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Electronic transport properties of metallic single-walled carbon nanotubes*

Cao Jue-Xian(曹觉先)[a)b)], Yan Xiao-Hong(颜晓红)[a)],
Xiao Yang(肖 杨)[a)], and Ding Jian-Wen(丁建文)[a)b)]

[a)] *Department of Physics, Xiangtan University, Xiangtan 411105, China*

[b)] *Institute of Mechanics and Material Engineering, Xiangtan University, Xiangtan 411105, China*

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We have calculated the differential conductance of metallic carbon nanotubes by the scatter matrix method. It is found that the differential conductance of metallic nanotube-based devices oscillates as a function of the bias voltage between the two leads and the gate voltage. Oscillation period T is directly proportional to the reciprocal of nanotube length. In addition, we found that electronic transport properties are sensitive to variation of the length of the nanotube.

Keywords: electronic transport properties, single-walled carbon nanotube, quantum interference effects
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Due to the development of micro-manufacture technology, miniaturization of microelectronic devices has led to intense research directed toward the development of molecular electronics.[1,2] The unique electrical[3,4] and mechanical[5] properties of carbon nanotubes (CNTs) have stimulated these efforts, because CNTs, especially single-walled carbon nanotubes (SWCNTs), exhibit a range of suitable properties for nanodevices.[6−10] To date, many basic microelectronic devices based on SWCNTs, such as molecular wires,[11] diodes,[12] field-effect transistors,[6,7,13] single-electron transistors[14] and elementary logic circuits,[15] have been invented. Experimental researches have shown that the length of SWCNTs,[8] dislocations,[16] and quantum interference effects play important roles in such devices.[15,17,18] A detailed theory is needed to describe the influence of these factors on electron transport in CNTs.

As an allotropic structure of carbon, CNTs exhibit rich electronic properties.[3−10] Band theory has predicted and experiments have confirmed the interplay between the geometry and electronic properties and that only the armchair SWCNTs are metallic.[3,4] Experiments based on scanning tunnelling microscopy (STM) have demonstrated the ballistic and coherent transport behaviour of SWCNTs,[19] which exhibit resonant tunnelling, quantum dot behaviour and standing waves in finite-sized tubes.[20,21] Previous experimental and theoretical studies have also indicated that metallic SWCNTs behave as a one-dimensional (1D) ballistic conductor whose conductance can be attributed to the two spin-degenerate 1D transport modes with linear dispersion.[19] Thereby, the conductance amounts to $4e^2/h$ when an electron passes through the nanotube–metal interfaces without reflection. However, the mean conductance values obtained by experiment are smaller than this predicted maximum, which provides evidence of electron scattering in nanotube devices.[26] In this paper, we devote our attention to the quantum interference effects in nanotube devices.

As in many experimental devices, the model in our study contains a single-walled armchair carbon nanotube with metallic contacts, a source and a drain,

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and a substrate gate contact as shown in Fig.1. At zero temperature, the normal conductance G of such a system is deduced from the Landauer formula [22]

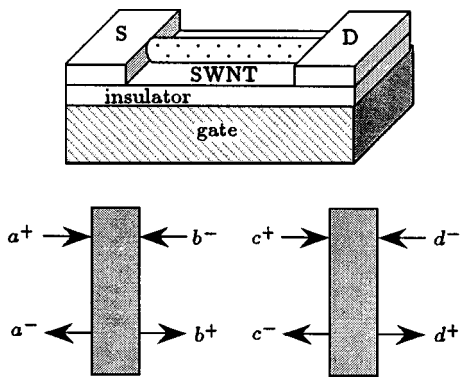


Fig.1. Description of a nanotube-based device in the calculation and dispersion relations for two propagating modes for metallic SWCNs.

$$G = \frac{2e^2}{h} \sum_{m=1}^{M} \sum_{m'=1}^{M} |t_{m'm}(E = E_{\mathrm{F}})|^2, \qquad (1)$$

where $t_{m'm}$ is the amplitude for an electron injected from the left into subband m and transmitted to subband m' on the right. M is the total number of modes that are occupied at the Fermi level E_{F}. In previous works, the transfer matrix method and recursive Green function technique [23,24] have been applied to obtain transmission coefficients $t_{m'm}$. Here, we obtain $t_{m'm}$ from the scattering matrix [25] of the device.

In general, the scattering matrix $[S]$ can be written as

$$[S] = \begin{bmatrix} t & r' \\ r & t' \end{bmatrix}, \qquad (2)$$

where t, t', r and r' are all $M \times M$ matrices. M is the number of propagating modes available at the Fermi level. It is defined as a matrix which gives the amplitude of the outgoing waves $[a^-]$ and $[b^+]$ from the scattering region relative to the amplitude of the incoming waves a^+ and b^-, where $[a^\pm]$ and $[b^\pm]$ are both $M \times 1$ column vectors. The overall scattering matrix $[S]$ for our model in Fig.1 is obtained by combining the scattering matrices of the successive sections as

$$[S_{\mathrm{T}}] = [S_{\mathrm{L}}] \otimes [S_{\mathrm{N}}] \otimes [S_{\mathrm{R}}]. \qquad (3)$$

Here S_{N} represents the electron propagation in the nanotube while S_{L} and S_{R} represent the electron transmission and reflection at the metal–nanotube interfaces, respectively. If $S = [S_1] \otimes [S_2]$, we can have the following relationship:

$$[S] = \begin{bmatrix} t_2[I - r_1' r_2]^{-1} t_1 & t_2[I - r_1' r_2]^{-1} r_1' t_2' + r_2' \\ r_1 + t_1'[I - r_2 r_1']r_2 t_1 & t_1'[I - r_2 r_1'] t_2' \end{bmatrix}. \qquad (4)$$

Following previous theoretical studies,[19−21] the electron propagates ballistically in two transport modes of the armchair nanotube. The electron scattering between the two modes inside the tube can be ignored. The matrix S_{N} is given by

$$S_{\mathrm{N}} = \begin{bmatrix} \mathrm{e}^{\mathrm{i}\phi_1} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\phi_2} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}\phi_1} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\phi_2} \end{bmatrix}, \qquad (5)$$

where ϕ_1 and ϕ_2 are the phases accumulated in travelling the two transport channels by the electrons in the nanotube segment. It is easy to obtain ϕ_1 and ϕ_2

$$\phi_{1,2} = k_0 L \pm \left(\frac{E}{\hbar v_{\mathrm{F}}} + \frac{\pi C_{\mathrm{L}} V_{\mathrm{g}}}{4e} \right) L, \qquad (6)$$

in which $k_0 = 2\pi/3a_0\mathrm{nm}^{-1}$ is the wave vector at the Fermi level (a_0=0.246nm is the lattice constant), L is the length of the CNT, E is the total energy of an electron at the Fermi surface, v_{F} ($= 8.1 \times 10^5 \mathrm{m/s}$) is the Fermi velocity inside the nanotube, and C_{L} ($= 2\pi\varepsilon/\ln\{[d + (d^2 - R^2)^{1/2}]/R\}$) is the capacitance per unit length of a nanotube, where $\varepsilon = 8.85 \times 10^{-12}\mathrm{F/m}$, d is the distance from the tube axis to the plane, and R is the radius of the nanotube. $\hbar$ is Planck's constant and V_{g} is gate voltage. Assuming a weak scattering potential ΔV at the metal–nanotube interfaces, the scattering matrix $S_{\mathrm{L,R}}$ can be written, using the Born approximation, as

$$[S] = I + \mathrm{i} \begin{bmatrix} a_{++} & a_{+-} \\ a_{-+} & a_{--} \end{bmatrix}, \qquad (7)$$

where I is the identity matrix of dimension 4×4, and the 2×2 matrices $[a_{\pm,\pm}]$ can be shown to be [25]

$$[a\pm, \pm] = -\frac{m^*}{\hbar^2 \sqrt{k_m k_n}} \int \mathrm{d}x \int \mathrm{d}y \psi^{\pm^*}{}_m(r) V(r) \psi_n^{\pm}(r). \qquad (8)$$

Here ψ_m represents the mode wavefunctions that propagate in the nanotube and k_m is the wavevector.

If γ is the parameter characterizing the strength of the interaction ΔV, the scattering matrix S is only unitary to order γ. In order to make it exactly unitary, one can use the following ansatz for S:

$$[S] = \mathrm{e}^{\mathrm{i}[a]}. \tag{9}$$

For our numerical simulations, the scattering matrix S is only unitary to the first order. So S_{R} and S_{L} may be reduced to a simple form [26]

$$S_{\mathrm{R}} = \exp\left(\mathrm{i}\begin{bmatrix} 0 & 0 & r_2 & r_1\exp(\mathrm{i}\delta_1) \\ 0 & 0 & r_1\exp(\mathrm{i}\delta_1) & r_2\exp(\mathrm{i}\delta_2) \\ r_2 & r_1\exp(-\mathrm{i}\delta_1) & 0 & 0 \\ r_1\exp(-\mathrm{i}\delta_1) & r_2\exp(-\mathrm{i}\delta_2) & 0 & 0 \end{bmatrix}\right), \tag{10}$$

and $S_{\mathrm{L}} = S_{\mathrm{R}}^{*}$. Here r_1 and r_2 are proportional to the magnitudes of the electron reflection matrix elements in the first-order Born approximation with and without the inter-mode hopping, respectively, and δ_1 and δ_2 signify the phases of these matrix elements. Since S_{T} is known, the differential conductance can be calculated by

$$\frac{\partial I}{\partial V}(V, V_{\mathrm{g}}) = \frac{2e^2}{h}\left[\sum_{i,j=1}^{2}\left|t_{ij}\left(\frac{eV}{2\hbar v_{\mathrm{F}}} + \frac{\pi C_{\mathrm{L}} V_{\mathrm{g}}}{4e}\right)\right|^2 + \sum_{i,j=1}^{2}\left|t'_{ij}\left(\frac{-eV}{2\hbar v_{\mathrm{F}}} + \frac{\pi C_{\mathrm{L}} V_{\mathrm{g}}}{4e}\right)\right|^2\right]. \tag{11}$$

Figure 2 shows the differential conductance ($\partial I/\partial V$) oscillations periodically with increasing gate voltage V_{g} around an average conductance of about $3.3e^2/h$ (the value of e^2/h is 38.8μs or $(25.8\mathrm{k}\Omega)^{-1}$) at different bias voltages. (The bias voltage is –4, –2, 2, 4mV for lines a, b, c, d, respectively.) From the figure, one can see that the period T does not change with the bias voltage in spite of the variation of conductance. Interestingly, the maximal differential conductance is about 3.8 e^2/h (shown in Fig.2). We know that the conductance of metallic SWCNTs is predicted to be 4 e^2/h by Landauer theory because the electrons pass through the nanotube ballistically. The results in Fig.2 indicate the existence of electron scattering at the nanotube–metal interface. Figure 3 shows the two-dimensional (2D) contour $\partial I/\partial V$ plots as a function of V and V_{g}, changing smoothly for the metallic SWCNT with different lengths. The peaks and troughs, which appear as white and black colours respectively in Fig.3, form a mesh of criss-cross dark lines. The conductance behaviour does not change although the V and V_{g} spacing between adjacent pitch-dark spots, called the oscillation period T, changes with the length of the nanotube. More detailed calculations show the linear relationship between the oscillation period T and the reciprocal length of the nanotube L^{-1}, as described in Fig.4.

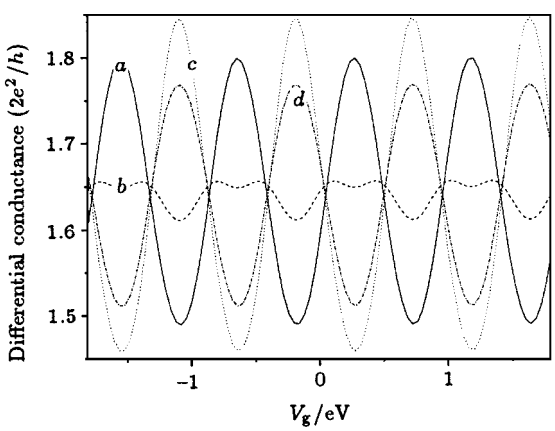


Fig.2. Differential conductance versus gate voltage V_{g} at different bias voltage V ((a, –4meV; b, –2meV; c, 2meV ; d, 4meV).

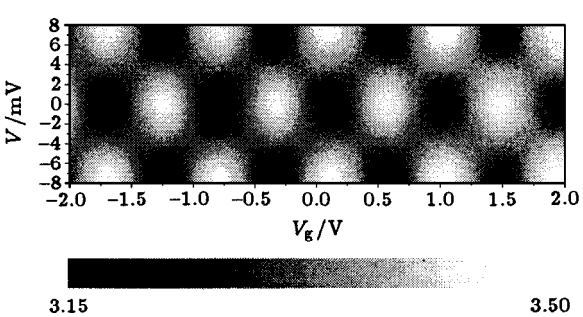


Fig.3. Two dimensional contour of $\partial I/\partial V$ plotted as a function of V and V_{g}.

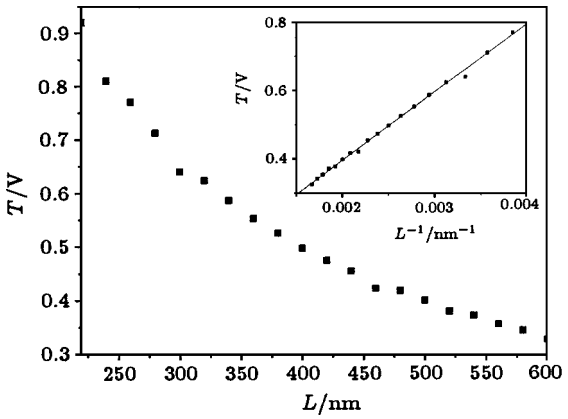


Fig.4. Linear relationship between oscillation period T and the reciprocal length of nanotube L^{-1}.

The effect of interfacial electron scattering coupled with ballistic transport within the nanotube indicates that the nanotube-device characteristics may be determined by quantum interference between electron waves multiply reflected between two nanotube–metal interfaces, just as in the case of transmitted intensity oscillations in an optical Fabry–Perot cavity. The results in Figs.2 and 3 show that the differential conductance oscillates as a function of V and V_g. The oscillation phenomenon may be attributed to the change of electron momentum and phase during the electron transport in the nanotube. Because V_g modulates the Fermi level in the nanotube, this modulation will control the potential energy of the electrons in the nanotube, and the electrons will be accelerated under the bias voltage, which controls their total energy. Therefore, both V and V_g modulate the kinetic energy of the electrons, which contributes to the current and the wavelength of an electronic wave. It is possible to make a nanoswitch based on the nanotube device by controlling the bias voltage V and gate voltage V_g. For example, for a 220nm length nanotube device, the differential conductance is about 3.69 e^2/h at V_g=0.28V and V=7.36mV, while it will be decreased to 2.90 e^2/h as the gate voltage increases to 0.72V. We can take the former for turn-on state and the latter for the turn-off state.

Figure 5 shows that the electronic transport properties are sensitive to variation of the length of nanotube. We find that the differential conductance does not vary in a smooth, monotonic way, instead it shows marked modulations with a certain period. It contributes to electron waves from two propagating modes of metallic SWCNT interfering at the port of the nanotube-based device because of their different phases. The intensity of the transmitted wave is a periodic oscillatory function of $1/\lambda$, where λ is the wavelength of the transmitted wave, with a period determined by the length of the nanotube L according to the rules of wave superposition.

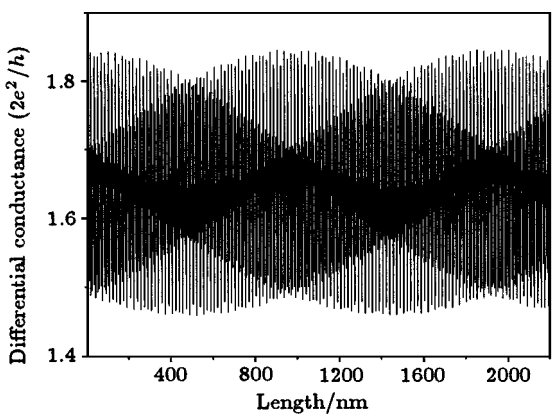


Fig.5. Differential conductance versus the length L of nanotube in a complex way.

In summary, by use of the scatter matrix, we have calculated the differential conductance of a metallic carbon nanotube with modulations of electric fields. It was found that the differential conductance of a metallic nanotube-based device oscillates as a function of the bias voltage between the two leads and the gate voltage. Oscillation period T is directly proportional to the reciprocal of the nanotube length. According to the transport properties of SWCNs, it is possible to make a nanoswitch based on nanotube devices by controlling the bias voltage V and the gate voltage V_g. In addition, the calculated differential conductance is sensitive to the variation of the length of nanotubes.

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