Excitons in metallic carbon nanotubes with Aharonov-Bohm flux

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Exciton effects in metallic carbon nanotubes with and without magnetic flux are studied in an effective-mass approximation. For parallel polarization, an exciton associated with the first excited bands has an appreciable binding energy even in the presence of strong screening of linear bands. The Aharonov-Bohm splitting of the exciton peak is slightly enhanced due to interaction effects. An Aharonov-Bohm gap in the linear bands is strongly enhanced, but the exciton binding energy tends to largely cancel this enhancement. For perpendicular polarization, there is essentially no exciton effect due to the absence of backscattering within linear bands and interband absorption is nearly suppressed by the depolarization effect.

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I. INTRODUCTION

Carbon nanotubes are rolled up two-dimensional (2D) graphite sheets and can be metallic or semiconducting depending on the chiral vector giving the circumference. Because of the quasi-one-dimensional nature of the electron motion, exciton effects play dominant roles in their optical properties. In this paper, we theoretically study exciton effects in metallic carbon nanotubes with and without Aharonov-Bohm (AB) magnetic flux in an effective-mass approximation.

In semiconducting nanotubes, it was predicted\(^1,2\) that the band gap is enhanced considerably by the Coulomb interaction and that exciton binding energy is comparable to but slightly smaller than this enhancement. As a result, the intensity of the optical absorption is focused on exciton energy levels lying higher than the band gap in the noninteracting case. This prediction has been confirmed both theoretically\(^3-8\) and experimentally\(^9-14\). The AB effect on the band gap, i.e., modulation by magnetic flux threading the cross section, is another intriguing subject.\(^15\) The splitting of absorption peaks in flux, predicted theoretically,\(^2,16,17\) was recently observed.\(^18-21\)

The development in photoluminescence measurement has enabled quantitative comparison between theories and experiments in semiconducting nanotubes.\(^12\) In metallic nanotubes, however, photoluminescence measurement is not possible and various other methods such as optical absorption,\(^9,10,22\) Raman scattering,\(^23-25\) and Rayleigh spectroscopy\(^26\) have been used. These experiments gave rich information on electronic states in metallic tubes, including possible assignment of observed spectra to different diameters and chirality, peak splitting due to trigonal warping effect, etc. Recently, exciton effects in metallic nanotubes were explicitly addressed.\(^27\)

Theoretically, excitons in metallic nanotubes were first studied in an effective-mass approximation.\(^1\) Optical absorption spectra of tubes with AB flux were shown and absence of excitonic instability was revealed for the linear bands in a limit of zero flux. Recent first-principles calculations showed that binding energies of excitons associated with the first excited bands are typically one-order-of-magnitude smaller than those of semiconducting nanotubes.\(^3,28\)

These experimental and theoretical studies motivate us to perform systematic analysis of excitons in metallic nanotubes. In this paper we theoretically carry out this task in an effective-mass approximation. It is organized as follows: In Sec. II, the model and method are described. Numerical results are presented in Sec. III and discussed in Sec. IV. Summary and conclusion are given in Sec. V.

II. MODEL AND METHOD

A. Energy bands and wave functions

An effective-mass theory of carbon nanotubes developed in previous papers\(^15,29\) is described again for metallic tubes for convenience of explanation. The structure of a 2D graphite sheet is shown in Fig. 1(a). In this system, the conduction and valence bands consisting of \(\pi\)-states cross at the \(K\) and \(K'\) points. Electronic states around these points are described by a \(\mathbf{k}\cdot\mathbf{p}\) equation.\(^15,29,30\) For the \(K\) point, it becomes

\[
\gamma (\sigma_x \hat{k}_x + \sigma_y \hat{k}_y)) \mathbf{F}^K (\mathbf{r}) = \varepsilon \mathbf{F}^K (\mathbf{r}),
\]

where the \(x\) and \(y\) coordinates are chosen in the circumference and axis directions, respectively, \(\gamma\) is a band parameter, \(\sigma_x\) and \(\sigma_y\) are the Pauli spin matrices, \(\mathbf{\hat{k}} = (k_x, k_y) \equiv -(\nabla)\) is a wave vector operator, and the energy origin is chosen at the crossing point of the valence and conduction bands.

Electronic states of a metallic nanotube with a sufficiently large diameter near the \(K\) point are obtained by imposing the periodic boundary condition around the circumference direction:\(^15,29\)

\[
\mathbf{F}^K (\mathbf{r} + \mathbf{L}) = \mathbf{F}^K (\mathbf{r}) \exp(2\pi i \varphi),
\]
with $\mathbf{L}$ a chiral vector shown in Fig. 1(a) and $\varphi = \phi / \phi_0$, where $\phi$ is magnetic flux passing through the cross section as shown in Fig. 1(b) and $\phi_0 = \hbar c / e$ is the magnetic flux quantum with $c$ the speed of light, $\hbar = 2\pi \hbar$, and $e$ the elementary charge.

The energy bands are specified by a set of quantum numbers $\alpha = (\pm, n)$ and the wave number $k$ in the axis direction, where $n$ is an integer giving the band index, ‘−’ denotes the valence band, and ‘+’ the conduction band. The wave function is written as

$$F^K_{\alpha,k}(x,y) = \frac{1}{\sqrt{AL}} \exp\left[i\kappa_{\varphi}(n)x + iky\right] F^\varphi_{\alpha,k}, \quad (3)$$

with $L = |\mathbf{L}| = \pi d$ where $d$ is the tube diameter, $A$ being the length of nanotube,

$$\kappa_{\varphi}(n) = \frac{2\pi}{L}(n + \varphi), \quad (4)$$

and

$$F^\varphi_{\alpha,k} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} b_{\varphi}(n,k) \\ s_\alpha \end{array} \right), \quad (5)$$

where

$$b_{\varphi}(n,k) = \frac{\kappa_{\varphi}(n) - ik}{\sqrt{\kappa_{\varphi}(n)^2 + k^2}}, \quad (6)$$

and

$$s_\alpha = \begin{cases} +1 & (\alpha = +, n), \\ -1 & (\alpha = -, n). \end{cases} \quad (7)$$

The corresponding energy is given by

$$\varepsilon_{\pm,n}(k) = \pm\gamma \sqrt{\kappa_{\varphi}(n)^2 + k^2}. \quad (8)$$

A $\mathbf{k} \cdot \mathbf{p}$ equation near the $K'$ point is given by Eq. (1) in which $\sigma_y$ is replaced by $\sigma^*_y$. The energy is the same as Eq. (8) and the wave function is given by Eq. (3) with $F^K_{\alpha,k}$ replaced with its complex conjugate. Effects of higher-order $\mathbf{k} \cdot \mathbf{p}$ terms, curvature, lattice strains, etc. will be briefly discussed in Secs. III and IV.

FIG. 2: Energy dispersions of a metallic nanotube at (a) $\varphi = 0$ and (b) 0.1. Numbers denote band index $n$. Arrows in $k < 0$ and $k > 0$ indicate optical interband transitions for parallel and perpendicular polarization, respectively. The transition between the linear bands with $n=0$ in (a) is not allowed.

B. Interband transition

Figure 2 shows energy dispersions of metallic nanotubes in the vicinity of the $K$ point (a) with and (b) without AB flux. In Fig. 2(a), the two linear bands with $n = 0$ cross at the energy origin and bands with $n$ and $-n$ are degenerate. While in Fig. 2(b) a small gap opens between the bands with $n = 0$ and the degeneracy of the bands between $n$ and $-n$ is lifted.

For parallel polarization, interband transition between the valence and conduction bands with the same index occurs which is shown by arrows in the $k < 0$ region of
Fig. 2. It should be noted that in the presence of the magnetic flux, the transition between the linear bands is prohibited.\textsuperscript{16,17,29} Then, the lowest transition is given by that between the valence and conduction bands with \( n = \pm 1 \). A magnetic flux makes the transition for \( n = 0 \) allowed only near the band gap induced by the flux.

For perpendicular polarization, the transition for which the band index changes by \( \pm 1 \) occurs as shown by arrows in the \( k > 0 \) region of Fig. 2. In the absence of flux, the lowest transition is given by that from the band with \( n = 0 \) to that with \( n = \pm 1 \) and vice versa. In the presence of flux, the energies for the transitions from the band with \( n = 0 \) to that with \( n = -1 \) and to that with \( n = 1 \) deviate from each other.

**C. Dynamical conductivity**

We shall use a screened Hartree-Fock approximation for interaction effect on the band structure and introduce an attractive electron-hole interaction using the Coulomb interaction screened by a static dielectric function.\textsuperscript{1,2,35} Excitons are obtained by solving an equation of motion for electron-hole pairs.\textsuperscript{1–8,33,34}

An exciton with the momentum zero and \( 2\pi \hbar /L \) in the axis and circumference direction, respectively, with integer \( l \) is written as

\[
|\psi\rangle = \sum_n \sum_k \psi_n^l(k)c_{+,n+l,k}^\dagger c_{-,n,k}|g\rangle,
\]

where \( c_{+,n,k}^\dagger \) and \( c_{n,k} \) are the creation and annihilation operators for electrons, respectively, and \( |g\rangle \) is the ground state.\textsuperscript{1,2} Solving an equation of motion for the exciton,\textsuperscript{1,2} \( \psi_n^l(k) \) and the exciton energy are obtained. Actually, coupling between different \( n \)'s turns out to be quite weak and excitons are associated well with each band. In principle, interband coupling gives rise to a finite life time of the exciton associated with the bands \( n = \pm 1 \) due to its decay into the linear bands \( n = 0 \). An estimate of the small broadening due to such decay processes will be briefly discussed in Sec. IV.

The dynamical conductivity characterizing optical absorption is calculated from the Kubo formula.\textsuperscript{1,2,33} For polarization perpendicular to the tube axis, the depolarization effect must be considered.\textsuperscript{16,17} It is taken into account in a self-consistent-field method where an optically induced current and electric field which electrons feel are determined self-consistently.\textsuperscript{16,17}

In the following, the equation of motion for the exciton wave function Eq. (9) is solved by discretizing \( k \), typically, with interval \( 3.75 \times 10^{-3} \times (2\pi /L) \). This forces us to introduce a phenomenological energy broadening \( \Gamma \) in the dynamical conductivity in such a way that it is larger than the separation of resulting discrete energy levels.\textsuperscript{1,2} Actually, the broadening is determined by various effects such as interactions with other electrons, phonons, impurities, etc. as well as possible inhomogeneity. The value of \( \Gamma \) required in the following calculation is larger than the broadening due to the exciton decay into continuum states associated with the linear bands as will be shown in Sec. IV.

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.,

\[
\frac{e^2}{\kappa L} \frac{L}{2\pi \gamma} \approx \frac{0.35}{\kappa},
\]

for \( \gamma \approx 6.4 \text{ eVÅ} \), corresponding to the nearest-neighbor hopping integral \( \gamma_0 = 3 \text{ eV} \) related through \( \gamma = (\sqrt{3}/2)\alpha_{\gamma_0} / \kappa \) with lattice constant \( a = 2.46 \text{ Å}. \textsuperscript{2} \) The static dielectric constant \( \kappa \) describes screening by electrons in \( \sigma \) bands, core states, and the \( \pi \) bands away from the \( K \) and \( K' \) points and by the surrounding material if any and therefore is independent of whether the nanotube is metallic or semiconducting. Since \( \kappa \) is considered to be of the order of unity, for example, \( \kappa = 2.4 \) in graphite, the typical strength of the Coulomb interaction is of the order of 0.1\textemdash0.2.

The infinitely extending energy bands in Eq. (8) are cut off by an energy \( \varepsilon_c \) which should be of the order of the half of the \( \pi \)-band width \( \varepsilon_{\gamma_0} \).\textsuperscript{1,2} Therefore, \( \varepsilon_c(2\pi\gamma/L)^{-1} \approx (\sqrt{3}/\pi)(L/a) = \sqrt{3}d/a \). Since excitation energy exhibits only weak dependence on the cutoff energy,\textsuperscript{2} we use a typical value \( \varepsilon_c(2\pi\gamma/L)^{-1} = 10 \) corresponding to a diameter \( \sim 1.4 \text{ nm} \) in the followings unless specified otherwise. For this typical nanotube with \( d \approx 1.4 \text{ nm}, \text{ the dimensionless magnetic flux is given by } \varphi \approx 3.7 \times 10^{-4}B \text{ where } B \text{ is a magnetic field in units of tesla.} \text{ Then, for example, } 100 \text{ T} \text{ corresponds to } \varphi \approx 0.04. \text{ }

**III. NUMERICAL RESULTS**

**A. Parallel polarization**

First, we consider excitons associated with the bands with \( n = \pm 1 \) for parallel polarization. Typical examples of optical absorption spectra for small flux \( \varphi = 0.001 \text{ and } 0.01 \text{ are shown in Figs. 3(a) and (b), respectively. At around energy } 2.4 \times (2\pi\gamma/L), \text{ a sharp exciton peak appears in Fig. 3(a) and splits into two peaks in Fig. 3(b). In the energy region higher than the band edges denoted by arrows, contributions from continuum states can be seen as a small and long tail.} \text{ In Fig. 4, solid lines show magnetic-flux dependence of the exciton energies. The band edges with and without the Coulomb interaction are also plotted by dashed and dotted lines, respectively. With decrease of the flux, the exciton energies associated with bands \( n = \pm 1 \) approach each other and take the same value in the zero flux limit. The band edges exhibit the same behavior. In the zero flux limit, there is a clear difference between the exciton energy and the band edge. Within the present } k \cdot p
FIG. 3: Dynamical conductivity for parallel polarization at (a) $\varphi=0.001$ and (b) 0.01. Arrows indicate edges of the bands for $n=\pm 1$ and numbers denote band index $n$. The phenomenological energy broadening $\Gamma(2\pi\gamma/L)^{-1}=0.005$ (solid lines), 0.02 (dotted lines), and 0.08 (dashed lines) is used.

The magnetic-flux dependence of the binding energy and the self-energy in Fig. 5 is larger than that for semiconducting tubes. The main origin of this dependence is the suppression of metallic screening associated with the band-gap opening induced by the flux. Because the gap opens linear in the flux, the shift increases in proportion to $|\varphi|$. It is interesting that the dependence on the flux approximately cancels between the self-energy and the exciton binding energy. As a result, the AB splitting of the exciton energies can be approximately the same as that in the absence of the interaction except for a slight enhancement, most of which may be absorbed into a change in the energy scale.

Figure 6 shows the dependence of the exciton energy (solid lines) and the band edge (dashed lines) on the strength of the Coulomb interaction in the zero-flux limit. The cutoff energy is chosen as $\varepsilon_c(2\pi\gamma/L)^{-1}=2$, 5, and 10. The dependence on the cutoff energy is logarithmic, because of the logarithmic divergence of the

The Hamiltonian is invariant under the special time reversal symmetry within each $K$ and $K'$ points in the absence of flux. Consequently, all states at each valley are doubly degenerate and therefore there is no splitting between excitons associated with the bands $n=\pm 1$. Note that this degeneracy can actually be lifted due to various effects as will be discussed in Sec. IV.

Figure 5 shows magnetic-flux dependence of the binding energies of the excitons and that of the self-energy shift of the band edges, i.e., difference between the dashed and dotted lines in Fig. 4. The binding energy approximately takes a nonzero value $\sim 0.05 \times (2\pi\gamma/L)$ in the zero flux limit, showing that the exciton effects survive at zero flux. It is approximately one-order-of-magnitude smaller than that for semiconducting nanotubes. The existence of excitons in metallic tubes is due to its strong binding and weak screening effect in one-dimensional systems in comparison with those in higher dimensions.

The magnetic-flux dependence of the binding energy and the self-energy in Fig. 5 is larger than that for semiconducting tubes. The main origin of this dependence is the suppression of metallic screening associated with the band-gap opening induced by the flux. Because the gap opens linear in the flux, the shift increases in proportion to $|\varphi|$. It is interesting that the dependence on the flux approximately cancels between the self-energy and the exciton binding energy. As a result, the AB splitting of the exciton energies can be approximately the same as that in the absence of the interaction except for a slight enhancement, most of which may be absorbed into a change in the energy scale.

Figure 6 shows the dependence of the exciton energy (solid lines) and the band edge (dashed lines) on the strength of the Coulomb-interaction in the zero-flux limit. The cutoff energy is chosen as $\varepsilon_c(2\pi\gamma/L)^{-1}=2$, 5, and 10. The dependence on the cutoff energy is logarithmic, because of the logarithmic divergence of the
A closer look of the results reveals that the exciton binding-energy becomes slightly smaller with the increase of the cutoff energy. This is the direct consequence of the increase of interband screening effects because more bands contribute to the screening. A small reduction of the effective mass due to interaction and its slight dependence on the cutoff also contributes to this dependence.

In Fig. 7, the result for $\varepsilon_c(2\pi\gamma/L)^{-1} = 10$ in Fig. 6 is compared with those of the first and second gaps in semiconducting nanotubes. The interaction dependence of the band edge of metallic tubes is weaker than that of semiconducting tubes. However, the small exciton binding-energy leads to the dependence of the exciton energy similar to those for semiconducting tubes.

B. AB gap in linear bands

In Fig. 8, a typical example of absorption spectra for parallel polarization is shown near an AB gap of the linear bands with $n = 0$ at $\varphi = 0.025$. The intensity is focused on the energy of the lowest exciton. A small peak below the band gap arises from its excited state.

Figure 9 shows the AB band gap and the exciton energy for the bands $n = 0$ as a function of the magnetic flux. The results depend weakly on cutoff-energy $\varepsilon_c$. Both exciton energy and band gap remain positive and converge to zero with the decrease of the magnetic flux, showing that there is no excitonic instability. The band gap is considerably enhanced by the Coulomb interaction (more than factor two), but the exciton energy lies closer to the gap in the absence of interaction. In a previous paper,$^1$ a similar result was presented for interaction parameter $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.1$.

In order to discuss quantitatively the gap enhancement due to the Coulomb interaction, we define a coefficient of
small $\varphi$ in the flux dependence of energy as

$$\varepsilon(\varphi) = \frac{4\pi\gamma}{L} C \varphi,$$  \hspace{1cm} (11)

where $\varepsilon(\varphi)$ is either the exciton energy or the band gap. In the absence of the interaction, we obviously have $C = 1$. This coefficient, determined by the numerical result for $\varphi = 0.01$, is plotted in Fig. 10. The gap enhancement increases with the interaction strength and becomes roughly $C \approx 2$ for $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.1$ and $C \approx 2.5$ for $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.2$. On the other hand, the enhancement of the exciton energy is insensitive to the interaction strength which remains roughly $C \sim 1.5$ for the wide parameter range.

The presence of a lattice distortion ($u_x, u_y, u_z$) causes a shift in $k_x$ and $k_y$ both in a tight-binding model and in the $kp$ scheme. The shift in the axis $y$ direction does not cause any appreciable effect. The shift in the $x$ direction can be replaced by an effective magnetic flux (its signature is opposite between the $K$ and $K'$ points). The flux for the $K$ point is written as

$$\frac{\phi}{\phi_0} = \frac{Lg_2}{2\pi\gamma}(u_{xx} - u_{yy}) \cos 3\eta - 2u_{xy} \sin 3\eta,$$ \hspace{1cm} (12)

where $u_{xy}$ etc. denote the lattice strain given by

$$u_{xx} = \frac{\partial u_x}{\partial x} + \frac{u_z}{R}, \quad u_{yy} = \frac{\partial u_y}{\partial y}, \quad u_{xy} = \frac{1}{2}(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}),$$ \hspace{1cm} (13)

with $R=L/2\pi$ being the tube radius, $g_2$ is the electron-phonon interaction given by $g_2 = (\alpha/2)\gamma_0$ with $\alpha \sim 1$, and $\eta$ is a chiral angle defined in Fig. 1(a).

The nonzero curvature also causes a shift in the origin of $k_x$ and $k_y$. This means that the curvature effect is exactly same as that of strain to the lowest order. For the $K$ point, for example, it was estimated as

$$\frac{\phi}{\phi_0} = -\frac{2\pi}{4\sqrt{3}^L} \rho \cos 3\eta,$$ \hspace{1cm} (14)

with $p = 1 - (3/8)(\gamma'/\gamma)$, $\gamma' = -(\sqrt{3}/2)\Gamma_{pp}^\sigma a$, and $\gamma = -(\sqrt{3}/2)(V_{pp}^x - V_{pp}^y) a$, where $V_{pp}^x = \Gamma_{pp}^\sigma a$ and $V_{pp}^y$ are the conventional tight-binding parameters for neighboring $p$ orbitals. The curvature effect is largest in zigzag nanotubes with $\eta=0$. For usual parameters, we have $\gamma'/\gamma \sim 8/3$ and therefore it is very difficult to make a reliable estimation of $p$ although we can safely assume $|p| < 1$. For example, the effective flux is $\phi/\phi_0 \sim 0.05 \times p \cos 3\eta$ for a typical nanotube with $d \sim 1.4$ nm.

In semiconducting nanotubes, the effective flux due to strain or curvature is different from a real magnetic flux. In metallic nanotubes, on the other hand, this flux can effectively be regarded as a magnetic flux because the sign difference between the $K$ and $K'$ points is irrelevant in determining the band structure. Therefore, the many-body enhancement of the AB gap and the corresponding exciton obtained above are directly applicable to the narrow gap due to strain and curvature. When a magnetic field is applied in the presence of a narrow gap due to strain or curvature, however, an effective flux becomes different between the $K$ and $K'$ points, leading to AB splitting.
C. Perpendicular polarization

Typical absorption spectra at the weak AB flux $\varphi = 0.001$ and 0.01 for perpendicular polarization are shown by solid lines in Figs. 11(a) and (b), respectively. For comparison, results without the depolarization effect are plotted by dashed lines. The conductivity without the depolarization effect shows peaks and they disappear when the depolarization effect is considered. This is quite in contrast to the case of semiconducting nanotubes, where a clear exciton peak is observable, although the intensity is approximately one-order-of-magnitude smaller than that for parallel polarization.\(^\text{5,7,47–49}\)

A potential with a range larger than the lattice constant, including that of the Coulomb interaction, cannot cause backward scattering within the linear bands.\(^\text{50,51}\) As shown in Fig. 2, either of an electron or a hole of the electron-hole pair is located at one of the two linear bands for the perpendicular polarization. Because it cannot be scattered between the positive and negative wave-vector region by the Coulomb interaction, the exciton consists of an electron-hole pair with the same sign of wave vectors. This leads to the extremely weak binding of the exciton for the perpendicular polarization.

IV. DISCUSSIONS

Interband mixing of the exciton wave function is usually very small and therefore each state in Eq. (9) is well approximated for fixed $n$. Weak interband mixing can give rise to broadening of an exciton level due to decay into continuum states in other bands. The relaxation time $\tau$ corresponding to the decay of an exciton associated with band $n$ into $m$ is given by

$$\frac{\hbar}{\tau} = 2\pi |\langle u_m | V | u_n \rangle|^2 D_m(\varepsilon_n),$$

where $|u_n\rangle$ is an approximate exciton bound state, $|u_m\rangle$ is a continuum state, $V$ is the screened Coulomb interaction, $\varepsilon_n$ is the exciton energy, and $D_m(\varepsilon_n)$ is the density of states of the continuum states.

Figure 12 shows the broadening of the excitons associated with the bands $n = \pm 1$ in the zero-flux limit. It
is more than one order of magnitude smaller than the exciton binding energy, showing that this process of the exciton decay into continuum states is not important. However, there can be other mechanisms of exciton decay such as interband scattering of a conduction electron or a valence hole caused by electron-hole pair excitations within the linear bands. The low energy excitation of metallic tubes with vanishing gap is described by the Tomonaga-Luttinger liquid.\textsuperscript{52–56} Such strong interaction effects can play important roles in excitons in metallic nanotubes, in particular, in the exciton broadening. This problem is left for a future study.

There are higher order corrections to the lowest order k·p equation in Eq. (1) such as the trigonal warping of energy bands\textsuperscript{29,57} and effects causing asymmetry of electron and hole energy dispersions in addition to curvature\textsuperscript{29,41,46,58} and strain.\textsuperscript{29,41,43–45} Such higher order corrections do not change the qualitative features of our results, but give rise to small modifications to the optical transitions associated with bands $n = \pm 1$. As has been discussed in the previous section, curvature and strain can be expressed in terms of an effective magnetic flux given by Eqs. (12) and (14). For bands with $n \neq 0$, further, the trigonal-warping effect can approximately be included as an effective flux,

$$\varphi_{\text{eff}} = \frac{\beta a}{4\sqrt{3}L} n^2 \cos 3\eta,$$

where $\beta$ is a constant of the order of unity.\textsuperscript{2,29} This leads to peak splitting for parallel polarization even at zero flux, as reported in recent experiments.\textsuperscript{56} More rigorous calculations including these corrections are left for a future study.

The first-principles calculations gave about 50 meV to the exciton binding energy of $n = \pm 1$ transitions in (12,0) and (10,10) tubes for parallel polarization.\textsuperscript{28} We have about 0.05 in units of $2\pi\gamma/L$ for both $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.1$ and 0.2. This gives 70 meV in a (12,0) tube and 50 meV in a (10,10) tube for $\gamma_0 = 3$ eV. It can be said at least that all these results are consistent with each other.

In the recently measured absorption spectrum of a (21,21) tube, exciton effects were discussed for the second excitation peak with $n = \pm 2$ by comparing the line shape with that obtained from the above first-principles calculations.\textsuperscript{27} In our results, exciton peaks for $n = \pm 2$, which are not shown here, approximately agree with the experiment when the energy scale $2\pi\gamma/L$ and the energy broadening $\Gamma$ are appropriately chosen.

Excitation energies measured in nanotube films are 0.8 and 1.4 eV for the first and second excitation of semiconducting tubes, respectively, and 1.9 eV for metallic tubes.\textsuperscript{10} Assuming that the diameter distribution in the film is the same between semiconducting and metallic tubes, the ratio among the three energies is 0.8 : 1.4 : 1.9 $\approx$ 1 : 1.8 : 2.4 in contrast to 1 : 2 : 3 in the absence of interaction. In Fig. 7, the three energies are about 0.87, 1.59, and 2.33 and about 0.94, 1.66, and 2.40 in units of $2\pi\gamma/L$ for $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.1$ and 0.2, respectively. They give the ratios 1 : 1.8 : 2.7 and 1 : 1.8 : 2.6, respectively, close to the experiments.

A previous calculation in a full random-phase approximation shows that the present screened Hartree-Fock approximation gives a slight overestimate of the band gap in metallic nanotubes.\textsuperscript{32} When such a correction is included, the ratio remains approximately the same for $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.1$, but becomes 1 : 1.8 : 2.5 for $(e^2/\kappa L)(2\pi\gamma/L)^{-1} = 0.2$.

Finally, we shall discuss the narrow band gap for $n = 0$. Energy bands of a (9,0) zigzag tube were calculated previously in a local-density approximation with many-body correction in a GW approximation.\textsuperscript{59} In the absence of the many-body correction, the band gap after geometry relaxation is 0.12 eV, and the many-body correction enhances it by 40% to 0.17 eV. The present calculation gives much larger enhancement of factor 2 $\sim$ 2.5 for $0.1 < (e^2/\kappa L)(2\pi\gamma/L)^{-1} < 0.2$ as shown in Fig. 10. The origin of this large difference is not known. Presumably, the (9,0) nanotube is extremely thin and therefore various other effects such as $\sigma$-$\pi$ mixing can be important. The dynamical nanotube is extremely thin and therefore various other effects such as $\sigma$-$\pi$ mixing can be important.

V. SUMMARY AND CONCLUSION

We have theoretically studied exciton effects in metallic carbon nanotubes with and without Aharonov-Bohm magnetic flux in the effective-mass approximation. For parallel polarization, an exciton associated with the first excited bands has an appreciable binding energy even in...
the presence of strong screening of metallic linear bands. The AB splitting of the exciton peak is slightly enhanced due to interaction effects. An AB gap in the linear bands is strongly enhanced, but the exciton binding energy tends to largely cancel this enhancement. For perpendicular polarization, there is essentially no exciton effect due to the absence of backscattering within linear bands and interband absorption is nearly suppressed if the depolarization effect is properly taken into account.

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