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Effects of Lattice Vacancy in Carbon Nanotubes Conductance Quantization

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Conductance of carbon nanotubes (CN's) with a lattice vacancy or strong and short-range impurity potential is studied within a tight-binding model. The conductance is quantized into zero, one, or two times the conductance quantum $e^2/\pi\hbar$ depending on the type of the vacancy if its size is much smaller than the circumference of CN.

Keywords: graphite; carbon nanotube; recursive Green's function technique; Landauer's formula; mesoscopic system

INTRODUCTION

Carbon nanotubes (CN's) were first discovered by Iijima in 1991.[1] They consist of coaxially rolled graphite sheets and their electronic states change critically from metallic to semiconducting depending on tubular circumferential vector. Because of the peculiarity of their geometric and electronic structure, they are considered as a new kind of quantum wires. The purpose of this work is to study effects of scattering by a vacancy in metallic nanotubes and to demonstrate the quantized conductance in its presence.

Recently, effects of scattering on impurity potential were studied theoretically and it was proved that a Born series for back-scattering vanishes identically for scatters having a potential with a range larger than the lattice constant.[2] This intriguing fact was related to Berry's phase acquired by a rotation in the wave-vector space in the system described by a $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian which is same as Weyl's equation for a neutrino.[3] The con-

ductance was calculated in a tight-binding model by varying the strength of the potential.[4] Effects of scattering by a vacancy in metallic armchair nanotubes in the presence and absence of a magnetic field were also studied.[5]

Some recent experiments suggest the existence of defective nanotubes of carpet-roll or papiermâché forms.[6,7] These systems have many disconnections of the π electron network governing transport of CN's and therefore are expected to exhibit properties different from those in perfect CN's.

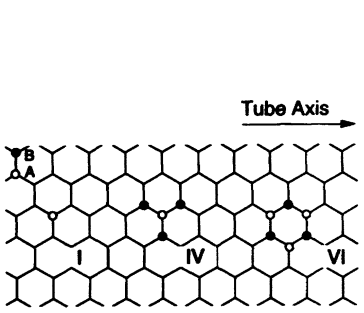
MODEL AND METHOD

We use a tight-binding model of a single π band with a nearest-neighbor hopping integral γ_0 and a lattice constant a. An armchair nanotube is known to be always metallic and has two bands in the vicinity of the Fermi energy crossing at $k_y = 2\pi/3a$ (K point) and $k_y = -2\pi/3a$ (K' point). The energy dispersion near the Fermi energy is approximately given by $\epsilon = \pm\gamma|k|$, where k is the wave vector measured from the K and K' point and $\gamma = \sqrt{3}a\gamma_0/2$. For a given energy $\varepsilon = \gamma k \geq 0$, for example, there are two channels denoted as K and K' with positive velocity $\gamma/\hbar$ and two with negative velocity $-\gamma/\hbar$.

A unit cell of two-dimensional graphite contains two carbon atoms denoted as A and B constituting a honeycomb network as shown in Fig. 1. We consider three typical vacancies: vacancy I, IV, and VI. In the vacancy I a single carbon site (site A) is removed, in the vacancy IV three B sites and one A site are removed, and in the vacancy VI three A and B sites on a ring are removed.

The conductance is calculated by multi-channel Landauer's formula,[8] given by $G = (e^2/\pi\hbar)\sum_{\mu,\nu}|t_{\mu\nu}|^2$, where μ and ν are out-going and in-coming channels, respectively. Transmission $t_{\mu\nu}$ and reflection $r_{\mu\nu}$ coefficients are calculated by a recursive Green's function technique.[8] In the following, we shall exclusively consider $\epsilon = 0$. In this case, the combinations of $\{\mu, \nu\}$ are given by {KK}, {K'K'}, {K'K}, and {KK'}. The former two correspond to intra-valley scattering within the K point or the K' point and the latter two correspond to inter-valley scattering between K and K' points.

The vacancies can be simulated by two models. In the first model (1), we consider the explicit disconnection of bonds around the vacancy. In the second model (2), on-site energy V is introduced at vacancy sites on the perfect network of CN's. In the following, we shall first choose the latter



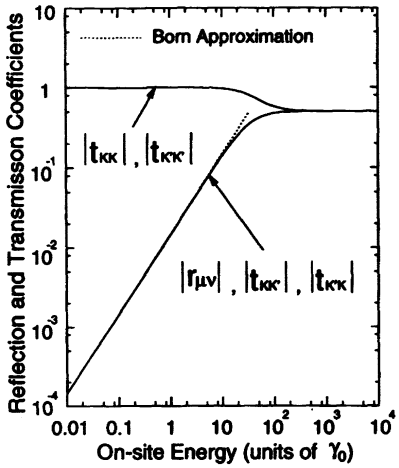


FIGURE 1 (Left) Three typical vacancies.

FIGURE 2 (Right) Transmission and reflection coefficients of armchair CN's with a vacancy I and circumference $L/\sqrt{3}a = 20$ as a function of on-site energy V.

model (2) and demonstrate that the results approach those of the former model (1) in the limit $V \to \infty$.

IMPURITIES WITH SHORT-RANGE POTENTIAL

Figure 2 shows calculated transmission and reflection coefficients for CN's with the vacancy I as a function of on-site energy V. For small V the magnitude of all reflection coefficients $|r_{\mu\nu}|$ and intra-valley transmission coefficients $|t_{K'K}|$ and $|t_{KK'}|$ increase in proportion to V in good agreement with those of the Born approximation. When V is much larger than the band width, both intra- and inter-valley components for transmission and reflection processes converge on a same value, i.e., $|t_{\mu\nu}|^2 = |r_{\mu\nu}|^2 = 1/4$ and therefore the conductance becomes $G = e^2/\pi\hbar$. In this case, the wave function vanishes at the defect site and therefore the results are exactly same as in the case of a vacancy.

In CN's with vacancy IV, $|r_{\mu\nu}|$, $|t_{K'K}|$, and $|t_{KK'}|$ increase in proportion to V following the result of the lowest Born approximation as shown in Fig.

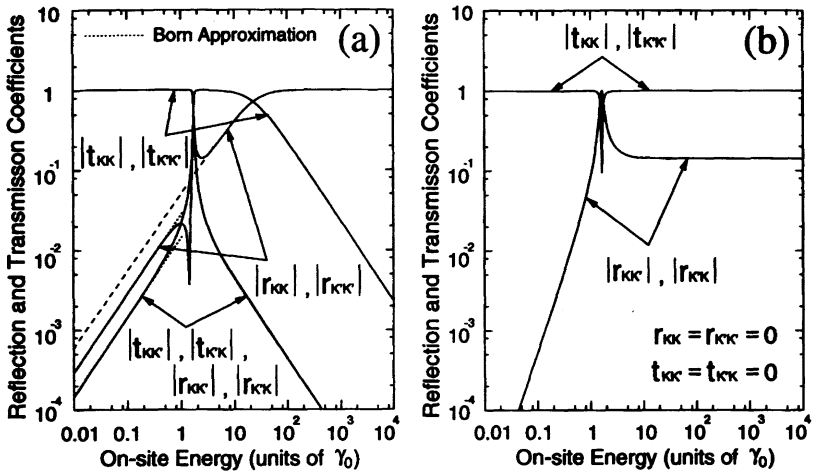


FIGURE 3 Transmission and reflection coefficients of CN's with a vacancy IV(a) and VI(b) as a function of on-site energy V, where $L/\sqrt{3}a = 20$. Dashed line shows $|r_{KK}|$ and $|r_{K'K'}|$ for a model with on-site energy on only three B sublattice sites of vacancy IV.

3(a). Both transmission and reflection coefficients show singular behavior around $V \simeq 3\gamma_0$, and $|t_{\mu\nu}|$, $|r_{KK'}|$, and $|r_{K'K}|$ decrease monotonically with further increasing of V. When V is large enough, we have $|r_{KK}| = |r_{K'K'}| = 1$ and the conductance vanishes. The resonance behavior around $V \simeq 3\gamma_0$ appears in various other kinds of impurities (see Fig. 3(b) also). It is difficult to explain the origin of this resonance intuitively.

The reflection coefficients $|r_{KK}|$ and $|r_{K'K'}|$ for a model with on-site energy only on three B sublattice sites of vacancy IV are denoted by dashed lines. When V is sufficiently large, they agree with those for vacancy IV, meaning that two models are equivalent as the vacancy. This is quite reasonable because the wavefunction cannot penetrate into the central A site through surrounding B sites due to the large on-site energy. Note that no resonance behavior is present in this case.

Figure 3(b) shows results for the vacancy VI. The back scattering within each valley r_{KK} and $r_{K'K'}$ and the transmission between different valleys $t_{KK'}$ and $t_{K'K}$ are absent because of a mirror symmetry about a plane containing the axis.[10] At $V \sim \gamma_0$, $|t_{KK}|$ and $|t_{K'K'}|$ have a dip and $|r_{KK'}|$ and $|r_{K'K}|$ reach a peak with height ~ 1, and therefore the conductance

becomes vanishingly small in a very narrow range of V. For $V \gg \gamma_0$ the conductance takes a value which is close to but slightly smaller than $2e^2/\pi\hbar$. The amount of the very small deviation is proportional to $(a/L)^2$. Because of this power-law dependence, we can neglect effects of the vacancy VI in sufficiently large CN's.

LATTICE VACANCY

Numerical calculations in the model (1) have provided completely the same results as those obtained in the model (2) discussed above for the vacancy I and IV.[5] Further, the results for the vacancy consisting of a pair of A and B sites[5] are essentially same as those for the vacancy VI presented above. In fact, in CN's with an AB pair vacancy, the conductance around $\epsilon = 0$ is slightly smaller than $2e^2/\pi\hbar$ and gradually increases and approaches $2e^2/\pi\hbar$ with the increase of the circumference. The deviation from the perfect transmission decreases with the increase of L almost in proportion to $(a/L)^2$.

Quite recently the conductance was calculated for CN's with over thirty thousand types of vacancies. The results show that the conductance is always quantized into zero, one, or two times $e^2/\pi\hbar$ depending only on the difference between numbers of sites on each sublattice and independent of the shape of the vacancy, when the vacancy is much smaller than the circumference of CN's and closely situated each other. These elaborate calculations will be reported elsewhere.

Although not shown explicitly, in the presence of a magnetic field perpendicular to the axis, the conductance is independent of the field and remains constant at $e^2/\pi\hbar$ for the vacancy I and zero for the vacancy IV. The conductance for the vacancy VI shows a large positive magnetoresistance, i.e., it decreases from $\approx 2e^2/\pi\hbar$ to zero with the increase of the field. A peculiar feature is the existence of a universal dependence on the field component in the direction of the vacancy.[5]

CONCLUSION

In this paper, we have studied the conductance as a function of the strength of the impurity potential based on a tight-binding model. When the strength

of the impurity is of the same order as the width of the π band, the transmission and reflection coefficients exhibit a complicated resonance behavior for many impurities. For a sufficiently strong potential the results are same as those of vacancies. In the case of vacancies, the conductance at $\epsilon = 0$ is quantized into zero, one, or two times $e^2/\pi\hbar$ depending on the difference between numbers of removed sites on each sublattice and independent of the shape of the vacancy. In the presence of a magnetic field perpendicular to the tube axis, the conductance depends only on the field component in the direction of the vacancy.

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