Impurity-Induced Conductance Anomaly in Zigzag Carbon Nanotubes

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Abstract. Impurities in carbon nanotubes give rise to rich physics due to the honeycomb lattice structure. We concentrate on the conductance through a point-like defect in metallic zigzag carbon nanotube via the Landauer-Büttiker approach. At low bias, the conductance is suppressed due to the presence of an additional impurity state existing only on one of the sublattices. In consequence, the suppression is exactly half of the perfect conductance without impurity. Furthermore, there exists a transport resonance at larger bias where the perfect conductance is recovered as if the impurity were absent. Implications of these conductance anomalies are elaborated and experimental detections in realistic carbon nanotubes are also discussed.

1. Introduction

Carbon nanotubes (CNTs)[1] can be constructed by rolling up the graphene sheet[2] with a particular chiral vector. Due to the extremely large aspect ratio, CNTs are naturally made quantum wire with lots of interesting transport properties. However, in practical systems, disorder/defects are inevitable. It is thus important to understand the role of the defect in CNTs, especially how the transport properties are affected. There are many types of defects including pentagon-heptagon pairs, vacancies and chemisorption adatoms[3]. One of the recent breakthroughs is the technique of covalent attachments[4] to CNTs, making the fabrication of single-molecule junctions possible. It is rather remarkable that one can use the conductance to monitor and manipulate the covalent attachments to the targeted CNT.

Inspired by these experiments, we investigate the quantum transport through a single impurity in CNTs. For quantitative comparison with experiments, the first-principles approach of the conductance is more appropriate. On the other hand, to reveal the close connections between the conductance, the transmission matrix and the current-induced charge accumulation, a phenomenological approach may prove to be useful. Furthermore, as long as the impurity potential is short-ranged, the detail profile is not crucially important and can be captured by the strength of the pseudo-potential, which is taken to be a delta-function for simplicity. These simplifications allow us to compute the scattering states in the metallic CNT and construct the transmission matrix exactly. Making use of the Landauer-Büttiker formula in the ballistic regime, we can compute the conductance within linear response regime.

It is quite interesting that the conductance sensitively depends on the strength of the impurity potential and the bias voltage. Note that in the absence of the impurity, the conductance is...
$G = 2G_0$, where $G_0 = 2e^2/h$ is the quantum conductance. The factor of two attributes to the presence of two Dirac fermions in low energy. However, it is known that the impurity in honeycomb lattice brings out peculiar evanescent modes. As a result, the transport properties are rather rich. In some energy regime, we found the backward scattering is greatly enhanced so that one of the conducting channel is totally blocked, leading to resonant backward scattering. On the other hand, in some other energy regime, the perfect conductance is recovered, signaling the conspiracy from the evanescent modes to make the impurity potential transparent. In the following, we would elaborate on the detail derivations that provides a firm ground for the rich physics of the conductance in CNTs.

2. Tight-binding model

In the following calculations, we concentrate on the metallic zigzag CNT that is well described by the tight-binding model,

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + c_j^\dagger c_i + V_0 c_0^\dagger c_0,$$

where $t$ is the hopping amplitude between nearest neighbors and $V_0$ is the strength of the impurity potential located at $(0,0)$ as shown in Fig. 1. Since no spin-flip scattering is present, the spin just gives rise to a factor of two and is suppressed in the above expression.

The above Hamiltonian can be solved by the generalized Bloch theorem. The key is to solve the tight-binding model without the impurity potential first. Then, by forming appropriate linear combinations of the obtained solutions, the impurity scattering can be transformed into a boundary constraint. In the following, we sketch how this is done in metallic zigzag CNT. In the absence of the impurity, the transverse momentum is a good quantum number, $k_m = 2\pi m/N$ with $m = 1, 2, \ldots, N$ and $N$ is the number of unit cells around the CNT. Performing a partial Fourier transformation for the wave function in the transverse direction, $\Phi(x, y) = \sum_k \Phi_k(x) e^{iky}$, the CNT is decomposed into $N$ decoupled effective 1D chains with definite transverse momentum $k_m$. In general, the wave function after partial Fourier transformation can take the form, $\Phi_k(x) \sim \phi_k z^x$. For $|z| = 1$, these solutions correspond to the familiar plane waves. However, in the presence of the impurity potential $|z| \neq 1$ solutions are also allowed and need to be taken into consideration. For given energy $\epsilon$ and momentum $k_m$, $z$ satisfies the characteristic equation,

$$tt_m(z + \frac{1}{z}) + (t^2 + t_m^2 - \epsilon^2) = 0,$$

where $t_m = 2t \cos(k_m/2)$. By forming appropriate linear combinations of all possible solutions of $z$, the scattering states can be constructed analytically and thus the transmission matrix is
obtained. Since there are only two scattering channels in a metallic zigzag CNT, the $4 \times 4$ $S$-matrix is

$$S(\epsilon) = \begin{bmatrix} r(\epsilon) & t'(\epsilon) \\ t(\epsilon) & r'(\epsilon) \end{bmatrix},$$

(3)

where $r, r', t, t'$ are $2 \times 2$ matrices. Finally, the Landauer-Büttiker formula gives the conductance as tracing over the square of the transmission matrix,

$$G(\epsilon) = G_0 \text{Tr} \left[ t(\epsilon) t^\dagger(\epsilon) \right].$$

(4)

Making use of the analytic expression of the transmission matrix, the conductance can be evaluated by numerical approach is a straightforward way.

3. Conductance, backward scattering and phase

We now turn to our numerical results as shown in Figs. 2 and 3. First of all, since the impurity potential only exists on one lattice site, one can always form an appropriate linear combination of the two channels so that one of them remains intact from scattering. This explains why the conductance is always larger than $G_0$. Even for weak impurity potential, the conductance already shows interesting behavior at different energies. For $V_0/t = 0.5$, the conductance is close to the perfect value $G \sim 2G_0$ at most energies. However, there exist two sharp dips down to exactly $G = G_0$. What happens is the presence of a resonant state due to the impurity potential that traps the itinerant carriers and completely blocks the conducting channel. By increasing the impurity strength, the resonant backward scattering is broadened, but there remains a dip with perfect suppression $G = G_0$. Finally, for extremely strong impurity strength, the system is close to the unitary limit and the particle-hole symmetry is restored as shown by the green curve in Fig. 2.

Another interesting feature is the resonant tunneling where the tunneling conductance becomes perfect. This may not look very surprising for weak impurity strength. However, even for $V_0/t = 50$, the strong impurity potential is still transparent at some particular energies. But, how can the scattering states ignore the strong impurity scattering and maintain the conducting channel perfect? To understand this phenomena, as shown in Fig. 3, we plot the conductance and the particle density on the impurity site together for comparison. The correlation between them is transparent. When the density on the impurity site is large, the conductance has a dip, while

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**Figure 2.** Conductance versus energy for the smallest $N = 3$ zigzag CNT. Various impurity strengths $V_0/t = 0.5, 5, 50$ are shown in blue, red and green curves respectively.

**Figure 3.** The energy dependence of the conductance (red) and the particle density on the impurity site (blue) with intermediate impurity strength $V_0/t = 5$ for $N = 9$ zigzag CNT.
when the density is zero, the conductance is perfect. This correlation can be understood from the Lippmann-Schwinger equation – with vanishing density on the defect site, the perturbed wave function remain the same as the unperturbed wave function and thus the impurity potential looks transparent.

To elaborate on the correlation between the current-induced particle density and the conductance, we resort to the Friedel sum rule that relates the accumulated density to the phase $\eta_t$ of the tunneling matrix. After some algebra, we can relate the backscattered conductance $G_b = 2G_0 - G$ and the phase $\eta_t$ in a simple way,

$$G_b = G_0 \sin^2 \eta_t,$$

(5)

where $\eta_t = \text{det} t/|\text{det} t|$. According to Friedel sum rule, the change of the particle number is related the the phase, $\Delta N = \eta_t/\pi$. Thus, we come to a useful relation $G_b = \sin^2(\pi \Delta N)$ that establishes the connection between the backscattered conductance and the charge accumulation.

4. Summary and Outlook

It was demonstrated[7] that the defect in CNT can turn opaque in the Coulomb blockade regime or transparent at other bias voltages, very much similar to our findings described in previous paragraphs. Furthermore, there exist controlled methods to fabricate the defects[8] systematically, or manipulate the effective impurity strength by a voltage pulse from the tip of the atomic force microscope on a carbon nanotube[9]. The interesting features, including resonant backward scattering, perfect tunneling and the relation between the conductance and the charge accumulation, can be relevant and observed in these experiments. We acknowledge support from the National Science Council of Taiwan through grants NSC-95-2112-M-007-009 and NSC-96-2112-M-007-004 and also from the National Center for Theoretical Sciences in Taiwan.

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