## Aharonov-Bohm effects on conductivity in carbon nanotubes: A tool for determination of a gap due to strain and curvature

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The Boltzmann conductivity is calculated for carbon nanotubes in the presence of an Aharonov-Bohm magnetic flux. Effects of strain or curvature manifest themselves as a prominent conductivity peak as a function of the flux. The appearance of the peak corresponds to the absence of backscattering in metallic linear bands and makes it possible to determine a gap due to curvature and strain.

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**1 Introduction** Carbon nanotubes (CN) are novel quantum wires consisting of rolled graphite sheets [1]. Their cylindrical shape leads to an Aharonov–Bohm (AB) effect in the band structure due to a magnetic field parallel to the axis [2, 3]. The purpose of this paper is to study conductivity in the presence of the AB flux and show that the AB effect is useful for the determination of a gap due to curvature and strain.

Intriguing electronic properties in CNs have been theoretically revealed in the  $\mathbf{k} \cdot \mathbf{p}$  scheme [4]. Metallic nanotubes are known as a ballistic conductor due to the absence of backward scattering as long as a potential range of scatterers is not smaller than the lattice constant of two-dimensional graphite [5, 6, 7]. A small gap is induced in metallic carbon nanotubes by effects of lattice strain or curvature. In the  $\mathbf{k} \cdot \mathbf{p}$  scheme, the presence of a lattice distortion can be incorporated as an effective flux [4, 8, 9] and the same is applicable to a nonzero curvature [4, 8, 10]. Therefore, this small gap is controlled by a magnetic field.

In this paper we calculate a Boltzmann conductivity in magnetic fields and demonstrate the manifestation of a strong AB effect on the conductivity due to the change in the small band gap. It is an extension of a previous work to the more general case in the presence of a perpendicular magnetic field [11].

**2** Effective-mass approximation In two-dimensional graphite, two bands having approximately a linear dispersion cross the Fermi level (chosen at  $\varepsilon = 0$ ) at K and K' points of the first Brillouin zone. The electronic states of the  $\pi$ -bands near the K point are described by the k·p equation [2, 4]:

$$\gamma(\sigma_x k_x + \sigma_y k_y) \mathbf{F}(\mathbf{r}) = \varepsilon \mathbf{F}(\mathbf{r})$$

where  $\gamma$  is a band parameter,  $\sigma_x$  and  $\sigma_y$  are the Pauli spin matrices, and  $\hat{\mathbf{k}} = (\hat{k}_x, \hat{k}_y) = -i\nabla$  is a wavevector operator. The two components of the wave function  $\mathbf{F}(\mathbf{r})$  correspond to the amplitude at sub-lattice sites in a unit cell. Electronic states of a metallic nanotube with a sufficiently large diameter are obtained by imposing generalized periodic boundary conditions around the circumference direction:

$$\mathbf{F}(\mathbf{r}+\mathbf{L}) = \mathbf{F}(\mathbf{r}) \exp(2\pi i \Phi).$$

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Fig. 1 (a) The coordinates for the nanotube. A magnetic field H is applied at an angle  $\theta$  with the axis direction of the nanotube. (b) The energy bands edges in a metallic nanotube in the presence of an effective flux  $\Phi$ . A flux due to curvature and strain,  $\phi_e$ , is opposite between the K and K' points and then a magnetic flux  $\phi$  shifts  $\Phi$  in the same direction. (c) A schematic view of the bands near the Fermi energy. In the absence of a magnetic flux shown by dotted lines, the energy gaps of  $4\pi\gamma|\varphi_e|/L$  are present at the K and K' point. As shown by solid lines, the band gap diminishes at the K' point and increases at the K point in the presence of magnetic flux  $\phi$  for  $\varphi_e > 0$ .  $k_0$  and  $k'_0$  are the Fermi wave-number measured from K and K' points, respectively. At  $\varphi = \varphi_e$  the dispersion becomes linear at the K' point.

where  $\Phi$  is an effective magnetic flux passing through the cross section and **L** is a vector corresponding to the circumference. For the K' point, Schrödinger equations are obtained by replacing  $\hat{k}_y$  by  $-\hat{k}_y$  and the effective flux can be different as will be discussed below.

A nonzero curvature causes a shift in the origin of  $\hat{k}_x$  and  $\hat{k}_y$  in the **k** · **p** Hamiltonian [4, 8, 10]. The shift in the y direction is irrelevant and that in the x direction can be replaced by an effective flux  $\varphi_c$  for the K point and  $-\varphi_c$  for the K' point. The flux is obtained as

$$\varphi_c = \frac{\phi_c}{\phi_0} = \frac{2\pi}{4\sqrt{3}} \frac{a}{L} p \cos 3\eta,\tag{1}$$

where  $\phi_0 = ch/e$  is the flux quantum, a is the lattice constant of the two-dimensional graphite, p is a dimensionless quantity of the order of unity determined by details of tight-binding parameters, and  $\eta$  is a chiral angle determining the structure of CN ( $\eta = 0$  for zigzag CNs and  $\eta = \pi/6$  for armchair CNs). This causes an opening of a narrow gap  $(2\pi\gamma/L)|\varphi_c| \propto L^{-2}|\cos 3\eta|$ . The presence of a lattice strain  $u_{\mu\nu}$  ( $\mu, \nu = x, y$ ) causes also an effective flux,  $\phi_s$  and  $-\phi_s$  for the K and K' point, respectively. It is estimated as [9]

$$\varphi_s = \frac{\phi_s}{\phi_0} = \frac{Lg_2}{2\pi\gamma} [(u_{xx} - u_{yy})\cos 3\eta - 2u_{xy}\sin 3\eta], \tag{2}$$

where  $g_2$  is the electron-phonon interaction energy. This flux gives rise to a band-gap opening also [12, 13].

In the presence of a magnetic flux  $\phi = \varphi \phi_0$  corresponding to an applied magnetic field *H* as shown in Fig. 1(a), the effective flux becomes  $\Phi = \varphi + \varphi_e$  for the K point and  $\Phi = \varphi - \varphi_e$  for the K' point, where  $\varphi_e = \varphi_c + \varphi_s$ . Figure 1(b) illustrates band edges as a function of  $\Phi$  and Fig. 1 (c) shows an example

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of the energy dispersion of the band near the Fermi energy. In the absence of magnetic flux  $\varphi$ , as shown by dotted lines in (b) and (c), the energy dispersions are the same between the K and K' points with gap  $2|\varphi_e|(2\pi\gamma/L)$ . When  $\varphi_e > 0$ , the gap diminishes at the K' point by applying  $\varphi$ , while it increases at the K point, as shown by solid lines. At  $\varphi = \varphi_e$ , the dispersion becomes completely linear at the K' point. The same thing happens for the K point at  $\varphi = -\varphi_e$ .

In the presence of a magnetic field H perpendicular to the axis, we have to introduce the vector potential  $\mathbf{A} = (A_x, A_y)$  with  $A_x = 0$  and  $A_y = (LH/2\pi)\sin(2\pi x/L)$  and replace  $\hat{\mathbf{k}}$  by  $\hat{\mathbf{k}} + (e/c\hbar)\mathbf{A}$ . Then, explicit calculations of the energy band in H can be performed only numerically [2].

**3 Impurity scattering** Most of scatterers including charged centers are characterized by a potential with range larger than the lattice constant *a*. For such scatterers, the Hamiltonian is given by a diagonal matrix for both K and K' points, and matrix elements between K and K' points are safely neglected [5]. It has been shown that the conductivity becomes infinitely large due to the absence of backward scattering in the metallic CNs characterized by linear bands [5]. These scatterers will be called *long-range* although their potential range can be comparable to the lattice constant and therefore can actually be much shorter than the electron wavelength typically of the order of the circumference. When the potential range becomes shorter than the lattice constant, the potential for two sub-lattice points in a unit cell can be different and matrix elements between K and K' points can no longer be neglected. These *short-range* scatterers cause backward scattering and make the conductivity finite [5].

In the lowest Born approximation the scattering strength for long- and short-range scatterers is characterized by the dimensionless quantity  $W_L$  and  $W_S$ , respectively, with

$$W_L = \frac{n_L \langle |u_L|^2 \rangle}{4\pi\gamma^2}, \quad W_S = \frac{n_S \langle |u_S|^2 \rangle}{4\pi\gamma^2}$$

where  $n_L$  and  $n_S$  are the concentration of long- and short-range scatterers in a unit area, respectively, and  $u_L$  and  $u_S$  are the corresponding integrated intensity of the potential [14]. Define the total strength  $W = W_L + W_S$  and the ratio  $\delta \equiv W_S/W$ . The Boltzmann conductivity is calculated under the conditions of fixed electron density  $k_+ = (k_0 + k'_0)/2$  where  $k_0$  and  $k'_0$  are the Fermi wave-number measured from the K and K' point, respectively, as shown in Fig. 1 (c).

Figure 2 shows some examples of the conductivity for  $\delta = 0.005$  and  $\varphi_e = 0.01$  with a fixed electron density. A fixed field H is applied and the angle  $\theta$  with the axis direction is varied from  $\theta = 0$  to  $\pi/2$ . In the left figure the field  $H (= 4\pi\phi_e/L^2)$  corresponds to the flux  $\varphi = \varphi_e$  at  $\theta = 0$  and in the right figure H corresponds to  $\varphi = 2\varphi_e$  at  $\theta = 0$ . When  $\varphi = \varphi_e$ , the magnetic flux cancels the effective flux  $\varphi_e$  due to curvature or strain, recovering a linear dispersion near the K' point, as shown by dashed lines in Fig. 1 (b). In this case the contribution of dominant long-range scatterers can be neglected and the conductivity is determined only by short-range scatterers for the K' point at the value of the flux. No significant change occurs in the conductivity for the K point. The appearance of the peak for the small electron density  $k_+$ corresponds to the absence of this backward scattering in metallic linear bands.

Such a prominent conductivity peak disappears when the electron density becomes larger. For the large electron density, where the dispersion at the Fermi level is nearly linear, the amount of the backward scattering is already small for long-range scatterers and the conductivity is limited mostly by short-range scatterers. As a result the conductivity becomes almost independent of the flux. The condition for the peak appearance is shown as  $\sqrt{\delta/(1-\delta)}(Lk_+/2\pi) < |\varphi_e|$  in the absence of a perpendicular magnetic field [11]. Explicit calculations for larger values of  $\varphi_e$  show that effects of the perpendicular component of the field starts to play important roles when  $\varphi_e$  becomes of the order of unity.

**4 Conclusion** The Boltzmann conductivity is calculated for carbon nanotubes in the presence of an Aharonov-Bohm magnetic flux with taking into account impurity scatterings. We have shown that effects of strains or curvature manifest themselves as a prominent conductivity peak as a function of the magnetic



Fig. 2 Calculated Boltzmann conductivity as a function of the direction of the applied magnetic field for several values of the electron density  $k_+$ , when electrons occupy the lowest conduction band of the K and K' points. The ratio of the short-range scatterers is chosen as  $\delta = 0.005$ .  $H = 4\pi\phi_e/L^2$  in the left figure and  $H = 8\pi\phi_e/L^2$  in the right figure.

flux in metallic carbon nanotubes. A careful analysis of possible gate-voltage dependence of the AB effect on the conductivity can reveal important information on curvature and strain effects and the potential range of dominant scatterers.

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## References

- [1] S. Iijima: Nature (London) 354 (1991) 56.
- [2] H. Ajiki and T. Ando: J. Phys. Soc. Jpn. 62 (1993) 2470; J. Phys. Soc. Jpn. 63 (1994) 4267 (Erratum).
- [3] H. Ajiki and T. Ando: Physica B **201** (1994) 349.
- [4] T. Ando: J. Phys. Soc. Jpn. 74 (2005) 777.
- [5] T. Ando and T. Nakanishi: J. Phys. Soc. Jpn. 67 (1998) 1704.
- [6] T. Ando, T. Nakanishi and R. Saito: J. Phys. Soc. Jpn. 67 (1998) 2857.
- [7] T. Nakanishi and T. Ando: J. Phys. Soc. Jpn. 68 (1999) 561.
- [8] C. L. Kane and E. J. Mele: Phys. Rev. Lett. 78 (1997) 1932.
- [9] H. Suzuura and T. Ando: Phys. Rev. B **65** (2002) 235412.
- [10] T. Ando: J. Phys. Soc. Jpn. 69 (2000) 1757.
- [11] T. Nakanishi and T. Ando: J. Phys. Soc. Jpn. 74 (2005) 3027.
- [12] L. Yang, M. P. Anantram, J. Han and J. P. Lu: Phys. Rev. B 60 (1999) 13874.
- [13] L. Yang and J. Han: Phys. Rev. Lett. 85 (2000) 154.
- [14] T. Ando and K. Akimoto: J. Phys. Soc. Jpn. 73 (2004) 1895.