Theoretical Study of Fano Resonance in Single-Walled Carbon Nanotubes

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Abstract

Electrical transport through single-walled carbon nanotubes (SWNTs) is investigated by using the nearest-neighbor tight-binding model coupled with two electron reservoirs. When the SWNT-electrode coupling is not axially symmetric, asymmetric resonance peaks are found in the conductance and are considered to be due to the interference between two transport channels. These Fano resonances are sensitive to the coupling with electrodes. When the coupling is axially symmetric, no asymmetric resonance peaks are observed.

Key words: Fano resonance, Carbon nanotube, C*-algebra, Nonequilibrium steady states, Tight-binding model

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1. Introduction

Fano resonance [1], a phenomenon that causes asymmetric conductance peaks due to interference between resonant and nonresonant states, is observed in several mesoscopic systems [2,3,4,5]. Recently, first observations of Fano resonances are reported in crossed carbon nanotubes [6]. Kim et al. claimed that Fano resonances can not be observed in single-walled carbon nanotubes (SWNTs) and only appear when two nanotubes cross each other because the Fano resonances are attributed to the resonant scattering by the crossed region. Fano resonances are observed in multi-walled carbon nanotubes (MWNTs) as well, and are considered to be due to impurities, defects or disorders [7,8]. Also theoretical prediction of Fano resonances for a multiply-connected carbon nanotube has been reported where asymmetric resonance peaks are originated from the scattering by the localized states on the heptagonal defects [9]. On the contrary, Babić et al. reported that, even in SWNTs without crossed contacts, Fano resonances can be observed due to the interference between narrow and wide orbitals [10].

In this report, we investigate the possibility of Fano resonances in a single armchair nanotube with the aid of the C*-algebraic method as in our previous work on the AB-ring [11]. The tight-binding Hamiltonian is adopted for describing the electronic states of SWNTs and only the linear response regime is considered. We show that, when the SWNT-electrode coupling is axially asymmetric, Fano-like resonances exist for an armchair SWNT.

2. Electronic States of Finite SWNTs

We consider a system consisting of the two-dimensional electrodes and a finite-size armchair SWNT without caps (see Fig.1(a)). In this section, the electronic structure of the finite-size SWNT is reviewed [12]. The nanotube can be regarded as a
rolled graphene sheet and it is convenient to adopt the primitive lattice vectors of the graphene sheet for specifying the atomic positions: 
\[ L^{(1)}_{n,m} = n\xi + m\eta, \]
\[ L^{(2)}_{n,m} = n\xi + m\eta + b, \]
where \( n \) and \( m \) are the integers, \( \xi = (\sqrt{3}/2, 3/2)b \), \( \eta = (-\sqrt{3}/2, 3/2)b \), \( b = (0, b) \) and \( b \) is the nearest-neighbor bond length. The armchair nanotube is constructed by rolling the graphene sheet along the \( y \)-direction in Fig.1(b). The nearest-neighbor tight-binding Hamiltonian is used to describe the nanotube:

\[ H_c = \sum_{n,m} \left\{ -t \sigma^{(1)} \sigma^{(2)} C_{n+m}^{(1)} \right\} + \sum_{n} \frac{\eta_0}{2} \sum_{i} C_{n+m}^{(i)} (\text{H.c.)} \} \]

where \( C^{(i)}_{n+m} \) (\( i = 1, 2 \)) is the annihilation operator of the \( \pi \) electron with spin \( \sigma \) at site \( L^{(i)}_{n,m} \), \( t \) is the nearest-neighbor hopping strength and the on-site energy \( \epsilon_0 \) linearly depends on the gate voltage applied to the nanotube. Throughout this report, the repeated spin index means the summation over it. The Coulomb interaction is neglected. In the case of the armchair nanotube, the site \( L^{(i)}_{n,m} \) is identified with \( L^{(i)}_{n+M,m+M} \) \( (M \in \mathbb{N}) \) and, then, the condition: \( C^{(i)}_{n+m} = C^{(i)}_{n+M,m+M} \) is imposed. In terms of new annihilation operators:

\[ e^{(i)}_{l|\sigma} = \frac{1}{\sqrt{M}} \sum_{n=0}^{N} \sum_{m=0}^{N} e^{-i4\pi(n+2m)\eta} S_m^{(i)} C_{n+m,m}^{(i)} \]

where \( S_m^{(i)} = \sqrt{2/(N+2)} \sin((n+1)|\theta_i| \), \( a_{l|\sigma} = \pi l/M \) and \( \theta_i = \pi(l+1)/(N+2) \), the Hamiltonian of an armchair SWNT of length \( \sqrt{3}/2bN \) becomes:

\[ H_c = \sum_{l=0}^{N} \sum_{l'=0}^{M-1} \left\{ -t e^{(1)}_{l|\sigma} \left( 1 + e^{-i\theta_l} + e^{-i\theta_{l'}} \right) \right\} + \sum_{n=0}^{N} \sum_{m=0}^{N} e^{(1)}_{l|\sigma} e_{l'|\sigma} \right\} + \text{(H.c.)}. \]

We remark that \( S_{nl} \) satisfies:

\[ \sum_{l=0}^{N} S_{nl} S_{lm} = \delta_{nm}. \]

The Hamiltonian \( H_c \) is then, diagonalized by a unitary transformation:

\[ f^{(1)}_{l|\sigma} = P_l e^{(1)}_{l|\sigma} + Q_l e^{(2)}_{l|\sigma}, \]

\[ f^{(2)}_{l|\sigma} = -Q_l e^{(1)}_{l|\sigma} + P_l e^{(2)}_{l|\sigma}, \]

and one has

\[ H_c = \sum_{l=0}^{N} \sum_{l'=0}^{M-1} \sum_{\gamma = \pm} e^{(\gamma)}_{l|\sigma} f^{(\gamma)}_{l|\sigma} f^{(\gamma)}_{l'|\sigma} \] (1)

where \( e^{(\gamma)}_{l|\sigma} = -\gamma l (1 + 2 \cos \theta_l + 4 \cos^2 \theta_l)^{1/2} \). Note that, as \( e^{(\gamma)}_{l|\sigma} = 0 \) for \( a_{l|\sigma} = 0, \theta_l = 2\pi/3 \), the armchair SWNT is metallic.

3. Steady States and Electrical Transport

Now we consider the effect of the electrodes. The total Hamiltonian is given by:

\[ H_{el} = \int dk \omega_{k\lambda} a_{k\sigma}^\dagger a_{k\sigma} \]

as the source-drain voltage. The second term \( H_c \) stands for the nanotube Hamiltonian (1) and

\[ V = \sum_{l=0}^{N} \sum_{l'=0}^{M-1} \sum_{\gamma = \pm} \{ h_{l|\sigma}^{(\gamma,\lambda)} (u_1^{l|\sigma} f^{(\gamma)}_{l|\sigma} + \text{(H.c.)}) \} \]

represents the tunneling between the nanotube and electrodes. We denote \( a_{k\lambda}^{(\lambda)}(u) = \int dk u_{k\lambda} a_{k\lambda} \) and \( h_{l|\sigma}^{(\gamma,\lambda)} \) are given by:

\[ h_{l|\sigma}^{(\pm,L)} = \frac{S_{nl}}{2M} \sum_{m=0}^{M-1} \left\{ \pm U_m^{(1)} e^{-i\theta_l} + \pm U_m^{(2)} e^{-i\theta_{l'}} \right\} e^{\pm i\pi l}, \]

\[ h_{l|\sigma}^{(\pm,R)} = \frac{S_{nl}}{2M} \sum_{m=0}^{M-1} \left\{ \pm U_m^{(1)} e^{-i\theta_l} + \pm U_m^{(2)} e^{-i\theta_{l'}} \right\} e^{\pm i\pi l}, \]

where \( \theta_l = 2\theta_l \pm \delta_{l|\sigma} \), \( \delta_{l|\sigma} = \theta_{l'} \pm a_{l|\sigma} N, \delta_{l|\sigma} = \frac{\pi}{3} \). \( \delta_{l|\sigma} \) is the phase of \((-1 + e^{-i\theta_l} (e^{i\theta_l} + e^{-i\theta_{l'}}))\) and the product \( U_m^{(1)} \cdot u_{k\lambda} \) stands for the tunneling strength between each edge site of the nanotube and the electrode \( \lambda \).

In order to calculate the steady-state current from the left to right electrodes, we derive the asymptotic incoming fields \( \beta_{k\sigma} \lambda \) that are solutions of the Heisenberg equation: \( [H, \beta_{k\sigma} \lambda] = -\omega_{k\lambda} \beta_{k\sigma} \lambda \). They are given by:
\[ \beta_{k\sigma\lambda} = a_{k\sigma\lambda} + \sum_{i=0}^N \sum_{\ell'=0}^{M-1} \sum_{\gamma \in \pm} \left\{ \frac{u_{k\lambda}^* \chi_{\mu\lambda}^{(\lambda)}(\Lambda(\omega_{k\lambda}) - \epsilon_{\mu\lambda}^{(\gamma)})}{\Lambda(\omega_{k\lambda})} \right\} \]
\[ + \int \frac{dk'}{(\omega_{k\lambda} - \omega_{k'\lambda} - i0)} \frac{u_{k'\lambda} u_{k\lambda}^{\ast}}{\Lambda(\omega_{k\lambda})} \]
\[ + \frac{u_{k'\lambda} u_{k\lambda}^{\ast}}{\Lambda(\omega_{k\lambda})} \right\} \]
\[ \langle \beta_{k\sigma\lambda}^{(\ast)} \rangle = F_\lambda(x) \delta(k - k') \delta_{\sigma\sigma'} \delta_{\lambda\lambda'} \]
\[ \langle \beta_{k\sigma\lambda}^{(\ast)} \rangle = F_\lambda(x) \delta(k - k') \delta_{\sigma\sigma'} \delta_{\lambda\lambda'} \]

where \( \eta_{\mu\lambda}^{(\lambda)}(\omega_{k\lambda}) = \nu(\omega_{k\lambda}) M_\lambda(\omega_{k\lambda}) + \chi_{\mu\lambda}^{(\lambda)}(\omega_{k\lambda}) \), \( \chi_{\mu\lambda}^{(\lambda)}(\omega_{k\lambda}) = h_{\mu\lambda}^{(\lambda)}(1 - g_{\lambda\lambda} M_\lambda(\omega_{k\lambda})) + h_\lambda^{(\lambda)} g_{\lambda\lambda} M_\lambda(\omega_{k\lambda}) \), \( \nu(x) = |g_{LR}(x)|^2 - |g_{LL}(x)|^2 - c_{RR}(x), \)
\[ \langle \beta_{k\sigma\lambda}^{(\ast)} \rangle = F_\lambda(x) \delta(k - k') \delta_{\sigma\sigma'} \delta_{\lambda\lambda'} \]

In the above, \( \Lambda = R, R = L \). As in [11], if the system admits no bound state, a nonequilibrium steady state (NESS) is rigorously constructed from the time-evolution. The NESS is found to satisfy Wick’s theorem and is fully specified by the two-point function:
\[ \langle \beta_{k\sigma\lambda}(x) \beta_{k'\sigma'\lambda'}(x') \rangle = F_\lambda(x) \delta(k - k') \delta_{\sigma\sigma'} \delta_{\lambda\lambda'} \]

where \( F_\lambda(x) \) indicates the Fermi-Dirac distribution function of the electrode \( \lambda \) with temperature \( T_\lambda \) and chemical potential \( \mu_\lambda \).

The current operator is the time-derivative of the left-electrode number operator: \( \vec{n}_{k\sigma L} = \int dk a_{k\sigma L}^{\dagger} u_{k\sigma L} \) and its average is
\[ \langle \hat{J} \rangle = \frac{e}{\hbar} \sum_{i=0}^N \sum_{\ell'=0}^{M-1} \sum_{\gamma \in \pm} \left\{ h_{\mu\lambda}^{(\gamma)} a_{\sigma}^{(L)}(u)^{\dagger} f_{\ell'\sigma}^{(\gamma)} + (c.c.) \right\} \]

By expressing \( a_{\sigma}^{(L)}(u) \), \( f_{\ell'\sigma}^{(\gamma)} \) with the asymptotic field operators \( \beta_{k\sigma\lambda} \) and by using (3), the steady-state current casts into the Landauer formula [13]:
\[ \langle \hat{J} \rangle = \frac{e}{\hbar} \int_{\omega_c}^{\infty} dx T(x) \times \{ F_L(x) - F_R(x) \} \]

where \( \omega_c \) is the density of states of the electrodes and other functions are defined after (2). Here, we are interested in the linear response regime at \( T_L = T_R = 0 \) and the variables \( u_{k\lambda L} \) and \( u_{k\lambda R} \) are taken to be the same and \( k \)-independent, i.e., \( u_{k\lambda L} = u_{k\lambda R} = u \).

4. Fano Resonances in SWNTs

As the nanotube length is finite, the integrand of (5) is a highly-oscillatory function of \( x \) with period \( \sim 3\pi t/N \). So we consider the average conductance: \( G = \langle \hat{J} \rangle / V \) where \( V \) is the source-drain voltage. In Fig. 2, the average conductance for \( eV/t \sim 0.3 \) as shown as a function of \( \epsilon_0 \) which corresponds to the gate voltage. The structural parameters of the nanotube are \( (N, M) = (7000, 15) \), which corresponds to the length of 1.72 \( \mu \)m and the diameter of 1.90 nm.

One can see that the envelope forms an asymmetric resonance peak around \( \epsilon_0 - \epsilon_F \approx -0.2t \). The case of \( \epsilon_0 = \epsilon_F \) corresponds to the half-filled SWNT band and the flat region observed from \( \epsilon_0 = \epsilon_F - 0.17t \) comes from the conduction band. The sharp peak below \( \epsilon_0 \) peaks -0.17t seems to arise from the van Hove singularity of the valence band nearest to the conduction band.

We remark that the conductance is suppressed just below the conductance maximum \( (\epsilon_0 - \epsilon_F)/t < -0.2 \). The dip seems to be caused by the interference between the two bands, the conduction and valence bands. This means that the valence band nearest to the conduction band contributes to the interference. In the system of the wave-guide geometry, even without the confined states, similar suppression of the transmission due to the interference has been reported [14].

We note that such asymmetric peaks are very sensitive to the coupling between the nanotube and electrodes. In the above calculation, four tunneling matrix elements \( \sum_{i=1}^{M-1} U_{\mu\lambda} \epsilon_{2\sigma} e^{-i2\pi \ell' M}(\lambda = L, R; i = 1, 2) \) involved in \( \chi_{\mu\lambda}^{(\gamma)} \) are taken as the same real numbers. This assumption implies that the nanotube contacts with both electrodes via single sites. This choice breaks the axial symmetry of the coupling, but the left and right contacts are equivalent. Indeed, when nanotube-electrode coupling is axially symmetric, Fano-like shapes disappear in the conductance. This could be understood as follows: Suppose that an asymmetric peak arises from the interference between axially symmetric and asymmetric states. Then, if the coupling is axially symmetric, non-symmetric nanotube states do not contribute to the transport and the asymmetric peak would disappear.
Fig. 2. One of the asymmetric conductance peaks in the linear response regime as a function of the gate voltage. The parameter is taken as $u^4 D^2 / t^2 = 1.0$ and $(N,M)=(7000,15)$.

5. Conclusion

We found that conductance shows Fano-like line shapes even in a single SWNT due to the interference between conduction and valence bands. These peaks are strongly affected by the contact condition.

Our analysis implies that, even for the same SWNTs, Fano resonances may or may not appear depending on the contact condition with electrodes. Therefore, we think that the observations by Kim et al. [6] and by the Babić [10] are consistent.

The exact form of the peaks depends on the nanotube structure and the contact conditions. Therefore, in order to reproduce experimentally observed conductance, more detail information on the experimental setting is required. Moreover, the neglected effects of the electron-electron interaction should be taken into account. In the present work, we have shown the possibility of Fano-like conductance peak and its dependence on the contact condition. We believe the essence of these features is not altered.

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