, ε_c and ε_d, respectively. In Fig. 1(a) and (b), we have depicted the structure of a CNT or AGNR in the real and mode spaces. The layered defect concentration in the device is, where N_d is the number of defect slices (see Fig. 1(c)). In this study, we ignore the electron–phonon and electron–electron interactions. Furthermore, the charging effect is neglected in the wire as it is assumed that the wire-lead coupling is not weak. In this article, we study only zigzag carbon nanotubes (ZCNTs) and armchair graphene nanoribbons (AGNRs), while this approach can also be generalized to other quantum wires.

2.1. Mode space approach

By mapping $(n, 0)$ nanotubes and $2n$-AGNRs from real space into mode space (q), we obtain n decoupled chain with two hopping parameters, $t_q = 2t\cos(\frac{\pi q}{m})$ and t with $m = n$ for CNTs [21,22] and $m = 2n+1$ for AGNRs [31], also $q = 1, 2, 3, \ldots n$. The decoupled electron Hamiltonian for the system is given by:

$$H = \sum_{q=1}^{n} H_q. \tag{1}$$

The one-dimensional tight-binding Hamiltonian H_q describes one chain with two sites per unit cell with on-site energy $\varepsilon_{carbon} = \varepsilon_c$ or $\varepsilon_{defect} = \varepsilon_d$. The geometry of the ZCNTs and AGNRs in the real space (RS) and the corresponding one-dimensional chains in the mode space is shown in Fig. 1(a) and (b), respectively. Also, in Fig. 1(c) we illustrate a system (a device connected to the two leads) with decoupled modes. Moreover, in this figure, we demonstrate

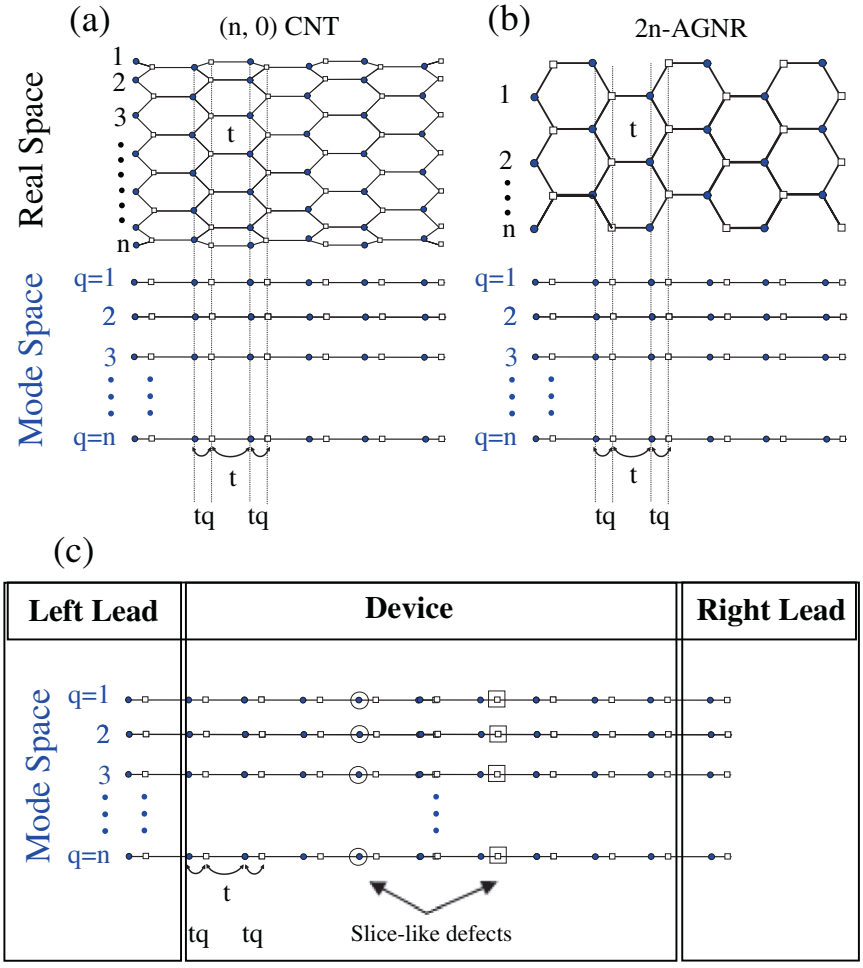

Fig. 1. (a) The schematic diagram of a $(n, 0)$ CNT in the real space and the corresponding one-dimensional chains in the mode space with two sites per unit cell. (b) The schematic diagram of a $2n$- AGNR. (c) The schematic diagram of a disordered system with slice-like defects and its decoupled modes. The on-site energy is taken as ε_{jw} and the hopping parameters are t_q and t in the mode space. The hopping parameter between the nearest neighbors in the system is t.