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CARBON NANOTUBES AS A PERFECT CONDUCTOR

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Effects of impurity scattering in carbon nanotubes (CN's) are studied in a $\mathbf{k}\cdot\mathbf{p}$ scheme and in a tight-binding model. The result obtained in a $\mathbf{k}\cdot\mathbf{p}$ scheme is shown to be essentially valid, including the complete absence of back scattering for scatterers with range larger than the lattice constant, unless the strength of the potential becomes comparable to the band width.

1 Introduction

Carbon nanotubes[1] are new kinds of quantum wires topologically different from conventional wires fabricated at semiconductor heterostructures. Further, electronic states in the vicinity of the Fermi level are quite different from those of free electrons. The purpose of this paper is to study effects of impurity scattering in CN's and to demonstrate the absence of back scattering in CN's except for scatterers with a potential range smaller than the lattice constant, suggesting that CN's can have an extremely high conductivity.

2 Effective-Mass Approximation

In a two-dimensional graphite, a unit cell contains two carbon atoms denoted as A and B and two bands having approximately a linear dispersion cross the Fermi level at K and K' points of the first Brillouin Zone. Therefore, electronic states in the vicinity of the Fermi level are described by a four-component envelope function $\mathbf{F}(\mathbf{r})$. In the absence of an impurity, it satisfies the equation the same as Weyl's equation for neutrinos:[2]

$$\mathcal{H}_0\mathbf{F}=\varepsilon\mathbf{F},\quad \mathcal{H}_0=\gamma\begin{pmatrix} 0 & k_x-ik_y & 0 & 0\\ k_x+ik_y & 0 & 0 & 0\\ 0 & 0 & 0 & k_x+ik_y\\ 0 & 0 & k_x-ik_y & 0\end{pmatrix},\quad \mathbf{F}=\begin{pmatrix} F_A^K\\ F_B^K\\ F_A^{K'}\\ F_B^{K'}\end{pmatrix}, \tag{2.1}$$

where γ is a band parameter, F_A^K and F_B^K are the envelope functions at A and B site related to the K point, $F_A^{K'}$ and $F_B^{K'}$ are those for the K' point,

the x axis is chosen in the circumference or chiral vector $\mathbf{L}$, and y in the axis direction.

In the presence of an impurity, the effective potential is written as[3]

$$\mathcal{H}' = \begin{pmatrix} u_A(\mathbf{r}) & 0 & e^{i\eta}u'_A(\mathbf{r}) & 0 \\ 0 & u_B(\mathbf{r}) & 0 & -\omega^{-1}e^{-i\eta}u'_B(\mathbf{r}) \\ e^{-i\eta}u'_A(\mathbf{r})^* & 0 & u_A(\mathbf{r}) & 0 \\ 0 & -\omega e^{i\eta}u'_B(\mathbf{r})^* & 0 & u_B(\mathbf{r}) \end{pmatrix} \tag{2.2}$$

where η is the chiral angle and $\omega = \exp(2\pi i/3)$. When the potential range is much shorter than the circumference $L = |\mathbf{L}|$, we have

$$\begin{aligned} u_A(\mathbf{r}) &= u_A\delta(\mathbf{r}-\mathbf{r}_0), \quad & u'_A(\mathbf{r}) &= u'_A\delta(\mathbf{r}-\mathbf{r}_0), \\ u_B(\mathbf{r}) &= u_B\delta(\mathbf{r}-\mathbf{r}_0), \quad & u'_B(\mathbf{r}) &= u'_B\delta(\mathbf{r}-\mathbf{r}_0), \end{aligned} \tag{2.3}$$

with $\mathbf{r}_0$ being the impurity position and

$$\begin{aligned} u_A &= \frac{\sqrt{3}a^2}{2}\sum_{\mathbf{R}_A} u_A(\mathbf{R}_A), \quad & u'_A &= \frac{\sqrt{3}a^2}{2}\sum_{\mathbf{R}_A} e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}_A}u_A(\mathbf{R}_A), \\ u_B &= \frac{\sqrt{3}a^2}{2}\sum_{\mathbf{R}_B} u_B(\mathbf{R}_B), \quad & u'_B &= \frac{\sqrt{3}a^2}{2}\sum_{\mathbf{R}_B} e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}_B}u_B(\mathbf{R}_B), \end{aligned} \tag{2.4}$$

where $\sqrt{3}a^2/2$ is the area of a unit cell, $u_A(\mathbf{R}_A)$ and $u_B(\mathbf{R}_B)$ are the impurity potential at site $\mathbf{R}_A$ and $\mathbf{R}_B$, respectively, and $\mathbf{K}$ and $\mathbf{K}'$ are the wave vector at the K and K' points.

In the vicinity of $\varepsilon = 0$, we have two right-going channels $K+$ and $K'+$, and two left-going channels $K-$ and $K'-$. The matrix elements are calculated as[3]

$$\begin{aligned} V_{K\pm K+} &= V_{K'\pm K'+} = \frac{1}{2}(\pm u_A + u_B), \\ V_{K\pm K'+} &= V^*_{K'\pm K+} = \frac{1}{2}(\mp u'_A e^{i\eta} - \omega^{-1}e^{-i\eta}u'_B), \end{aligned} \tag{2.5}$$

When the impurity potential has a range larger than the lattice constant, we have $u_A = u_B$ and u'_A and u'_B become much smaller and can be neglected because of the phase factor $e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}_A}$ and $e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}_B}$. This means that intervalley scattering between K and K' points can be neglected for such impurities as in the conventional $\mathbf{k}\cdot\mathbf{p}$ approximation. Further, the above shows that the back scattering probability within each valley vanishes in the lowest Born approximation. It has been proved mathematically that all back-scattering terms in the Born series vanish identically.[3] This has been ascribed to a spinor-type property of the wave function under a rotation in the wave vector space.[4]

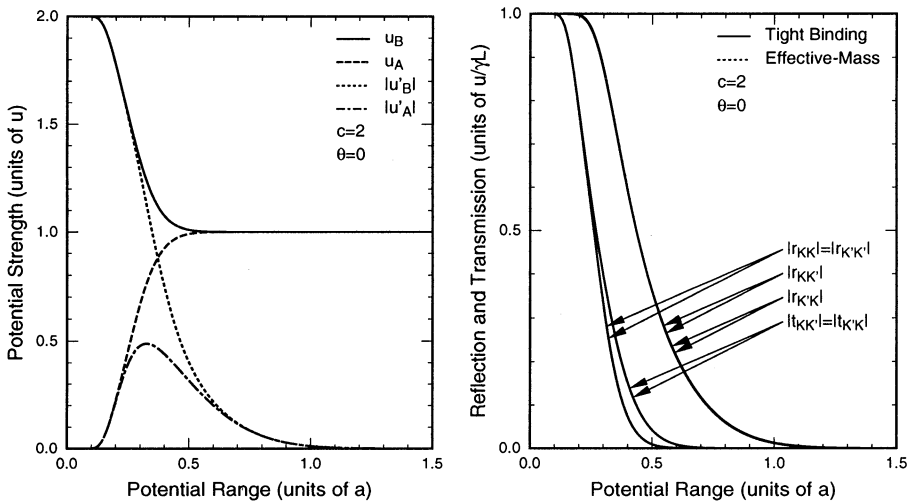

Fig. 1 (Left) Calculated effective strength of the potential for an anisotropic Gaussian impurity ($c=2$) at a B site.

Fig. 2 (Right) Calculated transmission and reflection coefficients versus the potential range at $\epsilon = 0$ for an anisotropic scatterer $c = 2$ and $\theta = 0$. The maximum potential is chosen as $0.01\gamma_0$ and $L=50\sqrt{3}a$. Results of the tight binding model and the effective-mass approximation overlap each other completely.

3 Tight-Binding Model

We consider armchair nanotubes which are known to be always metallic. We shall calculate transmission t_{nm} and reflection coefficient r_{nm}, where m and n denote in-coming and out-going channels, respectively, numerically using a recursive Green's function technique[5] as in a previous work.[6]

As a model of a scatterer, we consider an anisotropic Gaussian potential with its center at a B site and its range d which is much shorter than the circumference length L. The potential is given by

$$V(\mathbf{r}) = \frac{f(d/a,c)u}{\pi c d^2} \exp\Big[- \frac{(x\cos\theta + y\sin\theta)^2}{(cd)^2} - \frac{(-x\sin\theta + y\cos\theta)^2}{d^2} \Big], \qquad (3.1)$$

where $f(d/a,c)$ is determined by the normalization condition:

$$\sum_{i=A,B} \sum_{\mathbf{R}_i} \frac{\sqrt{3}a^2}{4} V(\mathbf{R}_i - \mathbf{R}_B^0) = u, \qquad (3.2)$$

where $\mathbf{R}_B^0$ is the impurity position.

4 Numerical Results

Figure 1 gives an example of calculated effective potential u_A, u_B, u'_A, and u'_B as a function of d/a for $c = 2$ and $\theta = 0$. When the range is sufficiently small, u_B and u'_B stay close to $2u$ because the potential is localized only at the impurity B site. With the increase of d the potential becomes nonzero even at neighboring A sites and u_A and u'_A start to increase and at the same time both u_B and u'_B decrease. The diagonal elements u_A and u_B rapidly approach u and the off-diagonal elements u'_A and u'_B vanish more slowly.

Figure 2 shows the calculated transmission and reflection coefficients. The back scattering probability decreases rapidly with d/a and becomes exponentially small for $d/a \gg 1$. The same is true of the intervalley scattering although the dependence is slightly weaker because of the slower decrease of u'_A and u'_B shown in Fig. 1. The difference from the result of the Born approximation plotted with dotted lines is negligible unless the strength of the potential becomes comparable to the band width.

5 Summary and Conclusion

In summary, we have studied the transmission and reflection coefficient of a CN with a scatterer. With the increase of the range of scatterers, the back scattering between states with $+k$ and $-k$ vanishes identically for the bands crossing the Fermi level in the absence of a magnetic field. This leads to an extremely large conductivity or mean free path. The absence of the back scattering disappears in magnetic fields,[3] which is likely to give rise to a huge positive magnetoresistance.

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