

Aharonov-Bohm effect on exciton absorption of perpendicular light in carbon nanotubes

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Abstract

The Aharonov-Bohm effect on optical absorption of light polarized perpendicularly to the tube axis in semiconducting carbon nanotubes is studied by taking account of exciton and depolarization effect in an effective-mass approximation. The magnetic-flux dependence of the excitation energy is weak and quadratic around zero in contrast to the linear dependence for light polarized parallel to the axis.

Key words: carbon nanotube, AB effect, optical absorption, exciton, depolarization effect

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In the presence of magnetic flux threading a carbon nanotube an Aharonov-Bohm (AB) effect on the energy-band gap was theoretically predicted [1]. Its manifestation in optical absorption spectra for light polarized parallel to the tube axis was theoretically shown [2–4] and experimentally observed [5,6]. In this paper we study the AB effect on optical absorption for perpendicular light taking account of exciton and depolarization effect in an effective-mass approximation.

In a one-particle model the optical absorption is proportional to a joint density of states with a typical one-dimensional van Hove singularity. For light polarized perpendicularly to the axis, this singularity disappears because of a depolarization effect [2,3]. However, both exciton effects and Coulomb interactions were shown to play decisive roles in optical spectra [7]. It was theoretically revealed [8–10] that exciton absorption peaks

of perpendicular light can appear due to large binding energy. Such peaks were recently observed experimentally [11]. In this paper we discuss the AB effect on optical absorption of perpendicular light in semiconducting nanotubes.

A carbon nanotube is a rolled-up two-dimensional (2D) graphite sheet where the conduction and valence bands consisting of π states cross at the K and K' points. Its arrangement of carbon atoms is determined by a chiral vector $\mathbf{L} = n_a \mathbf{a} + n_b \mathbf{b}$ where \mathbf{a} and \mathbf{b} are the primitive translation vectors of a 2D graphite sheet shown in Fig. 1(a) with n_a and n_b being integers.

In the effective-mass approximation the electron motion is described by a $\mathbf{k} \cdot \mathbf{p}$ equation which is equivalent to the Weyl equation with an appropriate boundary condition in the circumference direction [1,12]. The eigen energy for the K point is given by

$$\varepsilon_{\pm n}^K(k) = \pm \gamma \sqrt{\kappa_{\nu\varphi}(n)^2 + k^2}, \quad (1)$$

where ‘+’ and ‘-’ denote the conduction and valence

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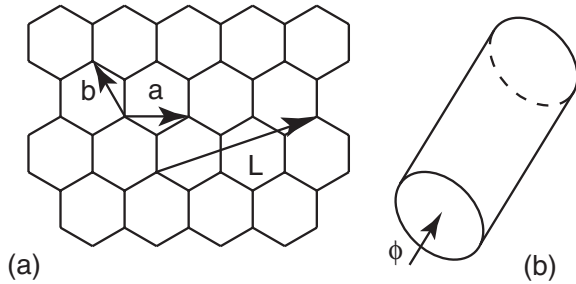


Fig. 1. Schematic illustration of (a) 2D graphite and (b) nanotube.

band, respectively, γ is a band parameter, k and $\kappa_{\nu\varphi}(n)$ are the wave number in the tube axis and circumference direction, respectively. The latter wave number is given by

$$\kappa_{\nu\varphi}(n) = \frac{2\pi}{L} \left(n + \varphi - \frac{\nu}{3} \right), \quad (2)$$

where $\varphi = \phi/\phi_0$ with ϕ and ϕ_0 being an AB magnetic flux passing through the cross section of the nanotube as shown in Fig. 1(b) and the flux quantum ch/e , respectively, and ν is an integer determined uniquely as $\nu = 0$ or ± 1 from $n_a + n_b = 3M + \nu$ with integer M .

For the K' point the energy is given by Eq. (1) with replacement $\nu \rightarrow -\nu$. Since the energy gap is given by separation between the valence and conduction bands with $n = 0$ at $k = 0$, tubes are metallic for $\nu = 0$ and semiconducting for $\nu = \pm 1$ in the absence of the magnetic flux. It should be noted that states associated with the K' point at $-\varphi$ are connected to those associated with the K point at φ by a time-reversal transformation [13,14].

The dynamical conductivity characterizing optical absorption is calculated in the linear response theory. We shall use a screened Hartree-Fock approximation to calculate interaction effect on the band structure and introduce an attractive interaction between a photo-excited electron and a remaining hole using the Coulomb interaction screened by a static dielectric function. Various approximation schemes were compared and this approximation was shown to be sufficient for single-wall nanotubes [15,16]. Actual calculations can be performed by solving equation of motion for an electron-hole pair [4,7,17].

Since states around the K and K' points are connected to each other by the time-reversal transformation, the dynamical conductivities associated with these points, $\sigma_{xx}^{Kl}(\omega)$ and $\sigma_{xx}^{K'l}(\omega)$, in the absence of

the depolarization effect are expanded as

$$\sigma_{xx}^{Kl}(\omega) = \sigma_{xx}^{K-l}(\omega) = a + b\varphi + c\varphi^2 + \dots, \quad (3)$$

$$\sigma_{xx}^{K'l}(\omega) = \sigma_{xx}^{K'-l}(\omega) = a - b\varphi + c\varphi^2 - \dots, \quad (4)$$

with $l = \pm 1$ indicating the wave number in the circumference direction, $(2\pi/L)l$, and a , b , and c being appropriate constants independent of the magnetic flux. Since the final conductivity is given by the sum of those for the K and K' point, that is,

$$\sigma_{xx}^l(\omega) = \sigma_{xx}^{Kl}(\omega) + \sigma_{xx}^{K'l}(\omega), \quad (5)$$

the odd order terms of φ cancel each other and $\sigma_{xx}^l(\omega)$ quadratically depends on the flux near zero.

For light absorption perpendicular to the tube axis, a depolarization effect has to be considered and the absorption is proportional to the real part of the conductivity [2,3]

$$\tilde{\sigma}_{xx}^l(\omega) = \frac{1}{2} [\tilde{\sigma}_{xx}^{l=1}(\omega) + \tilde{\sigma}_{xx}^{l=-1}(\omega)], \quad (6)$$

with

$$\tilde{\sigma}_{xx}^l(\omega) = \frac{\sigma_{xx}^l(\omega)}{\varepsilon_{xx}^l(\omega)}, \quad (7)$$

where the dielectric function $\varepsilon_{xx}^l(\omega)$ describing the depolarization effect is given by

$$\varepsilon_{xx}^l(\omega) = 1 + \frac{4\pi^2 |l|}{\kappa L \omega} \sigma_{xx}^l(\omega), \quad (8)$$

where κ is an effective dielectric constant describing screening by electrons in σ bands, core states, and the π bands away from the K and K' points and by surrounding materials if any.

Excitation energies with the depolarization effect are given by zero points ω_0 's of the dielectric function $\varepsilon_{xx}^l(\omega)$. Since the magnetic-flux dependence of $\sigma_{xx}^l(\omega)$ in Eq. (8) is quadratic near zero, ω_0 quadratically depends on the weak magnetic flux around $\varphi = 0$.

The strength of the Coulomb interaction in nanotubes is characterized by the dimensionless quantity given by the ratio of the typical Coulomb energy $e^2/\kappa L$ and the typical kinetic energy $2\pi\gamma/L$, i.e.,

$$\frac{e^2}{\kappa L} \frac{L}{2\pi\gamma} \approx \frac{0.35}{\kappa}. \quad (9)$$

Since κ is considered to be of the order of unity, for example, $\kappa = 2.4$ for graphite, the typical strength of the Coulomb interaction is of the order of 0.1~0.2.

The cutoff energy should be of the order of the half of the π -band width $3\gamma_0$, where γ_0 is the resonance integral between nearest neighbor sites and related to the

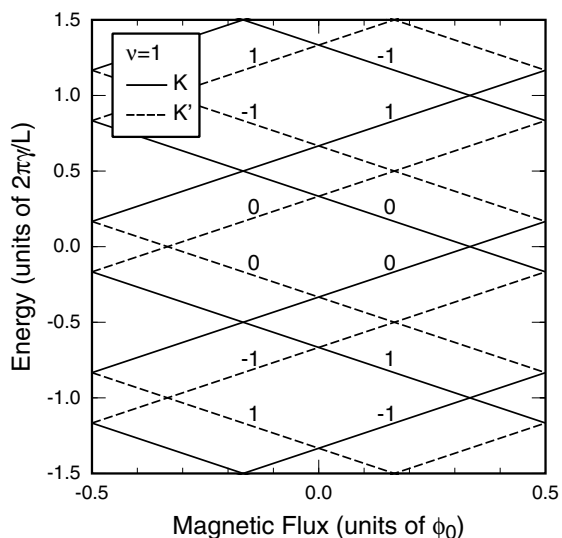


Fig. 2. Magnetic-flux dependence of energy-band edges at $k = 0$ for $\nu = 1$ without the Coulomb interaction. Solid and dashed lines indicate the band edges for the K and K' point, respectively. Numbers denote the energy-band index.

band parameter through $\gamma = \sqrt{3}a\gamma_0/2$ with $a = 2.46 \text{ \AA}$ being the lattice constant. Therefore, $\epsilon_c(2\pi\gamma/L)^{-1} \approx (\sqrt{3}/\pi)(L/a) = \sqrt{3}d/a$, with d being the diameter of the nanotube. For example, $\epsilon_c(2\pi\gamma/L)^{-1} = 10$ corresponds to a diameter $\sim 1.4 \text{ nm}$.

In the following the strength of the Coulomb interaction and cutoff energy are chosen as typical values $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.2$ and $\epsilon_c(2\pi\gamma/L)^{-1} = 10$, respectively. Results are qualitatively independent of these values.

Magnetic-flux dependence of band edges at $k = 0$ for $\nu = 1$ without the Coulomb interaction is shown in Fig. 2. Solid and dashed lines indicate those for the K and K' points, respectively, and numbers denote the integer n characterizing the wave number in the circumference direction in Eq. (2). All the band edges linearly depend on the flux and the absolute value of the slopes is same. The energy gap closes at $\varphi = 1/3$ for the K point and at $\varphi = -1/3$ for the K' point.

At the K point the smallest interband energy for the perpendicular polarization is associated with the transition between energy bands with $n = 0$ and 1 for $-1/2 < \varphi \leq 1/3$ and with $n = -1$ and 0 for $1/3 \leq \varphi \leq 1/2$. For the K' point it is given by the transition between bands with $n = 0$ and 1 for $-1/2 < \varphi \leq -1/3$ and with $n = -1$ and 0 for $-1/3 \leq \varphi \leq 1/2$. This

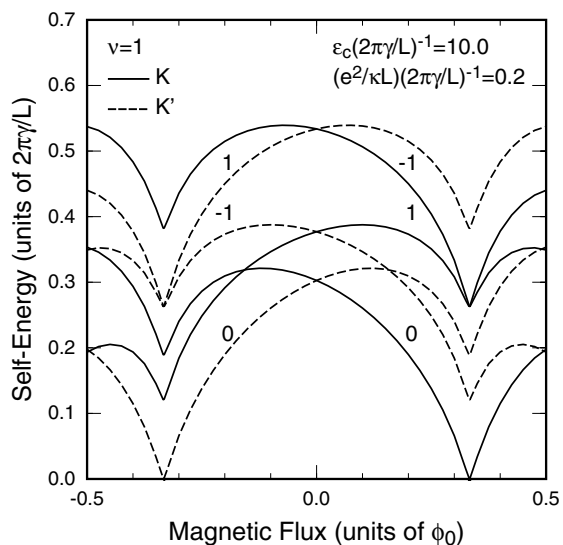


Fig. 3. Magnetic-flux dependence of self-energy for the conduction band edges at $k = 0$ for $\nu = 1$. Solid and dashed lines indicate the self-energies for the K and K' point, respectively. Numbers denote the energy-band index.

energy is $2\pi\gamma/L$ independent of φ , showing that the AB effect on the band gap is absent, if effects of the Coulomb interaction are neglected.

Figure 3 shows magnetic-flux dependence of the self-

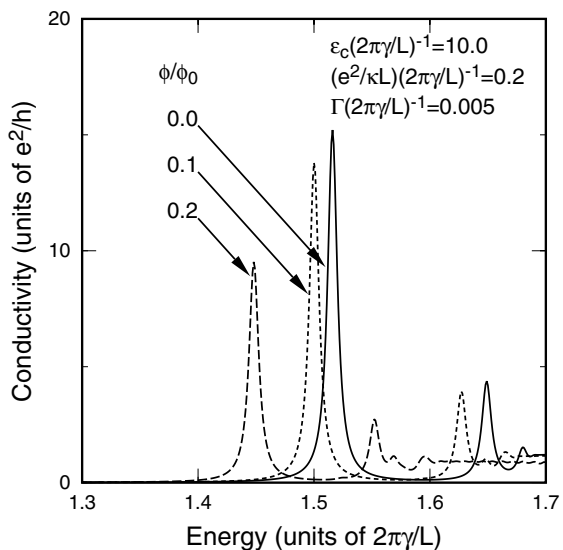


Fig. 4. Calculated dynamical conductivity at $\varphi = 0$ (solid line), 0.1 (dotted line), and 0.2 (dashed line) with the phenomenological energy broadening $\Gamma(2\pi\gamma/L)^{-1} = 0.005$.

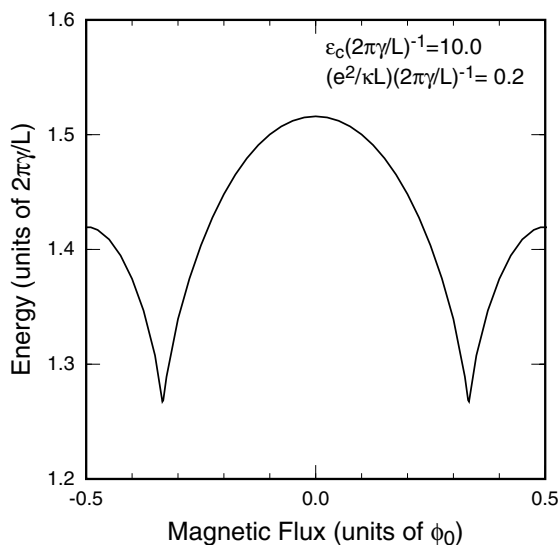


Fig. 5. Magnetic-flux dependence of excitation energy.

energy at each conduction-band edge for a tube with $\nu = 1$. The self-energy linearly depends on the magnetic flux around zero and this linear dependence is slightly larger for the lowest conduction band than the first excited band. For the valence bands the self-energy is given by inversion of the sign in that for the conduction band with the same index. Then, with increase of flux, the lowest transition energy for the K and K' point linearly depends on the flux near zero, giving rise to a small AB splitting.

Figure 4 shows the real part of the dynamical conductivity $\tilde{\sigma}_{xx}(\omega)$ at magnetic flux $\varphi = 0, 0.1$, and 0.2 in the energy range near the lowest band edge. At $\varphi = 0$ peaks appear due to exciton absorption. With increase of the magnetic flux, the peaks are shifted to the lower energy side and the intensity decreases.

The magnetic-flux dependence of the excitation energy for the largest peaks in Fig. 4 is shown in Fig. 5. It quadratically decreases with increase of the magnitude of the magnetic flux around zero, takes a minimum value at $|\varphi| = 1/3$, and increases for $|\varphi| > 1/3$. It is within a range between ~ 1.26 and ~ 1.52 in units of $2\pi\gamma/L$. This change is much smaller than that for parallel light lying between 0 and $2\pi\gamma/L$.

The narrow variation of the excitation energy caused by the magnetic flux is because the magnetic-flux dependence of band gap without interaction is absent and the Coulomb interaction is small comparing to the typ-

ical kinetic energy. Its quadratic dependence around zero magnetic flux is expected as described before.

Acknowledgments

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References

- [1] H. Ajiki and T. Ando, J. Phys. Soc. Jpn. **62** (1993) 1255.
- [2] H. Ajiki and T. Ando, Physica B **201** (1994) 349.
- [3] H. Ajiki and T. Ando, Jpn. J. Appl. Phys. Suppl. **34-1** (1995) 107.
- [4] T. Ando, J. Phys. Soc. Jpn. **73** (2004) 3351.
- [5] S. Zaric, G. N. Ostojic, J. Kono, J. Shaver, V. C. Moore, M. S. Strano, R. H. Hauge, R. E. Smalley, and X. Wei, Science **304** (2004) 1129.
- [6] L. J. Li and R. J. Nicholas, Internat. J. Mod. Phys. B **18** (2004) 3509.
- [7] T. Ando, J. Phys. Soc. Jpn. **66** (1997) 1066.
- [8] E. Chang, G. Bussi, A. Ruini, and E. Molinari, Phys. Rev. Lett. **92** (2004) 196401.
- [9] H. Zhao and S. Mazumdar, Phys. Rev. Lett. **93** (2004) 157402.
- [10] S. Uryu and T. Ando, Phys. Rev. B **74** (2006) 155411.
- [11] Y. Miyauchi, M. Oba, and S. Maruyama, Phys. Rev. B **74** (2006) 205440.
- [12] T. Ando, J. Phys. Soc. Jpn. **74** (2005) 777.
- [13] H. Suzuura and T. Ando, Phys. Rev. Lett. **89** (2002) 266603.
- [14] T. Ando, J. Phys. Soc. Jpn. **75** (2006) 054701.
- [15] H. Sakai, H. Suzuura, and T. Ando, J. Phys. Soc. Jpn. **72** (2003) 1698.
- [16] H. Sakai, H. Suzuura, and T. Ando, Physica E **22** (2004) 704.
- [17] T. Ando, J. Phys. Soc. Jpn., **75** (2006) 024707.