Inter-tube transfer of electrons in various double-wall carbon nanotubes

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Abstract. Conductance for inter-tube transfer in double-wall carbon nanotubes is calculated in a tight-binding model. The conductance remains extremely small with fluctuations around an averaged value independent of the tube length. This can be regarded as a direct manifestation of quasi-periodic nature of the system in the conductance.

Carbon nanotubes are often self-assembled to be complex systems such as multi-wall tubes and tube bundles. In these systems, inter-tube transfer of electrons can occur and become an important factor to modify electronic properties. The purpose of the present study is to clarify effects of inter-tube transfer on electronic transport properties of multi-wall tubes.

Using double-wall tubes, some experiments revealed a structural feature that lattices of tubes are incommensurate with each other and therefore, the system is quasi-periodic [1, 2]. Some theoretical studies suggested that effect of inter-tube transfer on electronic transport properties is small [3, 4]. However, the full understanding of inter-tube transfer effects has not been achieved yet. In this paper the conductance between the outer and inner tubes of a double-wall tube is calculated, because it is the quantity dominated by inter-tube transfer.

Figure 1 is a schematic illustration of our two-terminal system. A semi-infinitely long outer tube is attached to a reservoir on the right-hand side, while a semi-infinitely long inner tube is attached to another reservoir on the left-hand side. The two tubes are overlapped with each other in the middle double-wall-tube region with length A where inter-tube transfer occurs. Each tube plays a role of an ideal lead outside this region.

In numerical calculations we use a tight-binding model including only π orbitals and take into account transfers between nearest-neighbor sites in each wall and inter-tube transfers between all sites within the hopping range [Please refer to your paper if it contains more details on the model]. Conductance is calculated by using recursive Green's function method [5] and the Landauer formula.

In this paper conductance of (4,7)-(4,16) tube is presented as a typical result of incommensurate double-wall tubes with metallic inner and outer tubes. Energy is chosen as a value close to the Fermi energy throughout the paper.

Figure 2 shows length-dependence of conductance G in the lower panel and averaged conductance $\tilde{G}$ and conductance fluctuation ΔG in the upper panel. The result is in the case of short tubes $0 < A/L_{\rm out} \leq 0.8$ where $L_{\rm out}$ is the circumference of the outer tube. In the upper panel averaged values and fluctuations are calculated from the conductances of the lower panel in the ranges $0.2n \leq A/L_{\rm out} < 0.2(n+1)$ with $n = 0, 1, 2,$ and 3.

The conductance is extremely small in comparison with the quantum conductance and rapidly fluctuates as shown in the lower panel. In the upper panel the averages and fluctuations are essentially independent of the length.

A similar result in the case of long tubes is shown in Fig. 3. In the upper panel averages and fluctuations are calculated from the conductances in the ranges $500n \leq A/L_{\rm out} < 500(n+1)$ with $n = 0, 1, 2,$ and 3.

Averaged values and fluctuations are slightly enhanced as compared to those in the previous result. Similarly to the previous case, however, they are almost independent of the length in spite of the huge difference in the length scale (2500 times larger than that of the previous case), indicating that all the features of the conductance are independent of the length.

This result shows that the conductance due to inter-tube transfer exhibits quasi-periodic (and therefore fractal-like) behavior as a function of length. It is to be expected because double-wall tubes themselves are quasi-periodic except in some commensurate tubes. However, closer investigation of the length dependence of the conductance is needed in order to clarify more details on the quasi-periodicity and self-similarity. Details of the study will be published elsewhere.

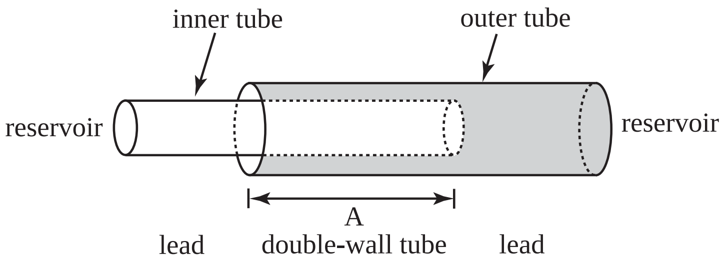

FIGURE 1. Schematic illustration of two-terminal double-wall tube.

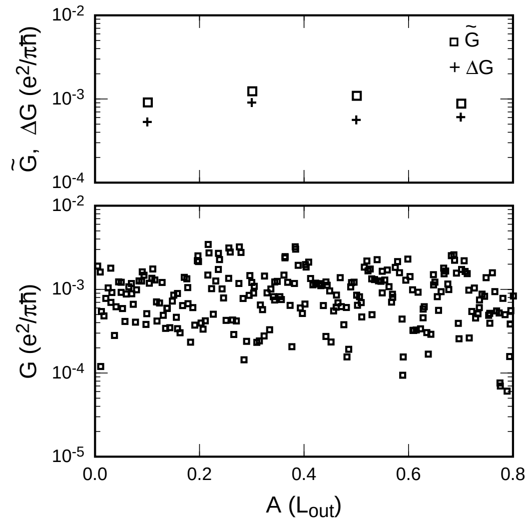

FIGURE 2. In lower panel length-dependence of conductance and in upper panel averaged conductance and fluctuation are plotted by squares and crosses, respectively, in the case of short tubes. The length is changed as finely as possible. Energy E is chosen as $EL_{\rm out}/2\pi\gamma = -0.04$ where the Fermi energy is set to zero and $\gamma = \sqrt{3}a\gamma_0/2$ with a being the lattice constant and γ_0 being the overlap integral between nearest-neighbor sites.

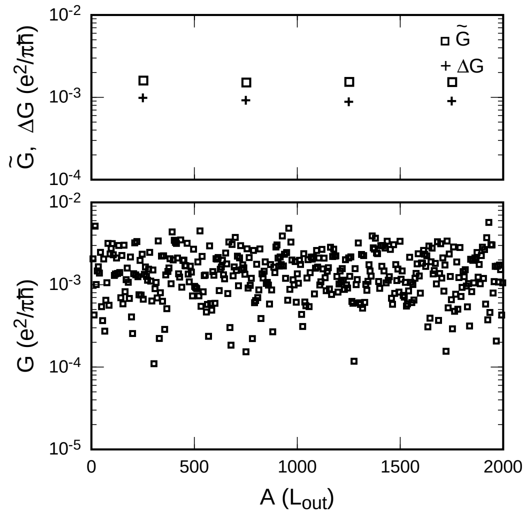

FIGURE 3. In lower panel length-dependence of conductance and in upper panel averaged conductance and fluctuation are plotted by squares and crosses, respectively, in the case of long tubes. In the lower panel the conductance is calculated at every $12T_{\rm out}$ length with $T_{\rm out}$ being the period of the outer tube in the tube axis direction, $T_{\rm out}/L_{\rm out} = 1/4\sqrt{3}$, and the conductances are plotted at every $36T_{\rm out}$ length for simplicity. The maximum length $2000L_{\rm out}$ is about 9 μm.

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REFERENCES

1. M. Kociak, K. Suenaga, K. Hirahara, Y. Saito, T. Nakahira, and S. Iijima, Phys. Rev. Lett. **89**, 155501 (2002).
2. J. M. Zuo, I. Vartanyants, M. Gao, R. Zhang, and L. A. Nagahara, Science **300**, 1419 (2003).
3. S. Roche, F. Triozon, A. Rubio, and D. Mayou, Phys. Rev. B **64**, 121401 (2001).
4. Y.-G. Yoon, P. Delaney, and S. G. Louie, Phys. Rev. B **66**, 073407 (2002).
5. T. Ando, Phys. Rev. B **44**, 8017 (1991).