Quantum Interference in Carbon-Nanotube Electron Resonators

Jie Jiang, Jinming Dong, and D. Y. Xing

Group of Computational Condensed Matter Physics, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China

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A new mechanism is proposed to explain the slow conductance fluctuations in the conductance-gate voltage plot observed in the nanotube electron resonators. It is found that the slow conductance fluctuation is an intrinsic quantum interference phenomenon and exists in all metallic nanotube resonators except zigzag ones. Analytical expressions for both slow and rapid oscillation periods of the conductance fluctuations have been derived, which are well consistent with the existing experiments. It is predicted that the ratio of the slow oscillation period to the rapid one is independent of the gate-voltage efficiency, and determined only by the nanotube length used in experiments.

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As electronic devices shrink to nanometer size, the quantum interference between electron waves becomes important [1–8]. The well-contacted single-walled carbon nanotubes (SWCNTs) [9–12] provide an example of the devices using the quantum coherence [13–15], in which the nanotube behaves as a coherent electron waveguide. Recently, it was reported that electron interference in the perfect-contacted nanotubes manifests as conductance fluctuations vs Fermi energy with an oscillation period determined by nanotube length [13,14]. Observation of two units of quantum conductance $4e^2/h$ [14] indicates the ballistic motion of electrons in the nanotubes [16]. The most interesting observation is that the rapid conductance fluctuations are superimposed on slow ones. Such a slow conductance fluctuation was attributed to possible disorder effects in the nanotubes [13,14]. In this Letter, we present a new mechanism to show that the slow conductance fluctuation is an *intrinsic phenomenon* in the nanotube electron resonators. It is found that both the rapid and slow conductance fluctuations are quantum interference phenomena. The latter comes from nonlinear terms in the energy dispersion relations of metallic nanotubes, while the former from linear ones. Furthermore, we predict that the zigzag nanotube resonators have no slow conductance fluctuations, which are a unique exception in all metallic carbon nanotube resonators because they have identical energy dispersion relations for two propagating modes.

A Fabry-Perot electron resonator based on an armchair nanotube is shown schematically in Fig. 1. The whole model system consists of two semi-infinite leads (left and right) and a central sample with a finite length, which, as usual, for simplicity are assumed to be made of the same kind of SWCNTs [17]. Each interface between a lead and the sample is simply represented by a highlighted ring of atoms in Fig. 1, which may be regarded as a kind of defect. We introduce on-site energies u_1 and u_2 to model the complicated barrier potential at the interface. It will be seen that the results obtained in this Letter do not depend on details of the leads and barrier potentials used above. For an electron injected from one channel in the left lead, its reflected and transmitted wave propagation trajectories in the two leads and the central sample are shown clearly in Fig. 1(c).

Armchair nanotubes (N, N) have a C_N rotational symmetry so that there are N slices along the circumference direction. A C-C bond in ring m and slice l can be labeled by (m, l). The armchair nanotube has two metallic bands a_1 and a_2 (see Fig. 1 of Ref. [16]) crossing the Fermi level at two Fermi points $\pm k_F = \pm 2\pi/3$. For a given energy,

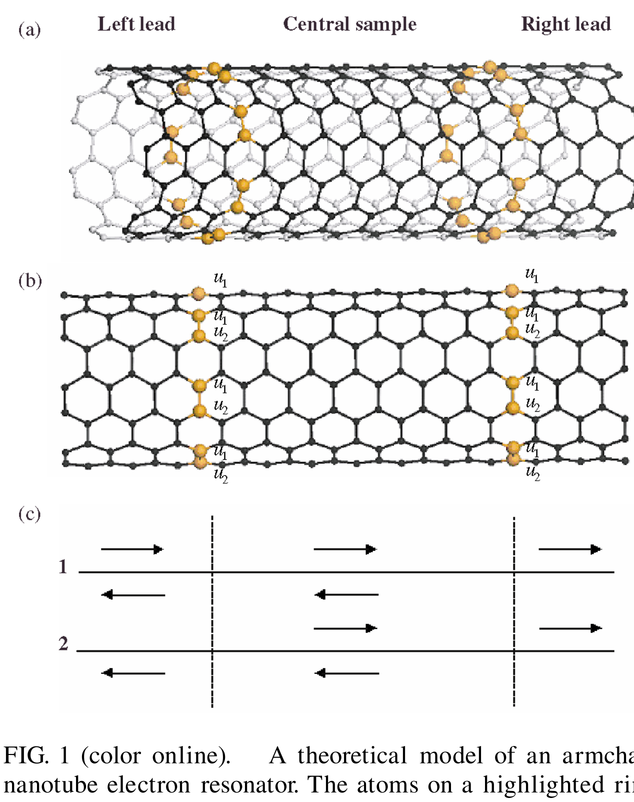

FIG. 1 (color online). A theoretical model of an armchair nanotube electron resonator. The atoms on a highlighted ring construct an interface. (a) and (b) are schematic three-dimensional and two-dimensional pictures, respectively. The electron trajectories for an electron injected from a channel are illustrated in (c).

there are four degenerate states in the two bands with wave vectors $\pm k_1$ and $\pm k_2$. Here k_1 and k_2 represent the states on band a_1 near k_F and band a_2 near $-k_F$, respectively. Under the tight-binding approximation, the wave functions of the four degenerate states are given by

$$\psi_{\pm k_1} = \frac{1}{\sqrt{2MN}} \sum_{m=0}^{M-1} \sum_{l=0}^{N-1} e^{\pm i k_1 m}(|ml;1\rangle + |ml;2\rangle),$$
$$\psi_{\pm k_2} = \frac{1}{\sqrt{2MN}} \sum_{m=0}^{M-1} \sum_{l=0}^{N-1} e^{\pm i k_2 m}(|ml;1\rangle - |ml;2\rangle), \quad (1)$$

where M is the total number of rings in the nanotube, $|ml;1\rangle$ ($|ml;2\rangle$) denotes the $|p_\perp\rangle$ orbital of the carbon atom labeled 1 (2) in the C-C bond (m, l).

At the zero-temperature and zero-bias limit, we set the wave vectors of incoming and outgoing waves to be the Fermi wave vector, i.e., $k_1 = -k_2 = 2\pi/3$. The Fermi energy in the nanotube waveguide can be changed by the gate voltage V_g, which introduces a potential energy $-\alpha V_g$ to the waveguide with α the gate efficiency factor [14]. Therefore, for an incident electron at the Fermi level, its kinetic energy in the waveguide becomes αV_g. From the energy dispersion relations in the armchair nanotube, the wave vectors in the waveguide can be determined by

$$-\alpha V_g = (1 + 2\cos k_1)|\gamma|, \qquad \alpha V_g = (1 + 2\cos k_2)|\gamma|, \quad (2)$$

where $\gamma \approx -2.7$ eV is the nearest-neighbor hopping amplitude [16]. With the help of Eq. (1), the boundary conditions are constructed through the continuity equations and the equations of motion [18] at sites on the boundary. Then, it is straightforward to analytically derive the transmission coefficients $t_{il,jr}$ for a wave going from the ith channel on the left electrode to the jth channel on the right electrode [19]. From the analytical expressions of $t_{il,jr}$, it follows that in the case of $u_1 \neq u_2$ the two propagating modes are coupled, whereas, if $u_1 = u_2$, the two modes are independent due to the symmetry of barrier potential [20,21].

After $t_{il,jr}$ is obtained, the conductance of the electron resonator can be calculated based on the multichannel Landauer-Büttiker formula [22–24]

$$G = (2e^2/h) \sum_{i,j=1}^{2} |t_{il,jr}|^2. \quad (3)$$

Figure 2 gives a plot of the conductance vs gate voltage ($G - V_g$) for $u_1 \neq u_2$, in which $u_1 = 1.0$ eV, $u_2 = 6.0$ eV, and M is taken as 1624, corresponding to a nanotube length of about 200 nm. The parameter α is taken to be 0.01, estimated from the capacitance of nanotube in Ref. [13], i.e., $C_L \approx 20\ electrons\,\mathrm{V}^{-1}\,\mu\mathrm{m}^{-1}$. It is seen that the rapid fluctuations are superimposed on a slow fluctuation background. The rapid oscillating period is found to be about 0.9 eV, corresponding well to the experimental result [13]. Moreover, as shown in the inset of Fig. 2, our calculated result reproduces the slow oscillating behavior in Fig. 1 of Ref. [13]. It is worthwhile pointing out that, since the gate voltage V_g used in Ref. [13] varies smaller, a full oscillating period of the slow conductance fluctuation was not observed; while with a larger variation of V_g, several slow oscillating periods were observed in Ref. [14]. It should be pointed out that, in order to reflect the significant contribution to the conductance from the scatterings between different modes, rather different values for u_1 and u_2 are taken in our simplified model, in which only two parameters of u_1 and u_2 are taken to model the real complex barrier potential. We should emphasize that, although the fine structure of the G vs V_g spectrum maybe changed by different values of u_1 and u_2, the phenomenon of the rapid fluctuations being superimposed on a slow fluctuation background does not depend on the values of u_1 and u_2. More importantly, it is found that both of the rapid and slow oscillation periods are independent of the choice of the u_1 and u_2 values, which can also be seen clearly from the later discussions.

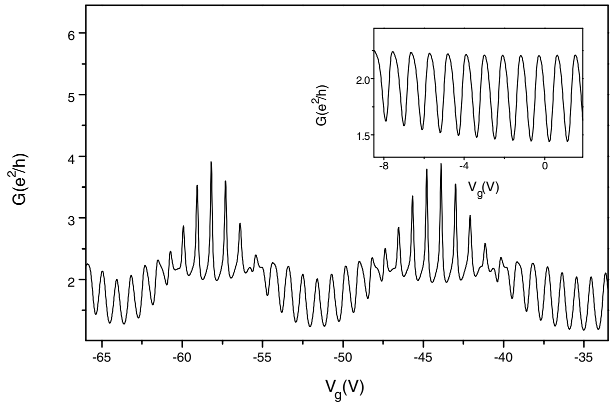

FIG. 2. Zero-bias conductance vs gate voltage of an armchair nanotube device with $\alpha = 0.01$, $u_1 = 1.0$ eV, $u_2 = 6.0$ eV, and $M = 1624$ rings of atoms. Inset, a plot in a narrower energy region near $V_g = 0$.

In both Refs. [13] and [14], the slow conductance fluctuations were argued to be induced by possible disorder in the nanotubes. However, in our model *no disorder* is introduced, but the slow fluctuations are still obtained in the armchair nanotube electron resonators. This indicates that such a slow conductance fluctuation arises mainly from intrinsic quantum interference effects in a perfect nanotube rather than from external impurities or defects. In order to make this point clear, we first analyze the wave behavior in a resonator without mode coupling. In this case ($u_1 = u_2 = u$), a wave injected from a channel must be transmitted to the same channel, forming a series of transmitted partial waves, each of which differs from the previous one by two extra reflections plus a round-trip between the barriers. Near the Fermi level, the simpler expressions of $t_{il,jr}$ can be approximately obtained as $|t_{1l,1r}| = |3/[(u/\gamma + \sqrt{3}i)^2 - (u/\gamma)^2 e^{i2k_1M}]|$ and $|t_{2l,2r}| = |3/[(u/\gamma + \sqrt{3}i)^2 - (u/\gamma)^2 e^{i2k_2M}]|$. Obviously, $|t_{1l,1r}|$ and $|t_{2l,2r}|$ have phase factors $e^{i2k_1M} = e^{i2(2\pi/3+\Delta k_1)M}$ and $e^{i2k_2M} = e^{i2(-2\pi/3+\Delta k_2)M}$, respectively, with $\Delta k_1 = k_1 - 2\pi/3$ and $\Delta k_2 = k_2 + 2\pi/3$, which can be obtained by the energy dispersion relations. From Eq. (2), we get

$$\begin{aligned} \alpha V_g/|\gamma| &= \sqrt{3}\Delta k_1 - \Delta k_1^2/2 + \cdots, \\ \alpha V_g/|\gamma| &= \sqrt{3}\Delta k_2 + \Delta k_2^2/2 + \cdots. \end{aligned} \tag{4}$$

In the first-order approximation, we have $\Delta k_1 = \Delta k_2 = \alpha V_g/\hbar v_F$ with $v_F = \sqrt{3}|\gamma|/\hbar$, so that $e^{i2k_1M} = e^{i[(2M/\hbar v_F)\alpha V_g + 4\pi M/3]}$ and $e^{i2k_2M} = e^{i[(2M/\hbar v_F)\alpha V_g - 4\pi M/3]}$. Thus, with V_g increased, both $|t_{1l,1r}|$ and $|t_{2l,2r}|$ will oscillate with a period of $\Delta V_g^r = \pi\hbar v_F/\alpha M$. But the phase difference between $|t_{1l,1r}|$ and $|t_{2l,2r}|$ keeps constant, making the total conductance fluctuate rapidly without slow fluctuations. To the second order,

$$\begin{aligned} \Delta k_1 &= \frac{\alpha V_g}{\hbar v_F} + \frac{\sqrt{3}}{6}\left(\frac{\alpha V_g}{\hbar v_F}\right)^2, \\ \Delta k_2 &= \frac{\alpha V_g}{\hbar v_F} - \frac{\sqrt{3}}{6}\left(\frac{\alpha V_g}{\hbar v_F}\right)^2, \end{aligned} \tag{5}$$

and we have

$$\begin{aligned} e^{i2k_1M} &= e^{i[4\pi M/3 + 2M(\alpha V_g/\hbar v_F) + (\sqrt{3}M/3)(\alpha V_g/\hbar v_F)^2]}, \\ e^{i2k_2M} &= e^{i[-4\pi M/3 + 2M(\alpha V_g/\hbar v_F) - (\sqrt{3}M/3)(\alpha V_g/\hbar v_F)^2]}. \end{aligned} \tag{6}$$

From Eq. (6), it follows that the phase difference between $|t_{1l,1r}|$ and $|t_{2l,2r}|$ varies with V_g, producing a slow fluctuation in G. Its oscillation period is approximately given by $\Delta V_g^s = (\hbar v_F/\alpha)(2\sqrt{3}\pi/M)^{1/2}(\sqrt{n} - \sqrt{n-1})$, where n is the number of the slow oscillating period labeled from $V_g = 0$. Next, we consider the case with mode coupling, which may complicate the wave behavior. For example, a wave injected from a channel can be transmitted to both channels. However, it is not difficult to show that in this case, $|t_{il,jr}|$ contains terms e^{i2k_1M}, e^{i2k_2M}, and $e^{i2(k_1+k_2)M}$. For the same reason mentioned above, the total conductance has only rapid fluctuations if only linear terms in Δk_1 and Δk_2 are taken into account, while it has the rapid oscillations superimposed on the slow ones if the nonlinear terms in Δk_1 and Δk_2 are included (see Fig. 2). The rapid and slow fluctuation periods are the same as those in the case of no mode coupling. From the analyses above, it follows that existence of slow fluctuations in $G - V_g$ plots is an *intrinsic* phenomenon of the armchair nanotube electron resonator. It is induced by the nonlinear terms in the energy dispersion relations, which causes the dispersion relations for band a_1 near $k_F = 2\pi/3$ to differ from those for band a_2 near $-k_F$. It is interesting to find that, although both the slow and rapid oscillation periods depend on α, their ratio, $(2\sqrt{3}M/\pi)^{1/2}(\sqrt{n} - \sqrt{n-1})$, is independent of α. It means that, for any two experiments with different gate efficiencies but the same tube length, there will be the same number of rapid oscillation periods within a slow oscillation period.

We have also studied the quantum interference in the electron resonators made of metallic zigzag nanotubes. It is found that the conductance has only rapid fluctuations with gate voltage, but, *NO slow fluctuation.* While at first glance it is surprising, this absence of slow fluctuations could be understood by the following argument. There are two completely coincided metallic bands in the zigzag nanotubes. Since the two modes have the same dispersion relations, electrons in a round-trip between two barriers will acquire the same phase shifts in the two modes. Therefore, the coefficients $|t_{il,jr}|$ contain only phase factor e^{i2kM} with k being determined from the dispersion relations,

$$-\alpha V_g = 2|\gamma|\sin(k/2). \tag{7}$$

As a direct result, there is no slow fluctuation.

The calculations made above are easily extended to arbitrary metallic nanotubes. For the same reasons discussed in armchair nanotube resonators, the nonlinear terms in the energy dispersion relations lead to slow conductance fluctuations. To the second order approximation, the slow fluctuation periods are approximately given by

$$\Delta V_g^s = (\hbar v_F/\alpha)[2\pi\tilde{r}/M\sin(3\theta)]^{1/2}(\sqrt{n} - \sqrt{n-1}). \tag{8}$$

Here $\tilde{r} = \sqrt{n_1^2 + n_2^2 + n_1 n_2}/N$ is the effective perimeter of metallic nanotube (n_1, n_2) with N the largest common divisor of n_1 and n_2, θ is the chiral angle of the nanotube, and M is the total C-C bond rings along the helical direction [25]. Equation (8) is a general result suitable for arbitrary metallic nanotubes. For $n_1 = n_2 = N$ and $\theta = \pi/6$, it reduces to the result of the armchair nanotube. The zigzag nanotube just corresponds to the case of $\theta = 0$.

In summary, we propose a new mechanism to explain the slow conductance fluctuations in the conductance-gate voltage plot observed in the nanotube electron resonators. It has been demonstrated that the slow conductance fluctuations are an *intrinsic quantum interference* phenomenon and exist in all metallic nanotube resonators *except zigzag ones.* We have analytically derived formulas for both the slow and the rapid oscillation periods of the conductance fluctuation, which are well consistent with the experimental observations. It is predicted that the ratio between the slow and the rapid oscillation periods is independent of the gate-voltage efficiency, and determined only by the nanotube length used in the experiment.

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