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The Study on Transmission Properties of Carbon Nanotubes by Recursive Green's Function Method

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The transmission properties of SWNT have been studied by the recursive Green's function method. The theoretical calculated results are not only in good agreements with the experiments, but also give a deep insight to the phenomena.
Key words: nanotube, transmission properties, Green's function

1. INTRODUCTION

Carbon nanotubes[1] as well-defined stable and rigid one-dimensional materials have attracted significant interests recently. Because of their potential application as one-dimensional (1D) quantum wires in carbon nanostructure electronics, many theoretical predictions and experimental proofs have been made for their electronic structure[2-4]. A single-wall carbon nanotube (SWNT) can be imagined by rolling up a single sheet of graphite along one of its two dimensional (2D) lattice vectors $R=mR_1+nR_2$ to form a (m,n) nanotube with radius $r=|R|/2\pi$, where R_1 and R_2 are primitive lattice vector. Armchair nanotubes are defined by rollup vector along the (n,n) direction, while zigzag nanotubes are defined by rollup vector along the $(n,0)$ direction. Armchair and zigzag nanotubes will possess reflection planes and be achiral, and all other SWNT will be chiral. The electrical properties of carbon nanotubes strongly depend on their diameter and the chiral angle of the atomic lattice: armchair tubes are predicted to be truly 1D metals, whereas zigzag or chiral nanotubes are expected to be semiconductors with either a substantial gap (~1eV) or a very low gap (~meVs). The measurement of transmission properties of carbon nanotubes has been the most challenging due to the small diameter of the tubes. Only very recently have ones been able to attach probes directly to individual tubes to measure their transmission properties[5-9]. In the case of multi-wall nanotubes, where many tubes are arranged in a coaxial fashing, the transmission properties of tubes have been shown to vary strongly from tube to tube[5]. However, in the case of SWNTs, the situation is quite different. C. Dekker *et al.*[7-9] succeeded in depositing individual SWNT molecules on metal leads and investigating their two-probe or four-probe resistance versus length, temperature, and gate potential. They find that SWNTs indeed act as genuine quantum wires, and the electrical conduction seems to occur through well separated, discrete electron states that is aligned with the Fermi energy E_f of the electrodes. Moreover, for multiprobe transport experiments they find also that it is electrically broken up into a chain of weakly coupled 1D quantum wires separated by local barriers.

It is the purpose of this paper to present a calculation of transmission properties of SWNT by the recursive Green's function method. It will be shown that the theoretical calculated results are not only in good agreement with the experimental ones, but also give a deep insight on the transmission properties of carbon nanotubes.

2. RECURSIVE GREEN'S FUNCTION METHOD

2.1 Basic algorithm

Consider a Tight-Binding Hamiltonian H given by

$$H = \sum_i \left(\hat{h}_i + \hat{v}_{i,i-1} + \hat{v}_{i-1,i} \right), \qquad (1)$$

where h_i describes the Hamiltonian in isolated region i, and $v_{i,i\pm1}$ corresponds to the hopping between regions i and $i\pm1$.

The Green's function $G(z)$ is defined as

$$G(z) \equiv (z - H)^{-1}, \qquad (2)$$

where z is a complex variable with a small imaginary part. The Green's function G_j^0 in the isolated region j and G in the whole system are related by the Dyson's equation:

$$G = G_j^0 + G_j^0 \hat{V}_j G \qquad (3)$$

with

$$\begin{cases} G_j^0(z) = (z - \hat{h}_j)^{-1} \\ \hat{V}_j = H - \hat{h}_j \end{cases} \qquad (4)$$

By taking matrix elements of Eq.(3) in region j, one obtains:

$$G_{j,j} = [(G_j^0)^{-1} - V_{j,j+1}G_{j+1}^R V_{j+1,j} - V_{j,j-1}G_{j-1}^L V_{j-1,j}]^{-1} \quad (5)$$

where the left (right) Green's function G^L_j (G^R_j) is the Green's function for a system in which all sites $i>j$ ($i<j$) are deleted. Then, the matrix recursion formula can be obtained as

$$\begin{cases} G_{j+1}^L = [(G_{j+1}^0)^{-1} - V_{j+1,j}G_j^L V_{j,j+1}]^{-1} \\ G_j^R = [(G_j^0)^{-1} - V_{j,j+1}G_{j+1}^R V_{j+1,j}]^{-1} \end{cases} \quad (6)$$

We can also obtain the non-diagonal block element of G from the Dyson's equation as follows:

$$\begin{cases} G_{j',j} = G_{j'}^L V_{j',j'+1} G_{j'+1}^L \ldots V_{j-1,j} G_{j,j} (j' < j) \\ G_{j',j} = G_{j'}^R V_{j',j'-1} G_{j'-1}^R \ldots V_{j+1,j} G_{j,j} (j' > j) \end{cases} \quad (7)$$

From the above equations, it can be seen that, all the Green's function G for the whole system can be calculated through the determination of the left and right Green's functions, which are the inverses of matrices with dimensions much smaller than the system matrix H.

The recursive procedure given above is a useful method for most Green's function applications, especially for some calculations where only parts of the Green's function for the system are necessary.

2.2 Boundary conditions

In many cases, we are interested in a particular finite system, which has some correlation with the environment, or a sub-system of an infinite system. In order to calculate the Green's function in the concerned system, we use the Dyson's equation again to evaluate the correlation with other systems.

Consider a system with the total Hamiltonian H written as:

$$H = H_0 + \sum_j (H_j + \hat{V}_{0j} + \hat{V}_{j,0}) \quad (8)$$

where H_j is the Hamiltonian for isolated system j ($j \neq 0$) and $V_{0,j}$ represents the hopping bwtween system 0 and j. By taking matrix elements of Eq.(3) in system 0, one obtains the following matrix equations:

$$G = [(G^0)^{-1} - \sum_j S_j]^{-1} \quad (9)$$

where

$$S_j \equiv \hat{V}_{0,j} G_j^0 \hat{V}_{j,0} \quad (10)$$

is the self-energy on the system 0, due to the presence of system j. G^0_j is the Green's function for the isolated system j.

We can also rewrite the above formula by considering the definition of the Green's function as follows:

$$H_{\text{eff}}(E) = H_0 + \sum_j S_j \quad (11)$$

where $H_{eff}(E)$ represents the effective Hamiltonian at a given energy E. This is a useful result for many boundary condition problems.

We conclude this section by noting that, in many application, it is not necessary to calculate all the elements of the Green's function, that will economize greatly both the storage space and the cpu time. And to consider the effect of the environment, we can just take the finite system as a sub-system connected with some semi-infinite systems to evaluate the characters of the finite sub-system in an infinite system.

3. RESULTS AND DISCUSSIONS

In this section, we study the transmission properties of single wall carbon nanotubes.

It is well known that the carbon system can be described well by the Tight-Binding (TB) parameters, so we use a simple TB representation of the electron states. m+n equivalent sites determined by the integer indices (m,n) are taken as the subsystem (defined as a slice) of the whole tube, which then gives $h_j = E_{site}\mathbf{I}$ where $\mathbf{I}$ is the unity matrix and E_{site} is the on-site energy. And it is the hopping matrix $v_{i,(i\pm1)}$ that describes the exact structure of the SWNT, which will vary for different integer indices (m,n). To study the transmission properties through this system, we attach two semi-infinite ideal leads to the SWNT from both sides. In order to make the representation simple, the on site energy E_{site} is taken as energy zero point, the hopping energy t between the neighbor carbon atoms is taken as energy unit, and the leads are taken to be 1D ones. Then, the Green's function at the edge site of the semi-infinite ideal leads is given by[10]

$$G^0(E) = E/2 - [(E/2)^2 - 1]^{1/2} \quad (12)$$

and the static conductance g through the SWNT is calculated by the Kubo formula[10-12]

Now, let us focus on the transmission properties in this system. Typical conductance-Fermi energy curves for some special integer indices (m,n) are shown in Fig. 1, where the total number of slices in the calculations is 121, which corresponds to a $12nm$ long tube. It is obvious that the tube is either a metal or a semiconductor, depending on the choice of m and n: the armchair tubes are always metals, as shown in Fig. 1(b); while the energy gap for the zigzag or chiral ones may be up to $1eV$. In order to compare directly with the experimental results, we map the integer indices (m,n) to the measurable values in the

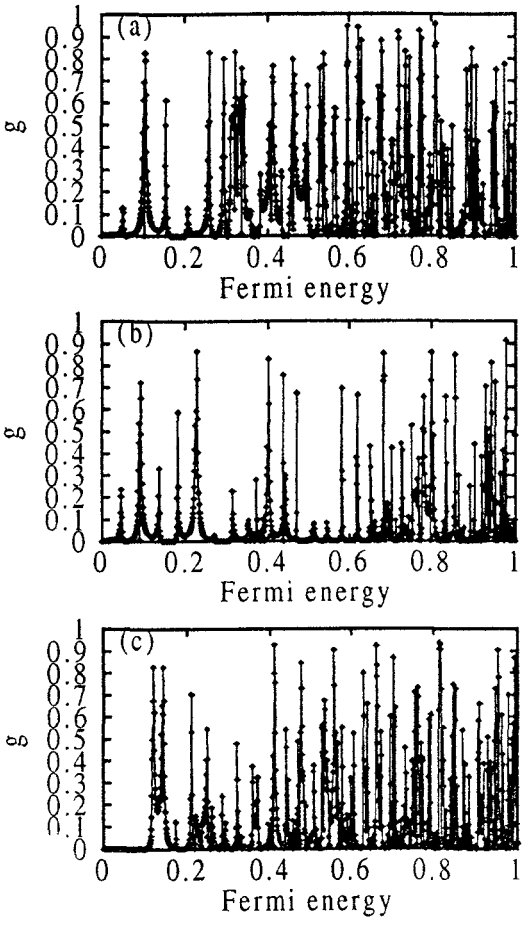

Figure 1. Conductance g (in units of e^2/h) as a function of the Fermi energy E_f for different chiral carbon nanotubes (*12nm* long). The marks give the calculated values of the conductance. (a) $m=18$, $n=0$ (zigzag); (b) $m=9$, $n=9$ (armchair); (c) $m=12$, $n=7$ (chiral).

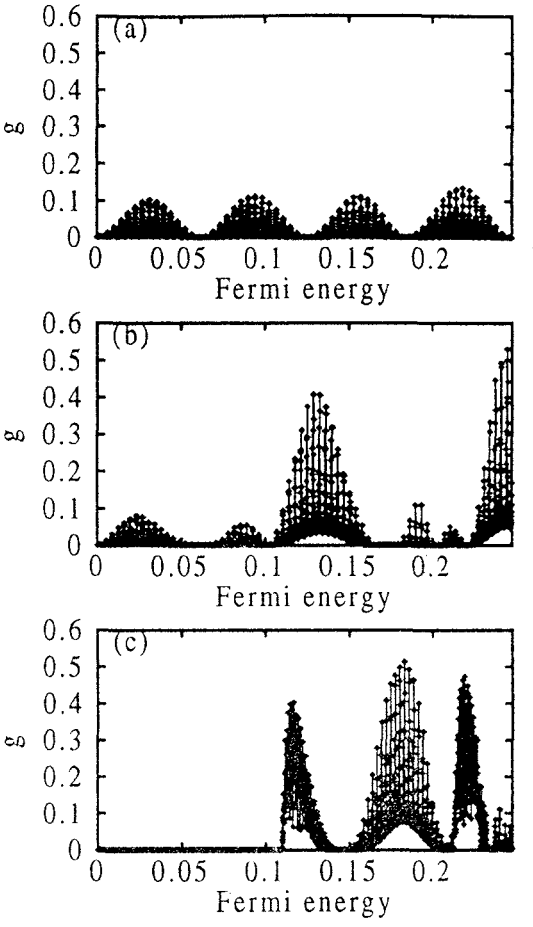

Figure 2. Conductance g (in units of e^2/h) as a function of the Fermi energy E_f for different chiral carbon nanotubes (*140nm* long). The marks give the calculated values of the conductance. (a) $m=18$, $n=0$ (zigzag); (b) $m=9$, $n=9$ (armchair); (c) $m=12$, $n=7$ (chiral).

experiments[13]. Then a (*12,7*) SWNT corresponds to a chiral angle (the wrapping angle to the armchair direction) $\phi=8^0$ and diameter $d=1.28nm$ tube. The experimental result[13] gives an energy gap of *0.60eV* (Tube no. *9* in the experiment) or *0.65eV* (Tube no. *19* in the experiment). If we take the value of $V_{pp\pi}$ (about *3eV*)[14] for carbon as *t*, it can be estimated the energy gap for this tube, as shown in Figs. 1(c) and 2(c), is about *0.65eV*, which is in good agreement with the experiement[13] and previous theoretical electronic structures calculations[15]. Moreover, it is shown that there exist many well-separated conductance peaks in a much wide range of the energy. It is well known that the conductance peak occurs in existence of resonant tunneling through a discrete electron level that is aligned with the Fermi energy E_f, which gives rises to that there do exist many discrete electron levels in the tube, as a genuine quantum wire.

In order to reveal the finite size effect of the nanotubes, we also calculated the electronic conductance for a much longer SWNT with *1400* slices, which corresponds to a *140nm* long tube in an earlier experiment[7]. The results are shown in Fig. 2. For a finite 1D tube of length *L*, the component of momentum along the axis will also be quantized, with an energy separation between levels of $\Delta E \propto 1/L$. In the figures, it is clear shown that with longer length *L*, the energy separations become smaller. With long enough length *L*, the details of the curves are dominated by the ΔE, where the conductance peaks are caused by the sub-energy-levels of the tube, while the envelope reflects the structure indices (*m,n*) of the tube. Because the zero-bias conductance peaks occur only when an electron level is shifted to the Fermi energy by the gate voltage, the energy separation ΔE between levels can be easily estimated from the experiment results. It has been deduced that *12mV* change in V_{gate} resulted in a change of tube potential of about *1meV*, and at the same time four main peaks can be found in a range of V_{gate} of *400mV*[7]. As a consequence, the energy separation can be calculated by *400/(12*3)* which gives $\Delta E \approx 11meV$. On the other hand, from our calculation results, it is found that the energy difference for adjacent conductance peaks is about

0.004t for the *140nm* long tube. Taking the value of $V_{ppπ}$ (about *3eV*)[14] for carbon as *t* again, it can be estimated the energy difference between levels is about *12meV*, which is in good agreement with the experiment result[7]. It is obvious that the energy separation between levels is caused by the *140nm* long tube between the electrodes, though it is expected to be caused by the whole *3μm* long tube[7]. Moreover, a more recent experiment[9] shows that the bending of the tube near the edge of electrodes may act as local barrier which separates the tube to many local parts without coherent interaction between them, which also means that the parts other than the one between the electrodes may not take effects to the conductance measurement.

4. SUMMARY

In conclusion, the transmission properties of SWNTs are studied with the help of a generalized recursive Green's function method. It is found that SWNTs indeed act as genuine quantum wires. The conductance peak occurs in existence of resonant tunneling through a discrete electron level that is aligned with the Fermi energy E_f of the electrodes. Our results are not only in good agreement with the recent experimental ones, but also give a deep insight on the phenomena.

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