Coherent Electronic Transport through the Single-Walled Carbon Nanotubes

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Summary: We present the results for coherent electronic transport through the single walled carbon nanotubes. A large value of conductance is obtained for strong coupling to the electrodes, which is close to the ideal transmission of $4e^2/h$ as in experiment. We also consider the system with ferromagnetic electrodes and analyze in detail conductance for separated channels in the coherent regime.

Keywords: carbon nanotubes; coherent transport; quantum conductance

Introduction

Electronic transport through carbon nanotubes (CNT) has recently became an objective of experiment [1-3] due to the technological progress in nanofabrication. It has been known that changing the length of the nanotube, one can change the character of the electronic transport. However, it became evident that the mode (strength) of coupling of the CNT to the electrodes is crucial for the transport properties. When the quality of the contacts is not good, and thus the coupling is weak, the resistances on the junctions are large, much exceeding 13 kΩ, and the transport exhibits an incoherent single-electron tunneling character with the Coulomb blockade effect.[1] If one improves the quality of the contacts, the resistances decrease, which results in higher values of the conductance of the system and one can observe the Kondo resonance, which is due to the exchange interactions between the conducting electrons and an uncompensated localized spin on the CNT.[2] Finally, for very good contacts, one achieves strong coupling to the electrodes and thus the coherent transport character, where the main role is assigned to the multiple scattering on the contacts, which leads to the Fabry-Perot interference.[3] The spin-dependent case measurements have been already performed on multiwalled CNT;[4] however, despite small resistance in that system, it is not possible to observe interference processes and it is very difficult to specify the mechanism of magnetoresistance.

The objective of our work is to determine the coherent transport properties through the system of

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a single-walled carbon nanotube (SWCNT) connected to metallic electrodes. We calculate the conductance of the systems with Au and Fe (ferromagnetic) electrodes. We show that the main contribution to the conductance spectrum should be ascribed to the superposition of the conducting channels rather than to the interference processes both in the paramagnetic and ferromagnetic systems.

Model description

We consider the system of the SWCNT of the armchair type [5,5], which has 5 carbon rings in the circumference. The dispersion relations of such SWCNT show metallic character with two crossing bands, which can be derived from the bonding (π) and antibonding (π^*) orbitals between neighboring carbon atoms. For the infinite SWCNT the dispersion curves are described by the relation[5]

$$E_m^a(k) = \pm\ t_{C-C}\left\{1 \pm 4\cos\left(\frac{m\pi}{5}\right)\cos\left(\frac{ka}{2}\right) + 4\cos^2\left(\frac{ka}{2}\right)\right\}^{\frac{1}{2}}, \tag{1}$$

where k is the wavevector along the SWCNT, m = 5, and a is the lattice constant. The curves (1) have equal slopes of opposite signs. One can say that the transport has an electronic as well as hole character. The Fermi level is assumed as $E_F = 0$ for the neutral SWCNT, and its position can be shifted by applying the gate potential. In the case of the nanotube of length L shorter than the electron-wave coherence length L_{coh}, the standing wave corresponding to $k_n \approx \frac{\pi n}{L}$ appears.

To determine the current through the system, we use the tight binding method, within which the Hamiltonian is expressed as

$$H = \sum_{ik,\alpha,\sigma} \varepsilon_{ik\alpha\sigma} c^+_{ik\alpha\sigma} c_{ik\alpha\sigma} + \sum_{ij,\sigma} t_{C-C}\left(c^+_{i\sigma} c_{j\sigma} + h.c.\right) + \sum_{\alpha i,\sigma} t_{\alpha i}\left(c^+_{ki\alpha\sigma} c_{i\sigma} + h.c.\right) \tag{2}$$

where the first term describes the electrons in the electrodes (α = L,R), the second one describes the electrons on the SWCNT, and the last one corresponds to the tunneling between the electrodes and SWCNT. The hopping integrals for C-C bonds are assumed as t_0 = -2.5 eV as it is accepted in the literature. The first and the last row of carbon atoms are connected with the electrodes, which are treated as ideal reservoirs. The hopping integral t between the electrodes and the SWCNT is treated as a parameter. Next, we apply the non-equilibrium Green functions in terms of which we express the current as

$$J = \frac{2e}{h} \sum_{\sigma} \frac{4}{\pi^2 \rho_{L\sigma} \rho_{R\sigma}} \int d\omega \; [f_L(\omega) - f_R(\omega)] \; \sum_{i,j} \left| G^r_{Li,Rj} \right|^2 , \tag{3}$$

where $G^r_{Li,Rj}$ is the retarded Green function connecting the channels in the electrodes, $\rho_{L\sigma}$ and $\rho_{R\sigma}$ are densities of states for electrons with the spin σ at the Fermi energy in the left (α = L) and right (α = R) electrode, respectively, and $f_\alpha(\omega)$ is the Fermi distribution function for electrons in the α electrode. The Green functions are obtained by numerical inversion of the matrix $\lfloor H - \omega\ I \rfloor$, where the bare Green functions in the electrodes $g^a_{\alpha\sigma} = i\pi\rho_{\alpha\sigma}$. The conductance of the system is given by $G = \left.\frac{dJ}{dV}\right|_{V \to 0}$.

Results

Conductance has been calculated numerically for the SWCNT of length $L = 90$ of atomic layers. Figure 1 presents the results for various couplings t, versus the incident electron energy E_F. In the weak coupling regime, G shows sharp resonant peaks, the positions of which correspond to the energies of standing electron waves. The theoretical maximal value of G for one conducting channel (energies lying on one of the branches) is $2e^2/h$. It can occur, however, that the energies on both branches lie close to each other, which causes G peaks to overlap (see the outer peaks on the right and left sides of the plot). With an increase in the coupling t, the width of the peaks grows, and the peaks change their positions. One can see the conductance exceeding the value of $2e^2/h$. In certain cases it can achieve the maximal value $4e^2/h$. This is the case of ideal transmission through the electron and hole channel simultaneously. We have made an effort to match the coupling parameter t to obtain the conductance level similar to the experimental measurements of $G \approx 3.3\ e^2/h$. We have achieved it for $t = 1.3$ eV, which is shown by the solid line in Fig. 1. The curve resembles the experimental one.[3] One can observe characteristic oscillations corresponding to standing electron waves. In the central part of the plot ($E \approx 0$), the conductance shows a fine structure. Similar features were observed experimentally,[3] and at this point we are in agreement. However, our interpretation of the correspondence of the character of theoretical and experimental curves is different. Liang et al.[3] have assumed the interference effect like in the Fabry-Perot etalon. In our opinion there is a superposition of the conductance for both channels only. Electron waves from both channels are of different symmetry and any matrix element between them is very small, which cannot lead to the interference.

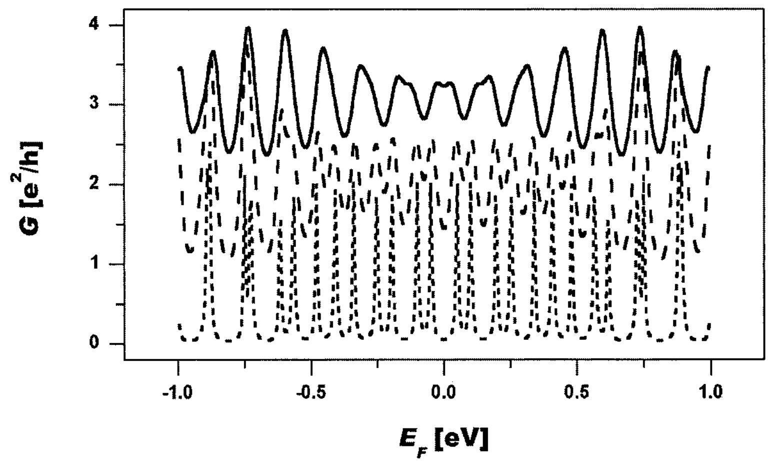

Figure 1. Conductance vs. incident electron energy in the Au-SWCNT-Au system for different couplings values. The solid curve corresponds to the strongest coupling, where the hopping integral is assumed as t = 1.3 eV, dashed line t = 0.9 eV, and short-dashed line t = 0.4 eV. The total density of states for gold at the Fermi level is taken as $\rho_L = \rho_R$ = 0.294 states/eV.[6]

The above example has encouraged us further to investigate other systems. The system with ferromagnetic metallic electrodes seems to be interesting. In this case we have different channels for the electrons with spin $\sigma = \uparrow$ and $\sigma = \downarrow$. In such system, the conducting channels for the opposite spin orientations are different. Now, G is a superposition of four components. In Fig. 2, we present the conductance G_P and G_{AP} for the parallel (P) and antiparallel (AP) orientations of polarization, respectively, and $G_{P\uparrow}$ and $G_{P\downarrow}$ corresponding to the electrons with spin $\sigma = \uparrow$ and $\sigma = \downarrow$ in the P configuration. The densities of states of ferromagnetic Fe were determined by the band structure calculations performed using the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation.[7] The density of states of ferromagnetic Fe for the majority electrons with spin $\sigma = \uparrow$ is $\rho_{Fe\uparrow} = 1.0275$ states/eV, and for the minority electrons $\rho_{Fe\downarrow} = 0.2631$ states/eV. In the parallel configuration, the $G_{P\uparrow}$ curve shows a bit smeared peaks, but still of resonant character of average value about 1 e^2/h, while $G_{P\downarrow}$ shows broad peaks at the level of 2 e^2/h, due to low density of states. In the antiparallel configuration, $G_{AP\uparrow} = G_{AP\downarrow}$ achieves the value slightly lower than 1 e^2/h, i.e. the total conductance G_{AP} takes values below 2 e^2/h. Magnetoresistance, MR = $(G_P - G_{AP})/G_P$, defined as the relative difference of the conductance in the P and AP configuration of spin polarization in the electrodes, shows large oscillations at energies corresponding to the standing waves. The maximal value of MR exceeds 50 %.

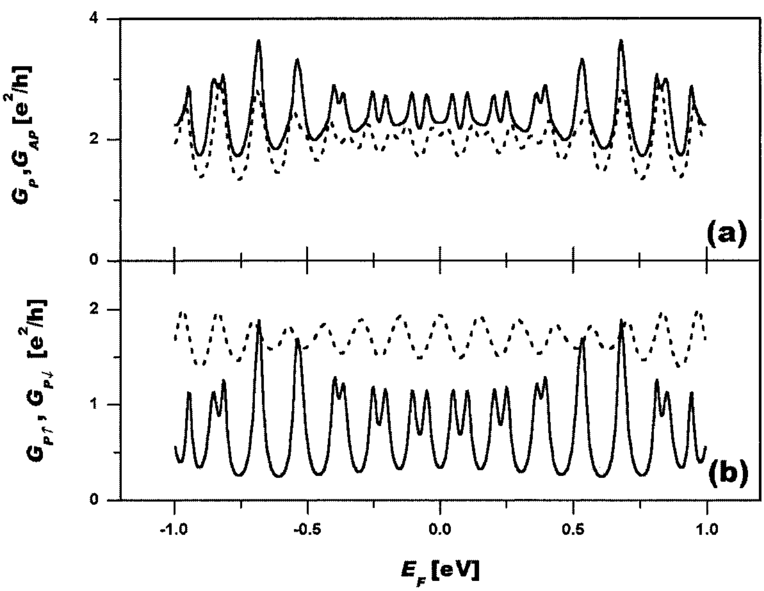

Figure 2. Conductance vs. incident electron energy in the Fe-SWCNT-Fe system. (a) Comparison of G_P (solid line) and G_{AP} (dashed line) for the parallel and antiparallel configuration of the polarization in the electrodes. (b) G_P for separated channels of the electrons with spin $\uparrow$ (solid line) and $\downarrow$ (dashed line). The parameters are as follows: $t = 1.9$ eV, $\rho_{Fe\uparrow} = 1.0275$ states/eV, and $\rho_{Fe\downarrow} = 0.2631$ states/eV.[7]

Conclusions

In our work, calculations of the conductance in the system of SWCNT connected to metallic electrodes have been presented. We have considered the cases of the system with paramagnetic and ferromagnetic electrodes. The obtained results indicate the leading role of the superposition of conductance for different channels and the negligible role of the interference processes between the modes. The method seems credible, as the obtained curves reflect experimental features.[3] We have also calculated magnetoresistance of the system, which shows large oscillations and achieves large values that can also be negative in some points. We believe the experiments on spin-dependent coherent transport through SWCNT can be realized and our theoretical predictions will be verified.

Acknowledgements

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[1]M. Bockrath, D. H. Cobden, P. L. McEuen, N. G. Chopra, A. Zettl, A. Thess and R. E. Smalley, *Science* **1997**, *275*, 1922; S. Tans, M. H. Devoret, R. J. A. Groeneveld and C. Dekker, *Nature* **1998,** *394*, 761.

[2] J. Nygard, D. H. Cobden and P. E. Lindelof, *Nature* **2000**, *408*, 342; W. J. Liang, M. Bockrath and H. Park, *Phys. Rev. Lett.* **2002**, *88*, 126801.

[3] W. J. Liang, M. Bockrath, D. Bozovic, J. H. Hafner, M. Tinkham and H. Park, *Nature* **2001**, *411*, 665.

[4] K. Tsukagoshi, B. W. Alphenhaar, H. Ago, *Nature* **1999**, *401*, 572.

[5] R. Saito, M. Fujita, G. Dresselhaus and M. S. Dresselhaus, *Phys. Rev. B* **1992**, *46*, 1804.

[6] J. M. Seminario, C. E. De La Cruz, P. A. Derosa, *J. Am. Chem. Soc.* **2001**, *123*, 5616.

[7] A. Szajek, unpublished; G. Krier, O. Jepsen, A. Burkhardt, O. K. Andersen, *The TB-LMTO-ASA Program*, source code version 4.7.