Perfect transmission from dirty electrode to carbon nanotube

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Abstract A contact resistance between a carbon nanotube and metallic electrode is studied in a tight-binding model. A model of dirty contact is employed for electrode weakly coupled to the carbon nanotube. Both weak coupling and large contact area make perfect transmission possible in two-terminal measurement.

1 Introduction

Carbon nanotubes (CN's) are new kinds of quantum wires topologically different from conventional wires fabricated at semiconductor heterostructures. Transport properties of CN's are interesting because of their unique topological structure. The absence of backward scattering was predicted even if there are scatterers having a potential range longer than the lattice constant [1], whose origin was related to Berry's phase [2].

For experimental measurement of transport properties in CN's themselves, it is important to know properties of contact between the CN and electrode, which are currently the subject of intensive theoretical study. For example, the transmission probability between a single-wall CN and a jellium metal was discussed [3] and explicitly calculated [4]. A coupling of CN with a copper chain was discussed using pseudopotential [5] and that with a metal in a jellium model [6]. The purpose of this paper is to study effects of the contact between a carbon nanotube and dirty electrode and to show the condition of the observation of a perfect conductance in two-terminal measurement.

2 Model of Contact

We consider a semi-infinite armchair nanotube with circumference $L=\sqrt{3}aM/2$ as shown in Fig. 1, where M is an integer and a is the lattice constant. We attach ideal leads to carbon atoms lying close to the left edge and calculate the conductance between the leads and CN. The conductance is proportional to the transmission probability from leads to the tube region infinitely away according to Landauer's formula.

The ideal leads consisting of a one-dimensional lattice are connected to many carbon atoms in CN as long as leads attached to different carbon atoms are independent of each other. The equation of motion for amplitude C_0 of a wave function at $j=0$ on the graphite sheet is given by

$$(\varepsilon-\Sigma)C_0+\gamma_0\sum_{i=1}^{3}C_{\boldsymbol{\tau}_i}=\frac{i\hbar\sqrt{|v(k')|}}{a'}. \tag{1}$$

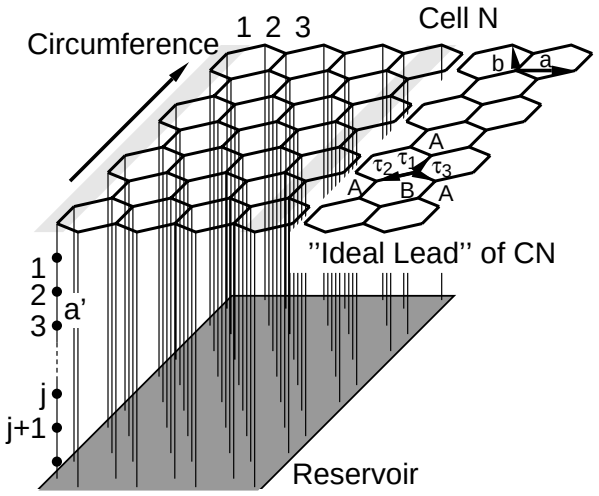

Fig. 1 Schematic illustration of the lattice structure of armchair CN and ideal leads. Only some part of CN is shown in the circumference direction. The cells $n=1$ and N are with shadow and the cell with $n=N+1$ is connected to an "ideal lead" of CN. Carbon atoms in cells $n=1$ to N are connected to a reservoir through an ideal lead characterized by the transfer integral t and lattice constant a'.

with

$$\Sigma=-t\exp(ik'a'), \tag{2}$$

where $v(k')$ is the group velocity of the states k' on the ideal lead and γ_0 is the transfer integral between three nearest-neighbor sites, which are connected by vectors $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$, and $\boldsymbol{\tau}_3$ in CN as shown in Fig. 1. The term Σ can be viewed as a self-energy arising from the interaction of CN with the ideal lead and $t=|\Sigma|$ is the parameter describing the coupling strength between the electrode and CN.

We introduce time $\tau_\phi=\hbar/|\mathrm{Im}\,\Sigma|$ during which an electron stays on a carbon atom in the contact region without going into ideal leads. By multiplying the velocity $\gamma/\hbar$ in CN, the corresponding length is defined by $l_\phi=\gamma\tau_\phi/\hbar$. This "phase coherence" length corresponds to the length of the nanotube covered by an electron before going into ideal leads in the contact region.

3 Numerical Results

Figure 2 shows calculated conductance as a function of t/γ_0 for several values of N. The conductance increases with t for small t, takes a maximum, and then starts to decrease. The value of t corresponding to the maximum conductance becomes smaller with the increase of

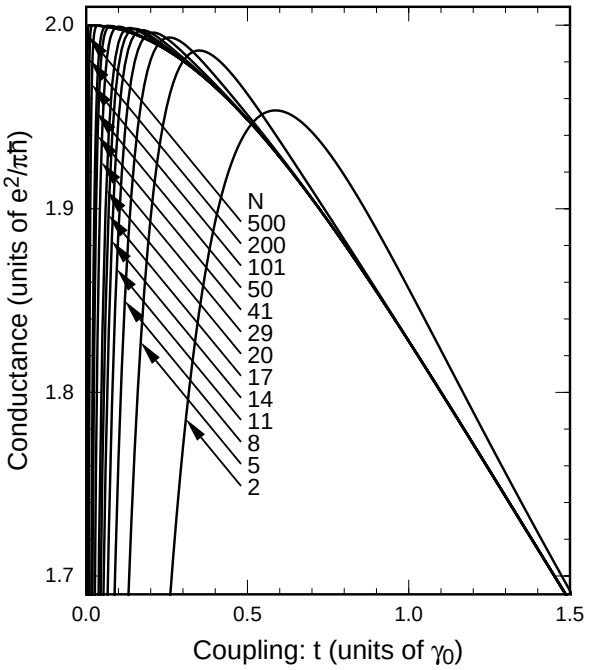

Fig. 2 Calculated conductance of CN with $L/a=50\sqrt{3}$ as a function of the coupling t for several values of N.

the length of the region connected to ideal leads. In the limit $N \to \infty$ the conductance comes up to the ideal value $G = 2e^2/\pi\hbar$ at $t/\gamma_0 = 0$ and decreases with the increase of t/γ_0. This reduction from the ideal value for nonzero t/γ_0 is due to reflection of the electron wave at the 'junction' between the nanotube with attached leads and the ideal nanotube lead. The results show clearly that a weak coupling between contacts and CN and a sufficiently large contact area are appropriate conditions for ideal electrodes, i.e., ideal for the observation of the conductance of a nanotube itself without any contact resistance.

Although not shown explicitly, the contribution to the conductance depends strongly on the lead position [7]. For small t and $Na/2 \lesssim l_\phi$, the conductance increases with N, where all cells contribute to the conductance almost equally. With the further increase of N, the conductance becomes independent of N when $Na/2 \gg l_\phi$. In this case, the contribution to the conductance is larger for a cell with large n, i.e., away from the left end, and becomes negligibly small for $n \ll N$. The reason is that an electron transmitted into the tube from a lead in a cell close to the left end is almost always scattered into other leads before being going into the region of the nanotube without leads.

The most crucial assumption of the model is that leads connected to different carbon atoms are completely independent of each other. Strictly speaking, this can be justified only when the phase coherence length in the metallic electrode is smaller than or of the same order as the lattice constant of CN. Even if such conditions are not completely satisfied, the model may describe essential features in the case that the electrode consists of dirty metals without translational symmetry. In actual experiments, various different metals are used as electrodes including liquid metals. They are mostly dirty metals without translational symmetry.

In realistic cases the transfer integral t' between a carbon atom and a metal atom can be quite different form t and may be reduced considerably by randomness of the contact surface or mismatch of a lattice constant. We find that the calculation can be extended easily to such a case and the important coupling parameter t is replaced by ${t'}^2/t$ which can be much smaller than t [7].

When a contact metal is not ideal, some carbon atoms are strongly coupled to electrode and others are weakly coupled due to randomness present in the contact region. Such disorder effects can be studied by varying the transfer integral t of ideal leads among different leads. In this case the effective coupling is characterized by the average transfer $t_{\rm av}$ and its width δt of the distribution. Explicit numerical calculations show that such disorder effect is not important and that t in the results should be replaced by $t_{\rm av}$ in the presence of randomness [7].

4 Summary and Discussion

We have studied the conductance between CN and a dirty metallic contact using the model in which a single ideal lead is attached to each carbon atom in the contact region. The result shows that the negligible contact resistance can be realized if we make the coupling between CN and the electrode sufficiently small, i.e., $t/\gamma_0 \ll 1$, and the contact area sufficiently large. For such contacts, fluctuations in the coupling strength due to randomness are not important because the effective coupling between CN and an electrode is essentially determined by an average over a large area.

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