Magnetoelectronic and optical properties of carbon nanotubes

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(Received 23 July 2002; published 17 January 2003)

We use the sp3 tight-binding model to calculate the magneto-electronic and optical properties of carbon nanotubes. These properties are studied within the sp3 tight-binding model and the gradient approximation. They strongly depend on the direction and the magnitude of the magnetic field, and the Zeeman splitting. The magnetic field leads to the change of energy gap, the destruction of state degeneracy, and the coupling of different angular momenta. Hence there are magnetic-field-dependent absorption frequencies and more absorption peaks. The types of carbon nanotubes predominate in the band structure and thus the range of absorption frequencies and the number of absorption peaks. The Zeeman splitting makes the semiconductor-metal transition occur at lower magnetic flux. It metalizes armchair carbon nanotubes in the presence of the perpendicular magnetic field. However, it does not affect the optical excitations except for metallic carbon nanotubes.

I. INTRODUCTION

Carbon nanotubes have prompted a lot of studies since their discovery by Iijima1 in 1991, such as electronic structures2–16 and optical properties.17–29 A single-wall carbon nanotube is a rolled-up graphite sheet,5 the structure of which is thus fully specified by a two-dimensional (2D) lattice vector R = m a1 + n a2, where a1 and a2 are primitive lattice vectors of a graphite sheet. The radius and the chiral angle of a (m, n) carbon nanotube are, respectively, (m+n)/[2πb(3m²+mn+n²)²π] and θ = tan⁻¹ [−v₃n/(2m+n)]. b = 1.42 Å is the C-C bond length. A carbon nanotube is a semiconductor or a metal, which depends on both radius and chirality.2–8 The electronic structure is strongly affected by the magnetic field.2–10 The optical excitations directly reflect its characteristics. In this work, the sp3 tight-binding model with the curvature effects is utilized to calculate the magnetoelectronic structure. Furthermore, the magneto-optical properties are studied by means of evaluating the optical-absorption function. The dependence on the nanotube geometry (R and θ), the direction and the magnitude of the magnetic field, and the Zeeman splitting are investigated.

There are three types of carbon nanotubes according to their energy gaps (Eₜ's).5–6,8–9 A (m, n) carbon nanotube is (I) a gapless metal for m = n, (II) a narrow-gap semiconductor for m ≠ n and 2m+n=3l (l is an integer), and (III) a moderate-gap semiconductor for 2m+n≠3l. Energy gaps are, respectively, inversely proportional to R and R for type-II and type-III carbon nanotubes. From the sp3 (2pₜ) tight-binding model,9 energy gaps of type-II carbon nanotubes are given by the approximate relation Eₜ = 5γ₀b²cos(3θ₁b²Rₐ) (3γ₀b²cos(3θ₁b²Rₐ) is the nearest-neighbor resonance integral of 2p orbitals). This model includes the curvature effects, the misorientation of p and sp3 orbitals, as well as the mixing of p and sp3σ orbitals. The predicted energy gaps are successful for understanding the experimental measurements of the low-frequency optical-absorption spectra (ω<0.1γ₀).20 Each carbon nanotube has many 1D parabolic subbands except that the subbands nearest to the Fermi level (Eₜ = 0) in an armchair (m, m) nanotube are linear. That is to say, all subbands have divergent density of states (DOS) in 1/√E form except the finite DOS of the linear subbands. The 1D van Hove singularities (vHs) in the DOS would play an important role on the optical-absorption spectra.

Electronic structures in the presence of the magnetic field are studied within the effective-mass approximation10 and the tight-binding model.11–18 The magnetic field would affect energy dispersions and energy gaps. Furthermore, it leads to the oscillatory behavior. Electronic structures exhibit the periodic Aharonov-Bohm (AB) oscillations with a period δ₀ = ℏc/e, if the magnetic field is parallel to the nanotube axis and the Zeeman splitting is neglected. The AB effect can be identified in the magnetophysical properties, e.g., magnetoresistance.17–18 Only 2p orbitals are taken into account in the above-mentioned studies. The sp3 tight-binding model, with the curvature effects and the Zeeman splitting, can reveal more detailed electronic properties.

There have been some experimental studies on the optical excitation spectra.19–25 These measurements show that the absorption spectra exhibit rich absorption peaks, owing to the 1D vHs. Such prominent peaks are determined by radius and chiral angle. For example, the first absorption peak, respectively, occurs at 10–20 meV (Ref. 22) and 0.5–0.7 eV (Refs. 20–21 and 23–25) for type-II and type-III carbon nanotubes with Rₐ≈6–7 Å. The theoretical studies are mainly focused on the p-electronic optical excitations.26–32 They could explain the experimental results, such as the first absorption peak31–32 and the special absorption peak at 2γ₀.31–32 The magneto-optical-absorption spectra are predicted to exhibit the periodic AB oscillations and depend on the direction of electric polarization and magnetic field.26–27

DOI: 10.1103/PhysRevB.67.045405
PACS number(s): 78.66.− w, 73.20.Mf

PHYSICAL REVIEW B 67, 045405 (2003)
netoenergy bands and the gradient approximation to evaluate the magneto-optical-absorption function. Comparison with the previous studies is also made. Our study of the magneto-optical-absorption function. Comparison with the previous studies is also made. Our study

II. The gradient approximation is used to evaluate the states of in the magnitude and the direction of the magnetic field, the nanotube geometry (radius and chiral angle), and the Zeeman splitting. The magnetic field would induce the change of energy gap, the destruction of state degeneracy, and the coupling of different angular momenta. Such effects are directly reflected in the optical excitations. There are magnetic-field-dependent absorption frequencies and more absorption peaks. The low-energy electronic structures are mainly determined by the types of carbon nanotubes, and so do the range of absorption frequencies and the number of absorption peaks. The Zeeman splitting could reduce the energy gap and destroy the periodicity of the AB oscillations. It thoroughly metalizes armchair carbon nanotubes when the magnetic field is perpendicular to the nanotube axis. On the other hand, the Zeeman splitting hardly affects the optical excitations except for metallic carbon nanotubes.

This paper is organized as follows. The magnetoelectronic structures are calculated from the sp$^3$ tight-binding model. The magnetic-field-dependent energy gap is studied in Sec. II. The gradient approximation is used to evaluate the optical-absorption function. The calculated magneto-optical spectra are discussed in Sec. III. Finally, Sec. IV contains the concluding remarks.

II. MAGNETOELECTRONIC PROPERTIES

We first see the sp$^3$ tight-binding model in the absence of the magnetic field. The number of carbon atoms in a primitive unit cell is $N_v = 4 \sqrt{(m^2 + mn + n^2)(p^2 + pq + q^2)/3}$. (p, q) corresponds to the primitive vector perpendicular to the vector of (m, n). As a result of the periodical boundary condition along the azimuthal direction, band structures without the magnetic field only involve two independent atoms, A and B. The calculations of band structure are similar to those done for a graphite sheet. The Hamiltonian is described by a 8×8 Hermitian matrix. According to A atom and B atom, it can be decomposed into four block matrices:

$$H_{Ai,Aj}(k) = H_{Bi,Bj}(k) = E_i \delta_{ij},$$

$$H_{Ai,Bj} = \sum_{l=1,2,3} h^{(l)}_{ij}(i, \mathbf{r}_j - \mathbf{r}_A),$$

$$H_{Bi,Aj} = \sum_{l=1,2,3} h^{(l')}_{ij}(i, \mathbf{r}_i - \mathbf{r}_B).$$

Each block matrix is a 4×4 matrix. $i$ represents the basis states of s and p orbitals. $\mathbf{r}_A$ and $\mathbf{r}_B$ are, respectively, positional vectors for the A atom and the B atom. The nearest-neighbor atom is at $\mathbf{r}_j$. The cylindrical coordinates $(r, \Phi, z)$ are convenient in taking into account the curvature effects. $\mathbf{r}_A = (R_d, 0, 0)$ and $\mathbf{r}_B = (R_d, \Phi_j, z_j)$. $\Phi_j$'s and $z_j$'s for the three nearest neighbors are $\Phi_1 = -b \cos(\pi 6 - \theta)/R_d$, $\Phi_2 = b \cos(\pi 6 + \theta)/R_d$, $\Phi_3 = b \cos(\pi 2 - \theta)/R_d$, $z_1 = -b \sin(\pi 6 - \theta)$, $z_2 = -b \cos(\pi 3 - \theta)$, and $z_3 = b \cos(\theta)$,

respectively. Similar results are obtained for $\mathbf{r}_B$. The matrix elements $h^{(l)}_{ij}$'s in Eq. (1) are given by

$$h^{(l)}_{ij} = V_{ppr} \cos(\Phi_j - 4(V_{ppp} - V_{ppa}) \sin^2(\Phi_j/2) R_d^2/b^2),$$

$$h^{(l)}_{ij} = V_{ppp} \sin(\Phi_j - 4(V_{ppp} - V_{ppa}) \sin^3(\Phi_j/2) R_d^2/b^2),$$

$$h^{(l)}_{ij} = -2(V_{ppp} - V_{ppa}) \sin^2(\Phi_j/2) R_d z_j/b^2,$$

$$h^{(l)}_{ij} = - (V_{ppp} - V_{ppa}) \sin(\Phi_j) R_d z_j/b^2,$$

$$h^{(l)}_{ij} = -2 V_{spp} \sin^2(\Phi_j/2) R_d z_j/b^2,$$

$$h^{(l)}_{ij} = V_{spp} \sin(\Phi_j) R_d z_j/b,$$

$$h^{(l)}_{ij} = V_{spp} \sin(\Phi_j) R_d z_j/b,$$

$$h^{(l)}_{ij} = V_{spp} \sin(\Phi_j) R_d z_j/b,$$

$$h^{(l)}_{ij} = V_{spp} \sin(\Phi_j) R_d z_j/b.$$

When a carbon nanotube is threaded by a uniform magnetic field, the angular momentum changes from $J$ into $J + \phi \hat{d}_0$. The magnetic flux is $\Phi = \pi R_d^2 B$. The angular momentum keeps decoupled; that is, $J$ is still a good quantum number. But on the other hand, the different $J$'s would couple one another as the magnetic field deviates from the nanotube axis. The angle between the magnetic field and the tube axis is assumed to be $\alpha$, i.e., $B = B \cos \alpha \hat{z} + B \sin \alpha \hat{d}$. The parallel magnetic filed ($B_\parallel$) induces the shift $[k_z - k_z + \phi \cos(\alpha)/(\Phi R_d)]$, and the perpendicular magnetic field ($B_\perp$) leads to the coupling of different $J$'s or $k_z$'s. For $B_\perp$, the total carbon atoms in a primitive cell are included in the band-structure calculations. The vector potential in the presence of $B_\perp$ is chosen as

$$A = R_d B_\perp \sin \left( \frac{x}{R_d} \right) \hat{z}.$$
where $x = R_d \Phi$. $A$ is independent of $z$, so the axial wave vector $k_z$ remains a good quantum number. The dependence on $x$ means that the different $k_z$'s or $J$'s are no longer decoupled. All the $k_z$'s need to be taken into account in the Hamiltonian matrix simultaneously. The vector potential will induce a phase factor $G_R = \int A(\mathbf{D}) \cdot d\mathbf{D}$ in the tight-binding function. Now, each Hamiltonian block matrix in Eq. (1) changes from a $4 \times 4$ matrix into a $2N_u \times 2N_u$ matrix. The Hamiltonian matrix element between site $A$ with $k_z$ state and site $B$ with $k_z'$ state is given by

$$
\langle \Phi_{k_z}^A | H | \Phi_{k_z'}^A \rangle = \frac{2h_{ij}}{N_u} \sum_{R^4} \sum_{R^8} e^{-i\Delta k_z^2} e^{-i(k_z' + \phi \cos \alpha \gamma/R_d) \Delta x} \times e^{-i\Delta z \gamma/\pi},
$$

where the phase difference due to $B_\perp$ is

$$
\Delta G = G_{R^4} - G_{R^8} = \frac{\phi \Delta z \sin \alpha}{\pi \Delta x} \left( \cos \frac{x}{R_d} - \cos \frac{x + \Delta x}{R_d} \right).
$$

$\Delta x \neq 0,$

$$
= \frac{\phi \Delta z \sin \alpha}{\pi R_d} \sin \frac{x}{R_d},
$$

$\Delta x = 0.$

$R^4 = (x, z), \quad R^8 = (x', z'), \quad$ and $\Delta R = R^8 - R^4 = (\Delta x, \Delta z).$ The effect of $B_\parallel$ is added in Eq. (4). The other three block matrices have the similar formula. The $4N_u \times 4N_u$ Hamiltonian matrix is thus constructed for any field direction.

By diagonalizing the Hamiltonian, we obtain energy dispersion $E^{\pm \alpha}(J,k_z,\phi)$ and wave function $\Psi^{\pm \alpha}(J,k_z,\phi)$. The superscripts $\alpha$ and $c$, respectively, represent the occupied valence bands and the unoccupied conduction bands. At $\alpha \neq 0^\circ$ ($\alpha = 0^\circ$), the wave function is the linear combination of the $4N_u$ (8) tight-binding functions, and it is composed of the different $J$'s (the same $J$). Although there exists the coupling of angular momenta, the wave function is principally dominated by $J$ at $\phi < \phi_B/3$. For simplicity, wave function and energy dispersion are denoted as a function of $J$. The magnetostate energy is the sum of the band energy plus the spin-$B$ interaction energy, i.e., $E^{\pm \alpha}(J,k_z,\sigma,\phi) = E^{\pm \alpha}(J,k_z,\phi) + E(\sigma,\phi).$ $E(\sigma,\phi) = g \sigma \phi / m^* R_d^2 \phi_B.$ The $g$ factor is taken to be the same as that ($\sim 2$) of the pure graphite. $\sigma = \pm 1/2$ is the electron spin and $m^*$ is the bare electron mass. The Zeeman splitting would lead to the rigid shift for the spin-up and spin-down states. It is neglected except that it has to be specially emphasized. For example, the Zeeman splitting affects the absorption spectra only when carbon nanotubes are gapless metals. The number of the total carriers is fixed during the variation of $\phi$. The $\phi$ dependence of the Fermi level is examined to be very weak, i.e., $E_F(\phi) = 0.$

Three types of carbon nanotubes, the type-I (10, 10) nanotube, the type-II (18, 0) nanotube, and the type-III (17, 0) nanotube, are chosen for a model study. They have the nearly same radii. We first see the type-I (10, 10) nanotube. The low-energy magnetoband structures, without $E(\sigma,\phi)$, are shown in Fig. 1(a). There are linear bands intersecting at the Fermi level in the absence of magnetic flux. The (10, 10) nanotube is a gapless metal at $\phi = 0$. The nondegenerate linear bands, which are described by $J = N_u/4 = 10$, exist at $k_z R_d \sim \pm 2 \pi /3$. The magnetic flux would make the linear bands change into the parabolic bands. It causes an energy gap and a blue shift in the wave vector of the band-edge state. A similar shift could also be found in nonzigzag carbon nanotubes ($m^* \neq 0$). The magnetic flux affects the state degeneracy. Energy bands of $J = N_u/2 - 2$ are doubly degenerate except for those of $J = N_u/4$ and $J = N_u/2$. The effects of $\phi$ on $J$ and $N_u/2 - 2$ are different, which thus leads to the destruction of the double degeneracy [Fig. 4(a)]. The above-mentioned effects due to the magnetic-flux dependence are relatively prominent, when the direction of the magnetic field approaches the nanotube axis. The magnetic flux at $\alpha \neq 0^\circ$ also induces the coupling of different $J$'s. Such coupling is strong only at large $\phi$ and $\alpha$. It is weak for the type-I (10, 10) nanotube at $\phi = \phi_B/12$; therefore each energy band is approximately described by the decoupled angular momentum.

The variation of energy gap with magnetic flux deserves a closer investigation. Figure 1(b) presents the magnetic-flux-dependent energy gap for the type-I (10, 10) nanotube at $\phi = \phi_B/3$ and different $\alpha$'s. $E_g$, without the Zeeman splitting, increases with $\phi$ monotonously except at large $\alpha$. The oscil-
The metallic behavior occurs at large $\alpha$, e.g., at $\alpha=90^\circ$. It is associated with the oscillatory feature of the phase difference $\Delta \phi$ in the Hamiltonian matrix element [Eq. (4)]. The energy gap decreases with increasing $\phi$. This result means that the energy gap is comparatively easily modulated by the parallel magnetic field. Energy dispersions near the Fermi level, the dependence of the band-edge state on $\phi$, and the zero or nonzero $\phi_{\text{MST}}$ are plotted from $\phi_{\text{MST}}=0$. Such transition occurs more frequently at large $\phi$. The spin-$B$ interaction causes the splitting of the spin-up and spin-down states and thus reduces energy gap. It metalizes the (10, 10) nanotube at any magnetic flux for sufficiently large $\alpha (>81^\circ)$, since the double spin-$B$ interaction energy $[2/\hbar^2m^*R_0^2\phi_0]$ is in excess of energy gap due to the magnetic field. All type-I armchair nanotubes exhibit the metalization behavior in the presence of the perpendicular magnetic field, mainly owing to the Zeeman splitting. The metallic carbon nanotubes have free carriers, so they are expected to own the low-frequency collective excitations. This problem is under current investigation.

At $\phi=0$, the type-II (18,0) nanotube has parabolic energy dispersions near the Fermi level and a small energy gap, as shown in Fig. 2(a). The curvature effects are the main cause. The two parabolic bands correspond to $J=12$ and $J=24$. The double degeneracy is clearly destroyed by the magnetic flux. However, the band-edge state keeps at $k_z=0$ during the variation of $\phi$. The energy gap, as shown in Fig. 2(b), decreases as $\phi$ gradually grows. $E_g$ without the spin-$B$ interaction vanishes at small $\phi_{\text{MST}}$, where energy dispersions are linear. The main effects of the Zeeman splitting are to reduce $\phi_{\text{MST}}$ and metalize the type-II nanotubes at sufficiently large $\phi$ and $\phi_{\text{MST}}$. There are three important differences between type-I carbon nanotubes and type-II carbon nanotubes (or type-III carbon nanotubes). They include the destruction of the double degeneracy for the energy bands nearest to the Fermi level, the dependence of the band-edge state on $\phi$, and the zero or nonzero $\phi_{\text{MST}}$.

The magnetoband structures of the type-III (17,0) nanotube are shown in Fig. 3(a). It has a large energy gap in the absence of $\phi$. The magnetic flux leads to the splitting of the doubly degenerate energy bands, but not the shift of the $k_z=0$ band edge. It could effectively reduce the energy gap, as shown in Fig. 3(b). $E_g$ decreases with $\phi$ monotonously even at large $\alpha$. The oscillatory $\phi$ dependence, as seen in type-I and type-II carbon nanotubes at large $\alpha$ [Figs. 1(b) and 2(b)], is not present. The MST of the type-III carbon nanotubes happens at $\phi_{\text{MST}}=\phi_0/3$. However, for all carbon nanotubes, the variation of $E_g$ with $\phi$ is relatively quick at small $\alpha$. The above-mentioned magnetoband gap can be directly verified by scanning tunneling spectroscopy, transport measurements, and optical-absorption spectroscopy.

Our study is compared with the previous studies. From the $sp^3$ tight-binding model, the $\phi$ dependence of the energy gap is different for type-I, type-II, and type-III carbon nanotubes [Figs. 1(b), 2(b), and 3(b)]. Energy gaps of type-I carbon nanotubes grow in the slow increasing of $\phi$, while the opposite is true for type-II carbon nanotubes. Such difference...
mainly comes from the curvature effects.\textsuperscript{9} It cannot be found in the \(2\rho \sigma\) tight-binding calculations.\textsuperscript{16,13} An energy gap at \(\phi = 0\) would determine whether carbon nanotubes are paramagnetic or diamagnetic.\textsuperscript{11,12} The curvature effects might dominate over magnetic properties of type-II carbon nanotubes. A simple relation between the nanotube radius and the \(\phi\)-dependent energy gap is examined. The previous study by Lu\textsuperscript{16} shows that \(E_\sigma(\phi)\) is inversely proportional to \(R_d\) for any field direction. However, there is no simple relation in another study by Ajiki and Ando.\textsuperscript{13} This work is consistent with the latter. For the perpendicular magnetic field, the Zeeman splitting can thoroughly metalize type-I carbon nanotubes. It is very important in clarifying the low-energy physical properties, such as magnetoplasmons and magnetization. The metalization behavior is absent in the previous studies. The spin-B interaction energy increases with magnetic field linearly. The Zeeman splitting apparently destroys the periodical \(AB\) oscillations in electronic\textsuperscript{10,16} and optical properties.\textsuperscript{26–27}

### III. MAGNETO-OPTICAL SPECTRA

The above-mentioned features of the magnetoband structures will be directly reflected in the optical excitations. At \(T=0\), electrons are excited from the occupied valence bands to the unoccupied conduction bands. The magneto-optical absorption function of the \((m, n)\) carbon nanotube is given by\textsuperscript{34}

\[
A(\omega; \phi) \approx \sum_{f,\beta} \int_{1stBZ} \frac{dk_z}{2\pi} \frac{\left| \langle \Psi_f (J', k_z; \sigma \phi) | \hat{E} | \Psi_{\beta} (J, k_z; \phi) \rangle \right|^2}{\omega^2 (J, J', k_z; \phi) \left( \omega - \omega_{\text{xc}} (J, J', k_z; \phi) \right)^2 + \Gamma^2} \cdot \Gamma,
\]

\[
D(\omega; \phi) = 2 \sum_{f, \beta, \sigma, \nu} \int_{1stBZ} \frac{dk_z}{2\pi} \frac{\Gamma}{\left( \omega - E\nu (J, k_z; \phi) \right)^2 + \Gamma^2}.
\]
excitations between the band-edge states of the two parabolic bands with the same \( J \) produce the asymmetric absorption peaks. These peaks are divergent in the square-root form at \( G \to 0 \), mainly owing to the vHs in the conduction and valence bands. For the first absorption peak, its frequency (\( \omega_1 \)) is energy gap without the spin-B interaction, but not that with the spin-B interaction [Fig. 1~]. Both frequency and intensity increase as \( f \) grows. The enhancement of intensity is caused by the less dispersive parabolic bands. The magnetic flux also leads to double absorption peaks at higher frequency.

The nanotube geometry affects band structures and thus absorption peaks. Figure 5(a) shows DOS for different carbon nanotubes at \( \phi = \phi_0 / 12 \) and \( \alpha = 0^\circ \). The type-I (10, 10) nanotube, the type-II (13, 7) nanotube, and the type-II (18, 0) nanotube have the different chiral angles. Their DOS’s exhibit asymmetric peaks at \(|\omega| < 0.05 \gamma_0 \) and \( 0.25 \gamma_0 < |\omega| < 0.35 \gamma_0 \). That is to say, the energy range of peaks is the same for type-I and type-II carbon nanotubes. On the other hand, the differences in DOS’s are mainly determined by armchair or nonarmchair structures (\( \theta = -30^\circ \) or others). Armchair nanotubes have half the peaks compared with nonarmchair nanotubes. This result could be understood from the simple zone folding model.\(^{31}\) Moreover, the DOS is higher for the former. Armchair nanotubes thus exhibit fewer but stronger absorption peaks [Fig. 5(b)]. The number of interband excitation channels is proportional to the nanotube radius or the number of 1D subbands, as shown in Fig. 5(a) for the type-I (20, 20) and (10, 10) nanotubes. The large nanotubes have more absorption peaks and lower threshold frequency [Fig. 5(b)]. As for the energy spacing between the two neighboring peaks, \( \omega_x \) decreases in the increasing of radius or chiral angle.

The direction of the magnetic field plays an important role on electronic and optical properties. DOS of the type-I (10, 10) nanotube is shown in Fig. 6(a) at \( \phi = \phi_0 / 12 \) and different \( \alpha \)’s. The main effect of \( B_\parallel \) is to induce the subband splitting except for the two energy bands near \( E_F \). The larger \( B_\parallel \) is (the smaller \( \alpha \) is), the wider the energy spacing between the two neighboring peaks is. The coupling of different \( J \)'s due to \( B_\perp \) is negligible at \( \phi = \phi_0 / 12 \). Only the optical excitations from the symmetric energy bands produce the strong absorption peaks, as shown in Fig. 6(b). To get the additional absorption peaks, the magnetic flux needs to be sufficiently high, e.g., \( \phi = \phi_0 / 3 \). At \( \alpha = 90^\circ \), the perpendicular magnetic field hardly affects the state degeneracy. There are fewer absorption peaks. It is very special that the first absorption peak is absent. The main reasons are as follows. The energy bands nearest to the Fermi level are linear except at the neighborhood of band edges [Fig. 6(a)]. The Zeeman splitting makes the (10, 10) nanotube metallic, so there are no allowable optical excitations from the band-edge states with the different spin states. Moreover, the linear energy dispersions, as discussed earlier, have no contributions to absorption spectra. In addition, the type-II (18, 0) nanotube exhibits the similar...
DOS and $A(\omega)$ except that the first absorption peak is present at $\alpha = 90^\circ$ and $\phi = 0^\circ$ [Fig. 8(b)].

DOS of the type-III (17, 0) nanotube exhibits eight peaks at $0.08 \gamma_0 < |\omega| < 0.22 \gamma_0$, as shown in Fig. 7(a). As a result, at $\phi = 0^\circ$, the symmetric conduction and valence bands yield four absorption peaks at $0.16 \gamma_0 < \omega < 0.44 \gamma_0$ [Fig. 7(b)]. When the magnetic field deviates from the nanotube axis, each energy band is made up of different angular momenta ($J$ and $J+1$). The optical excitations from the asymmetric energy bands are allowed; therefore the coupling of different $J$’s causes two new absorption peaks at $0.3 \gamma_0$. Such peaks become stronger as $\alpha$ increases; that is, the coupling effect is more important at large $\alpha$. They hardly exist in the type-I (10, 10) nanotube or the type-II (18, 0) nanotube [Fig. 6(b)]. It is relatively easy to see the coupling of different $J$’s in the type-III carbon nanotubes.

The $\alpha$-dependent absorption frequencies are important in understanding the characteristics of absorption peaks. The frequencies ($\omega_i$’s) of absorption peaks are shown in Fig. 8 for the type-I (10, 10) nanotube at $\phi = 0^\circ$. The frequency of the first peak is $\omega_1 \sim 0.05 \gamma_0$ at $\alpha = 0^\circ$. $\omega_1$ is equal to the energy gap in the absence of the Zeeman splitting, and it decreases with $\alpha$. The first peak is absent at sufficiently large $\alpha$ ($\geq 81^\circ$), where the (10, 10) nanotube is a gapless metal. The two neighboring peaks, the second peak and the third peak, have the largest energy spacing at $\alpha = 0^\circ$. Their frequencies are, respectively, $\omega_2 \sim 0.57 \gamma_0$ and $\omega_3 \sim 0.67 \gamma_0$. They gradually merge together in the increasing of $\alpha$, since the double degeneracy would be restored. The type-II (18, 0) nanotube is similar to the type-I (10, 10) nanotube, such as the frequency range of absorption peaks ($0.5 \gamma_0 < \omega_i < 0.7 \gamma_0$) and the merger of a pair of peaks at $\alpha = 90^\circ$. However, the number of absorption peaks is double for the former [Fig. 8(b)]. The absorption peaks of the type-III (17, 0) nanotube occur at the different frequency range [$0.16 \gamma_0 < \omega_i < 0.44 \gamma_0$ in Fig. 8(c)]. The two additional peaks with $\omega_i \sim 0.3 \gamma_0$ could survive at sufficiently large $\alpha$, when the coupling of different angular momenta is strong. The difference in absorption frequency range is useful in distinguishing type-III carbon nanotubes from type-I or type-II carbon nanotubes. The Zeeman splitting does not affect the number of absorption peaks and absorption frequencies except the disappearance of the first peak from type-I and type-II carbon nanotubes. The experimental measurements on the magnetooptical properties can verify the predicted absorption frequencies.

The effective-mass approximation had been used to study magnetoelectronic and optical spectra. There are some similar results. The optical spectra strongly depend on the direction and the magnitude of the magnetic field. Moreover, all the absorption peaks can exist in the parallel electric polarization. However, such works do not involve the Zeeman splitting and the curvature effects. The present work can provide more detailed optical properties, e.g., the absorption frequencies and the number of absorption peaks.
are significantly affected by the nanotube geometry (radius and chiral angle), the magnitude and the direction of the magnetic field, and the Zeeman splitting. The predicted physical properties, energy gap, density of states, and absorption spectrum can be tested by scanning tunneling spectroscopy, transport measurements, and optical-absorption spectroscopy. The curvature effects and the Zeeman splitting are included in the calculations. There exist certain important differences between the present study and the previous studies such as the dependence of energy gap for type-II carbon nanotubes, the relation between energy gap and magnetic field, and the metalization of type-I carbon nanotubes in the perpendicular magnetic field.

The nanotube geometry dominates the electronic properties, energy gap, state degeneracy, and number of energy bands. The differences among type-I, type-II, and type-III carbon nanotubes are directly reflected in the optical excitations, e.g., the number of absorption peaks and the range of absorption frequencies. The magnetic field results in the change of energy gap, the destruction of state degeneracy, and the coupling of different angular momenta. Hence there are magnetic-field-dependent absorption frequencies and more absorption peaks. The Zeeman splitting can effectively reduce energy gap, so it makes the semiconductor-metal transition display at lower magnetic flux. It can completely metalize type-I carbon nanotubes in the presence of the perpendicular magnetic field. The Zeeman splitting is expected to play an important role on the low-energy physical properties, e.g., magnetoplasmons and magnetic susceptibility. However, it has no effect on the optical excitations except for metallic carbon nanotubes.

**IV. CONCLUDING REMARKS**

In this work, we have studied the magnetoelectronic and optical properties of single-walled carbon nanotubes. They

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