Negligible inter-wall interaction in sliding double-wall carbon nanotubes

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Abstract. The inter-tube conductance is quite small in double-wall carbon nanotubes. When both edges are present in the outer tube or the inner tube, the conductance exhibits wild and discrete fluctuations as a function of the tube length and varies smoothly with a small oscillation as a function of the shift in the relative position of the outer and inner tubes. When one edge is in the outer tube and another in the inner tube like in telescoping tubes, the conductance exhibits a smooth but irregular oscillation as a function of the length corresponding to a certain combination of the length and position change.

1. Introduction
In double-wall carbon nanotubes the lattice of an outer tube and that of the inner tube is incommensurate [1, 2]. The situation is same in multi-wall nanotubes. Because each tube is weakly coupled to others through a weak van der Waals force, inner core tubes can be mechanically slid with low friction [3]. This fact was used in the measurement of the inter-tube conductance as a function of the position of core tubes (telescoping tubes) [4, 5]. In this paper, the inter-wall conductance in such sliding double-wall tubes is calculated for different configurations. In the configuration corresponding to telescoping tubes, in particular, the conductance is shown to exhibit a smooth but irregular oscillation as a function of the tube length.

2. Model and method
We consider double-wall tubes consisting of metallic outer and inner tubes near the Fermi energy in a nearest-neighbor tight-binding model including only π orbital [6]. The resonance integral between π orbitals at \( \mathbf{R}_1 \) and \( \mathbf{R}_2 \) of adjacent walls is chosen as

\[
-t(\mathbf{R}_1, \mathbf{R}_2) = \alpha \gamma_1 \exp \left( -\frac{d - c/2}{\delta} \right) \left( \frac{\mathbf{p}_1 \cdot \mathbf{d}}{d} \right) \left( \frac{\mathbf{p}_2 \cdot \mathbf{d}}{d} \right) - \gamma_0 \exp \left( -\frac{d - a_0}{\delta} \right) \left[ (\mathbf{p}_1 \cdot \mathbf{e})(\mathbf{p}_2 \cdot \mathbf{e}) + (\mathbf{p}_1 \cdot \mathbf{f})(\mathbf{p}_2 \cdot \mathbf{f}) \right],
\]

where \( a_0 \) is the distance between neighboring carbons in two-dimensional graphite given by \( a_0/a = 1/\sqrt{3} \) with \( a \) the lattice constant, \( c \) the lattice constant along the c axis in graphite given by \( c/a = 2.72 \), and \( \delta \) the extent of π orbital. Further, \( \gamma_0 \) is the resonance integral between nearest-neighbor sites in each layer and \( \gamma_1 \) is that of neighboring layers. Vectors \( \mathbf{p}_1 \) and \( \mathbf{p}_2 \) are...
Unit vectors directed along $\pi$ orbitals at $\mathbf{R}_1$ and at $\mathbf{R}_2$, respectively, $\mathbf{d}$ a vector connecting the two sites with the length $d$, and $\mathbf{e}$ and $\mathbf{f}$ unit vectors perpendicular to $\mathbf{d}$ and to each other.

Figure 1 shows illustration of four-terminal double-wall tubes considered in the following. Inter-tube transfer is present only in hatched double-wall regions, while tubes are independent outside the region and connected to reservoirs. This geometry is ideal for revealing essential features of inter-wall interaction because of the absence of boundaries which tend to obscure them through the strong reflection and interferences of the electron wave [6].

In a telescoping tube used experimentally [3], the left edge of the outer tube and the right edge of the inner tube are fixed and the length of the overlapping region is changed continuously. This can be simulated well by the configuration shown in Fig. 1(c), where the left edge of the outer tube and the right edge of the inner tube are sharply defined. Although it is difficult to realize experimentally, we can consider the configuration shown in Fig. 1(a), where both left and right edges of the outer tube are sharply defined. Figure 1(b) is similar except that the sharp edges are defined in the inner tube.

In a telescoping tube shown in Fig. 1(c), the length of the double-wall region changes if the inner tube slides relative to the outer tube. In tubes shown in Figs. 1(a) and (b), on the other hand, a shift of the inner-tube position changes only the relative position between the outer and inner tubes and the length change is achieved by adding or removing carbon atoms at the edges. Because the inter-tube coupling is weak and has a strong tendency to cancel each other among neighboring sites, the inter-wall conductance can be calculated using Landauer’s formula with effects of inter-wall hopping being included to the lowest order.

**3. Results and discussion**

In the following, calculated conductance is shown for tubes consisting of an outer (6,15) tube with diameter $\sim 1.5$ nm and an inner (4,7) tube as a typical case. Figure 2 shows calculated...
length dependence of the inter-tube conductance for tubes with two sharp edges on (a) the outer tube and (b) the inner tube. Both results show that the conductance remains much smaller than $e^2/\pi\hbar$ [a typical value is $10^{-4}(e^2/\pi\hbar)$] and exhibits a wild and irregular oscillation as a function of the length. Its average and fluctuation are independent of the length and this feature prevails even in longest nanotubes realized experimentally.

This behavior can be understood as follows: The phase of the wave function at the Fermi energy is given by the wave vector at the $K$ and $K'$ points located at the corner of the hexagonal first Brillouin zone and therefore jumps by an amount $\pm 2\pi/3$ when the position changes by a primitive lattice vector. Because of this rapid phase jump and the quasi-periodic nature due to incommensurate lattice structure, almost all inter-tube transfers cancel out and remain nonzero only because of an incomplete cancellation due to the presence of sharp edges. In fact, when inter-wall interaction is turned on smoothly over the distance of the order of the lattice constant, the inter-wall conductance becomes several order of magnitude smaller [6]. As a result the inter-tube conductance is extremely sensitive to edges of the double-wall region. Both average and fluctuation in Fig. 2(a) are approximately four times as large as those in Fig. 2(b). This difference is a typical example showing this sensitivity.

Figure 3 shows the dependence of the conductance on the position of inner tube for several long tubes. Figure 3(a) corresponds to the presence of sharp edges in the outer tube and (b) in the inner tube. Upper horizontal axes in Figs. 3(a) and (b) are in units of the period of the inner tube $T_2$ and that of the outer tube $T_1$, respectively. The conductance oscillates with period $T_2$ in (a) and $T_1$ in (b) as is expected. The conductance changes smoothly as a function of the position with less fluctuations as compared to that in Fig. 2. This reduction of fluctuation is expected because the change in an effective inter-tube coupling at a site due to slide of the inner tube tends to cancel that at another site. The distribution of the conductances for various
lengths are the same as those in Fig. 2, however.

Figure 4 shows the length dependence of the conductance for telescoping tubes shown in Fig. 1(c). Three typical examples are plotted, which are chosen from among many results for tubes with different edges, because qualitative feature is independent of tube edges. The conductance changes continuously but in a somewhat irregular manner with the increase of the length. Its average is smaller than that in Fig. 2(a) while larger than that in Fig. 2(b). The fluctuation is smaller than that in Fig. 2(a), similar to that in Fig. 2(b), and larger than that in Figs. 3(a) and (b).

In the telescoping tube the conductance is determined by effective inter-tube couplings at the right sharp edge on the inner tube and those at the left sharp edge on the outer tube because of the cancellation except near edges. When the inner-tube position is shifted, the position of the other tube is shifted smoothly as in the case shown in Figs. 3(a) and (b) and at the same time the length of the double-wall region changes. Therefore, the conductance fluctuates from one curve to another for tubes with different lengths in Fig. 3, exhibiting an irregular oscillation with amplitude larger than that shown in Fig. 3(a).

It was reported in experiments [4, 5] that inter-tube conductance in telescoping tubes can be as large as \(0.03 \times \frac{e^2}{\pi \hbar}\) without any fluctuations. This conductance is much larger than our typical value \(10^{-4} \times \frac{e^2}{\pi \hbar}\) for tubes with about 1.5 nm outer diameter. A part of this discrepancy may be attributed to the presence of tube ends in actual telescoping nanotubes. Their presence can enhance the conductance by more than one order of magnitude due to strong reflection and interferences of the electron wave [6]. Possible dephasing effects present in actual systems also enhance the conductance [6]. It is hardly possible to account for the huge discrepancy between the theory and the experiments, however.

Multi-wall nanotubes used in the experiments have a thickness much larger than double-wall tubes considered here and are likely to contain lots of defects making the transport in each wall diffusive rather than ballistic. It is a hard task to study theoretically inter-wall conductance in such thick multi-wall nanotubes used experimentally.

4. Summary and conclusion
The inter-tube conductance in double-wall tubes with sliding inner tubes have been studied taking account of three kinds of edge configurations. The small conductance of the order of \(10^{-4} \times \frac{e^2}{\pi \hbar}\) arises due to the presence of sharp edges making the cancellation of inter-wall transfer incomplete. When both edges are present in the outer tube or the inner tube, the conductance exhibits wild and discrete fluctuations as a function of the tube length and varies smoothly with a small oscillation as a function of the shift in the relative position of the outer and inner tubes. When one edge is in the outer tube and another in the inner tube like in telescoping tubes, the conductance exhibits a smooth but irregular oscillation as a function of the length corresponding to a certain combination of the length and position change.

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