

Electronic Properties of Carbon Tori in External Fields

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Electronic states of carbon tori in electric and magnetic fields are studied by the tight-binding model with the curvature effect. Electronic properties, such as electronic states, energy gaps, and density of states, are very sensitive to the changes in the direction and the magnitude of the external fields. The electric field can widen the π -electron energy width; furthermore, there are more low- and extreme-energy states. Energy gaps are drastically modulated by $\mathbf{E}$. The zero-gap transition ($E_g \neq 0 \rightarrow E_g = 0$) happens more frequently when $\mathbf{E}$ deviates from the symmetric axis, or its magnitude is sufficiently large. The electric field could change the state degeneracy. Moreover, the modulation of electronic states is enhanced by the magnetic field.

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1. Introduction

Since carbon nanotubes were discovered in 1991 by Iijima,¹⁾ they have attracted a lot of theoretical and experimental studies because of their particular geometric structures^{2,3)} and electronic properties.⁴⁻⁹⁾ Due to the nano-scaled size and the diversified conductivity, carbon nanotubes have bright prospects in nanoelectronic devices. A single-walled carbon nanotube (SWCNT) is formed by rolling a graphite sheet from the origin to the vector $\mathbf{R}_x = m\mathbf{a}_1 + n\mathbf{a}_2$. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive lattice vectors of a graphite sheet. The parameters (m, n) specifically define a SWCNT. From the theoretical calculations,⁸⁾ carbon nanotubes are divided into three types: (I) gapless metals for $m = n$, (II) narrow-gap semiconductors for $2m + n = 3I$ and $m \neq n$ (I an integer), and (III) moderate-gap semiconductors for $2m + n \neq 3I$. Electronic structures are predicted¹⁰⁻¹²⁾ to be strongly affected by the transverse electric field ($\mathbf{E}_\perp$) perpendicular to the nanotube axis. The electric field significantly changes the low-energy bands; furthermore, it could induce the semiconductor-metal transition (SMT).

A carbon toroid (CT), which was recently found by Liu *et al.*,¹³⁾ is closely related to a straight SWCNT. The scanning force microscopy image shows that a CT has height or width of 1.0–1.2 nm and diameter 300–500 nm. Carbon tori have stimulated many studies, such as electronic properties,¹⁴⁻¹⁸⁾ magnetic properties,¹⁸⁻²⁴⁾ and optical properties.²⁵⁻²⁷⁾ Experimentally, the low-temperature magneto-resistance (MR) measurement on carbon nanotube ring was performed.²⁸⁾ The coherence length, determined by the measured MR, revealed characteristic of dephasing through weakly inelastic electron–electron interaction at the low temperature. Moreover, the small carbon nanotube rings on the Si substrate exhibit the characteristics of the field-effect transistor with the sharp switching behavior.²⁹⁾ This result

means the high potential in the nanoscaled electronic circuits.

A CT is formed by bending a cylindrical SWCNT along the tubular axis and further connecting the origin to the vector $\mathbf{R}_y = p\mathbf{a}_1 + q\mathbf{a}_2$ (the axial periodic vector of a SWCNT). That is to say, a CT corresponds to a rolled-up graphite sheet which satisfies the transverse ($\|\mathbf{R}_x$) and the longitudinal ($\|\mathbf{R}_y$) periodical boundary conditions simultaneously (details in ref. 14). The geometric structure is characterized by the parameters (m, n, p, q) , such as height, radius and chiral angle. The height and the radius are, respectively, $2r = |\mathbf{R}_x|/\pi = b\sqrt{3(m^2 + mn + n^2)}/\pi$ and $R = |\mathbf{R}_y|/2\pi = b\sqrt{3(p^2 + pq + q^2)}/2\pi$. $b = 1.42 \text{ \AA}$ is the C–C bond length. The chiral angle of a (m, n, p, q) toroid is $\theta = \tan^{-1}[-\sqrt{3}n/(2m + n)]$. It is confined to $-30^\circ \leq \theta \leq 0^\circ$. A CT has a lot of discrete states which are described by the longitudinal (L) and the transverse (J) angular momenta. According to energy gaps, there are four types of carbon tori in the presence of the curvature effect:^{14,17)} (I) $E_g = \gamma_0 b/r$ for $2m + n \neq 3I$ ($\gamma_0 \sim 3 \text{ eV}$), (II) $E_g = 0$ for $m = n$, (III) $E_g = \gamma_0 b/R$ for $m = n$, and (IV) $E_g \propto \gamma_0 (b/r)^2$ for others. Only a little armchair $(m, m, p, -p)$ carbon tori are type-II gapless systems. When carbon tori exist in the magnetic field parallel to the symmetric axis ($\mathbf{B}_\parallel$), the longitudinal angular momentum L would become $L + \phi/\phi_0$ (ϕ is magnetic flux and $\phi_0 = hc/e$). The theoretical results^{14,23,24)} show that $\mathbf{B}_\parallel$ causes the drastic modulations of energy gaps and destroys the state degeneracy. The perpendicular magnetic field $\mathbf{B}_\perp$ leads to the coupling of different L 's. The effect of $\mathbf{B}_\perp$ on energy gap is weaker than that of $\mathbf{B}_\parallel$. However, the state degeneracy is recovered for $\mathbf{B}_\perp$.

In this work, we use the tight-binding model to investigate electronic properties of achiral carbon tori in the presence of electric and magnetic fields. The curvature effect is included in the calculations. Electronic properties, such as electronic states, energy gaps, and density of states, are strongly

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affected by the direction and the magnitude of electric and magnetic fields. Our study shows that the electric field could induce the zero-gap transition (ZGT), i.e., energy gap changes from a finite value to zero, or *vice versa*. Such transition happens more frequently, when the electric field is oriented closer to the toroidal plane or its magnitude is sufficiently large. The π -electron energy width is widened, and there are more low- and extreme-energy states. The state degeneracy is destroyed by the electric field. The modulation of electronic states is enhanced by the magnetic field.

2. The Tight-Binding Model in Electric and Magnetic Fields

Achiral carbon tori, $(m, m, p, -p)$ armchair tori and $(m, 0, p, -2p)$ zigzag tori, are chosen for a model study. The π -electronic states are calculated from the nearest-neighbor tight-binding model with the curvature effect. There are $N = 4pm$ carbon atoms in each armchair or zigzag toroid. The Hermitian Hamiltonian matrix is built from the subspace spanned by the N wave functions of $2p_z$ orbitals. Under electric and magnetic fields, the nearest-neighbor Hamiltonian is given by

$$H = \sum_i \epsilon_i(\mathbf{E}) \mathbf{c}_i^\dagger \mathbf{c}_i - \sum_{i,j} \mathbf{t}_{ij}(\mathbf{B}) \mathbf{c}_i^\dagger \mathbf{c}_j, \quad (1)$$

where $\epsilon_i(\mathbf{E})$ is the on-site energy due to the electric field, and $\mathbf{t}_{ij}(\mathbf{B})$ is the nearest-neighbor hopping integral associated with the magnetic field. $\{\mathbf{c}_i^\dagger, \mathbf{c}_j\}$ are creation and annihilation operators of fermions. Due to the curvature effect (the misorientation of the $2p_z$ orbitals on the cylindrical surface), $\mathbf{t}_{ij}$'s would be different along the longitudinal and the transverse directions: $\gamma_1 = \gamma_0(1 - b^2 \sin^2 \theta / 8r^2)$, $\gamma_2 = \gamma_0[1 - b^2(\sin \theta + \sqrt{3} \cos \theta)^2 / 32r^2]$, and $\gamma_3 = \gamma_0[1 - b^2(\sin \theta - \sqrt{3} \cos \theta)^2 / 32r^2]$. γ_0 (~ 3 eV) is the resonance integral without the curvature effect.^{14,17)}

For $(m, m, p, -p)$ armchair carbon tori, there are $2m$ atoms along $\mathbf{R}_x$ and $2p$ atoms along $\mathbf{R}_y$. The atom position is represented by the coordinates (x_i, y_i) in a graphite plane, where $i = 1, 2, 3, \dots, N$. The distance between the i th atom and the j th atom is $\Delta_{ij} = \sqrt{\Delta x^2 + \Delta y^2}$, where $\Delta x = |x_i - x_j|$ and $\Delta y = |y_i - y_j|$. The Hamiltonian matrix elements in the absence of $\mathbf{E}$ or $\mathbf{B}$ are given by

$$H_{ij} = \begin{cases} -\gamma_3 = -\gamma_0(1 - b^2/8r^2) & \text{if } \Delta_{ij} = b, \Delta y = 0, \\ -\gamma_1 = -\gamma_0(1 - b^2/32r^2) & \text{if } \Delta_{ij} = b, \Delta y \neq 0, \\ 0 & \text{if } \Delta_{ij} \neq b. \end{cases} \quad (2)$$

As to $(m, 0, p, -2p)$ zigzag carbon tori, the Hamiltonian matrix elements are

$$H_{ij} = \begin{cases} -\gamma_1 = -\gamma_0 & \text{if } \Delta_{ij} = b, \Delta x = 0, \\ -\gamma_2 = -\gamma_0(1 - 3b^2/32r^2) & \text{if } \Delta_{ij} = b, \Delta x \neq 0, \\ 0 & \text{if } \Delta_{ij} \neq b. \end{cases} \quad (3)$$

When carbon tori exist in an electric field, its main effect is to change the on-site energy. The effective electric field is assumed to be $\mathbf{E} = E \cos \alpha_E \hat{\mathbf{Z}} + E \sin \alpha_E \hat{\mathbf{X}} = \mathbf{E}_\parallel + \mathbf{E}_\perp$, where α_E is the angle between $\mathbf{E}$ and the toroidal axis ($\hat{\mathbf{Z}}$). The unit of E is $\gamma_0/\text{\AA}$, here and henceforth. It is convenient in using the rectangular coordinates (X, Y, Z) . The center of toroid is chosen as the origin. The coordinates (x_i, y_i) of the i th atom in a graphite plane are transferred to (X_i, Y_i, Z_i) . Such coordinates are further expressed as $X_i = R_i \cos \Phi$,

$Y_i = R_i \sin \Phi$, and $Z_i = r \sin \beta$. R_i is the perpendicular distance between the i th atom and the toroidal axis. $\Phi = y_i/R$ and $\beta = x_i/r$ are azimuthal angles of carbon toroid and carbon nanotube, respectively. Due to the electric field, the diagonal elements of the Hamiltonian matrix are changed from zero to

$$H_{ii} = -E \cos \alpha_E Z_i - E \sin \alpha_E X_i. \quad (4)$$

In the presence of magnetic field, the hopping parameter is modified by the Peierls phase (G_{ij}).³⁰⁾ The magnetic field is assumed to be $\mathbf{B} = B \cos \alpha_B \hat{\mathbf{Z}} + B \sin \alpha_B \hat{\mathbf{R}} = \mathbf{B}_\parallel + \mathbf{B}_\perp$. α_B is the angle between $\mathbf{B}$ and the symmetric axis. The cylindrical coordinates (R, Φ, Z) are used for simplicity. The vector potential is chosen to be $\mathbf{A} = RB \cos \alpha_B / 2 \hat{\Phi} + RB \sin \alpha_B \sin \Phi \hat{\mathbf{Z}}$. It causes the magnetic phase factor $G = \int \mathbf{A} \cdot d\mathbf{R}$. Therefore, the hopping parameter t_{ij} would change into $t_{ij} e^{iG_{ij}}$. The magnetic phase is $G_{ij} = G_\parallel + G_\perp$, where

$$G_\parallel = \frac{\phi}{\phi_0} \cos \alpha_B \left(\frac{y_i - y_j}{R} \right), \quad (5)$$

and

$$G_\perp = \begin{cases} \frac{2\phi \sin \alpha_B (Z_j - Z_i)}{\phi_0 (y_j - y_i)} \left[\cos \left(\frac{y_i}{R} \right) - \cos \left(\frac{y_j}{R} \right) \right] & \text{if } \Delta y \neq 0, \\ \frac{2\phi \sin \alpha_B (Z_j - Z_i)}{\phi_0 R} \sin \left(\frac{y_i}{R} \right) & \text{if } \Delta y = 0. \end{cases} \quad (6)$$

Electronic state energies of achiral carbon tori could be obtained by diagonalizing the $4pm \times 4pm$ Hamiltonian matrix. They could be expressed as $E^{c,v}(M, \mathbf{E}, \mathbf{B})$, where M ($= 1, 2, 3, \dots, 4pm$) represents the discrete state. c and v , respectively, correspond to unoccupied and occupied states. The low-energy electronic states can be further understood from the density of states (DOS). It is defined as

$$D(\omega, \phi) = \sum_{M=1}^{4pm} \frac{2}{\pi} \frac{\Gamma}{[E^{c,v}(M, \mathbf{E}, \mathbf{B}) - \omega]^2 + \Gamma^2}, \quad (7)$$

where $\Gamma = 5 \times 10^{-5} \gamma_0$ is the broadening parameter.

3. Electronic Properties

We first see the electronic structure of the $(5, 5, 100, -100)$ armchair toroid ($R = 39 \text{\AA}$ and $2r = 6.8 \text{\AA}$). The discrete states in the absence of $\mathbf{E}$ are simply reviewed. Each state is described by the longitudinal and transverse angular momenta (L, J) .^{23,24)} The low-energy electronic states are doubly degenerate [Fig. 1(a)]; that is, $E(L, m) = E(p - L, 2m)$. Also noted that the high energy states might have fourfold degeneracy [$E(L, J_1) = E(L, 2m - J_1) = E(p - L, J_2) = E(p - L, 2m - J_2)$; not shown]. The occupied and unoccupied states are symmetric to the Fermi level ($E_F = 0$). It might have an energy gap between the lowest unoccupied state (LUS) and the highest occupied state (HOS), e.g., $E_g = 0.04 \gamma_0$ at $\mathbf{E} = 0$. The total π -electron energy width (E_w), the energy difference between the lowest occupied state and the highest unoccupied state, is $\sim 6\gamma_0$.

The low-energy states in the presence of $\mathbf{E}$ are detailedly investigated. For the electric field $E = 0.02 \gamma_0/\text{\AA}$, the maximum electric potential differences along the toroid diameter and the toroid height are about 4.6 and 0.4 V, respectively. For the parallel electric field ($\alpha_E = 0^\circ$),

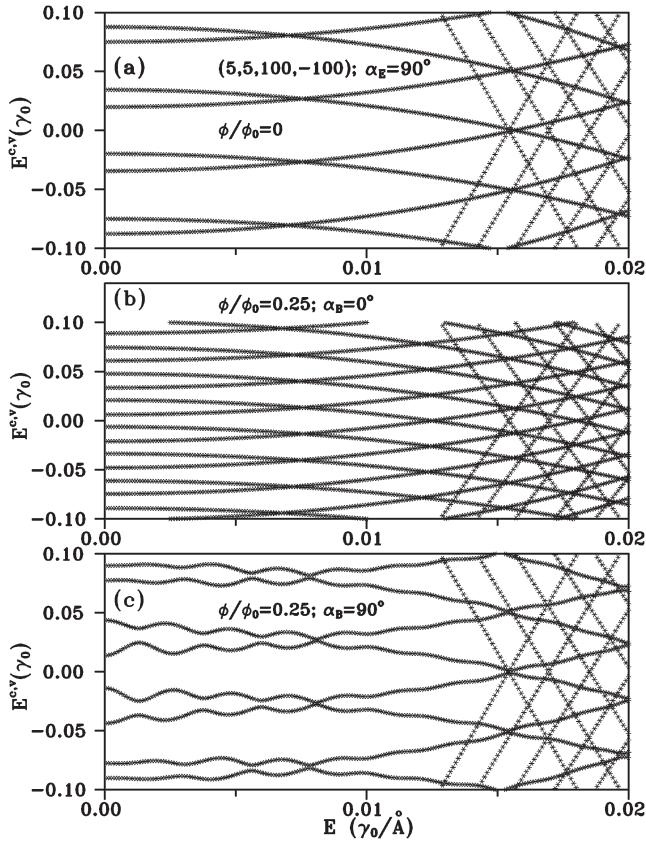


Fig. 1. The low-energy states of the (5,5,100,-100) toroid at $\alpha_E = 90^\circ$ and (a) $\phi = 0$, (b) $(\phi = 0.25 \phi_0, \alpha_B = 0^\circ)$; (c) $(\phi = 0.25 \phi_0, \alpha_B = 90^\circ)$.

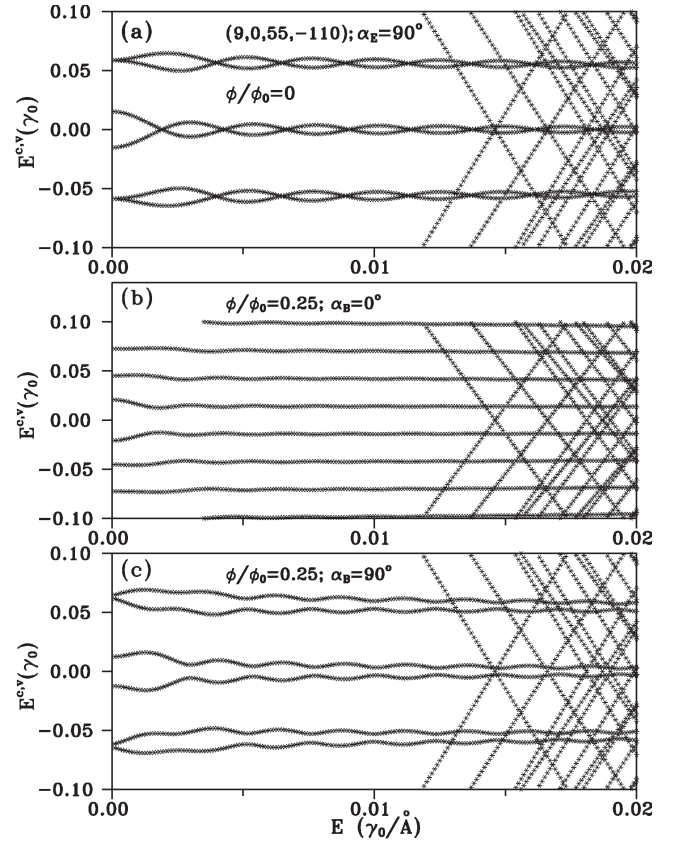


Fig. 2. Same plot as Fig. 1, but shown for the (9,0,55,-110) toroid.

electronic structures are hardly changed for $E < 0.02 \gamma_0/\text{\AA}$ (not shown here). That $\epsilon_i(\mathbf{E}_\parallel)$ at $E < 0.02 \gamma_0/\text{\AA}$ is much smaller than the typical hopping integral γ_0 is the main reason. On the other hand, state energies are gradually affected by the large electric field, e.g., $E > 0.05 \gamma_0/\text{\AA}$ (not shown). Only the large $\mathbf{E}_\parallel$ have a strong effect on electronic properties, such as state energy, energy width, energy gap, and wave function. From the perturbation point of view, each state is mainly characterized by the superposition of the wave functions $|L, J\rangle$, $|L, J+1\rangle$, and $|L, J-1\rangle$ in the absence of electric field. However, the state symmetry about $E_F = 0$ is not destroyed by $\mathbf{E}_\parallel$. This result remains unchanged even for other electric and magnetic fields.

As for the perpendicular electric field, electronic states are drastically modulated even for the weak field, as shown in Fig. 1(a). State energies would become large or small in the increasing of $\mathbf{E}_\perp$; therefore, there exist state crossings. Such crossings happen more frequently at large $\mathbf{E}_\perp$. Energy gap is vanishing at certain electric fields. More electronic states are grouped into the low- and extreme-energy regions. $\mathbf{E}_\perp$ would make the longitudinal angular momentum change from the separate L into the superposition of L , $L+1$, and $L-1$. The coupling amplitudes are different for $L+1$ and $L-1$. The perpendicular electric field has different effects on the doubly degenerate states ($|L, m\rangle$ and $|p-L, 2m\rangle$) so that state degeneracy is clearly destroyed by $\mathbf{E}_\perp$ at sufficiently large field ($E \sim 0.05 \gamma_0/\text{\AA}$) [Figs. 5(b)–5(d)]. The effects of $\mathbf{E}_\perp$ on electronic structures are much stronger than those of $\mathbf{E}_\parallel$, since the electric potential difference is large in the equatorial plane. This result clearly reflects the geometric feature, i.e.,

the radius is much larger than the height.

Electronic states of carbon tori are further changed by the magnetic field. For the applied magnetic flux $\phi = 0.25 \phi_0$, the corresponding magnitude of the magnetic field is about 21 T. It could be effectively reduced as the toroid radius increases. The parallel magnetic field causes the rigid shift of the longitudinal angular momentum from L to $L + \phi/\phi_0$. The doubly degenerate states are split up by $\mathbf{B}_\parallel$, as shown in Fig. 1(b). The energy spacing between two electronic states is reduced. The modulation of energy spectra is enhanced by $\mathbf{B}_\parallel$ and thus leads to more state crossings [Fig. 1(b)]. The vanishing energy gaps would occur at the smaller electric fields. On the other hand, the perpendicular magnetic field induces the coupling of different L 's. $\mathbf{B}_\perp$ has weaker effects on changing electronic states [Fig. 1(c)], compared with $\mathbf{B}_\parallel$. $\mathbf{B}_\perp$ strengthened the modulation of electronic structures [Fig. 1(c)], while it does not destroy state degeneracy.

The external electric and magnetic fields induce the similar effects in zigzag carbon tori [Figs. 2(a)–2(c)], as seen in armchair carbon tori [Figs. 1(a)–1(c)]. However, there are two main differences between zigzag and armchair tori. At vanishing fields, a zigzag carbon toroid has fourfold degeneracy [$E(L, J_1) = E(L, 2m - J_1) = E(p - L, J_2) = E(p - L, 2m - J_2)$] except for the doubly degenerate HOS and LUS. The electronic-state modulation due to the perpendicular electric field is stronger for a zigzag carbon toroid. There are more state crossings [Fig. 2(a)], and energy gap vanishes at the smaller electric fields. Moreover, state degeneracy could be destroyed at $(\phi = 0 \text{ and } \mathbf{E}_\perp \rightarrow \mathbf{0})$ or $(\phi = 0.25 \phi_0, \alpha_B = 90^\circ \text{ for any } \mathbf{E})$.

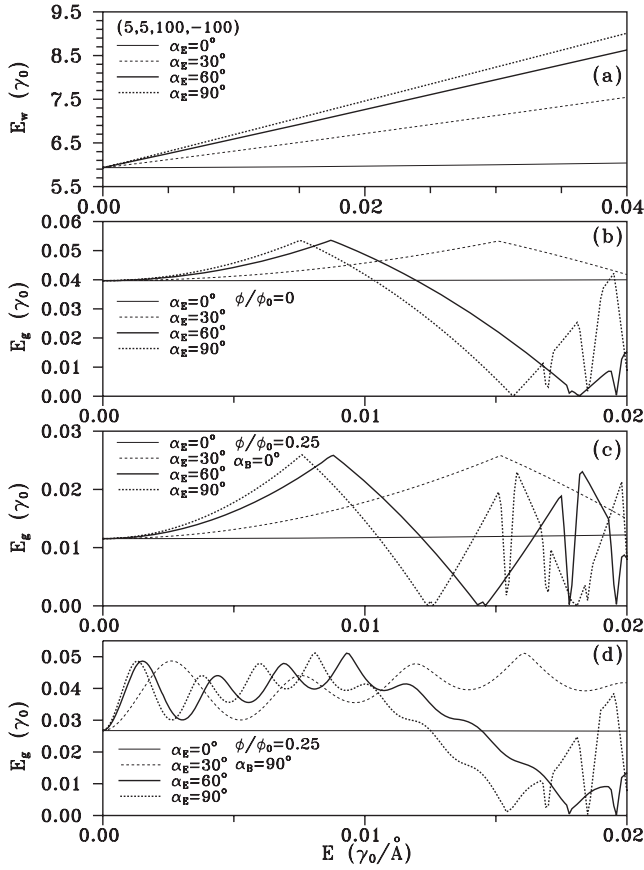


Fig. 3. (a) The electric-field-dependent π -electron energy width of the (5,5,100,−100) toroid for different field directions. The electric-field-dependent energy gap at different field directions for (b) $\phi = 0$, (c) ($\phi = 0.25 \phi_0$, $\alpha_B = 0^\circ$); (d) ($\phi = 0.25 \phi_0$, $\alpha_B = 90^\circ$). The Zeeman effect is taken into account.

The total π -electron energy width is drastically changed by the electric field. E_w strongly depends on the magnitude and the direction of $\mathbf{E}$, as shown in Figs. 3(a) and 4(a) for armchair and zigzag carbon tori, respectively. E_w linearly grows with the increasing electric field. The perpendicular electric field could widen energy width very effectively. This result clearly illustrates that electronic states are grouped into the two extreme-energy regions in addition to the low-energy region (close to $E_F = 0$).

In order to understand the zero-gap transition, the variation of energy gap with the direction and the magnitude of the electric field is investigated. Fig. 3(b) presents the electric-field-dependent energy gap for the (5,5,100,−100) armchair toroid at $E \leq 0.02 \gamma_0/\text{\AA}$. At $\alpha_E = 0^\circ$, energy gap is hardly changed by the electric field (the light solid curve); that is, the energy-gap modulation is negligible for the parallel electric field. When the electric field gradually deviates from the symmetric axis, the energy-gap modulation is getting stronger. The zero-gap transition occurs at the electric field with larger perpendicular components (the heavily solid and dashed curves). In general, there are more ZGT's for the large E and the corresponding threshold electric field is reduced as α_E increases. The energy-gap modulation is greatly strengthened by the magnetic field, as shown in Figs. 3(c) and 3(d). The spin- B interaction, $g\sigma\phi/m_e R^2 \phi_0$, is included in the calculations. The g factor is equal to 2, $\sigma = \pm 1/2$ is the electron spin, and m_e is the

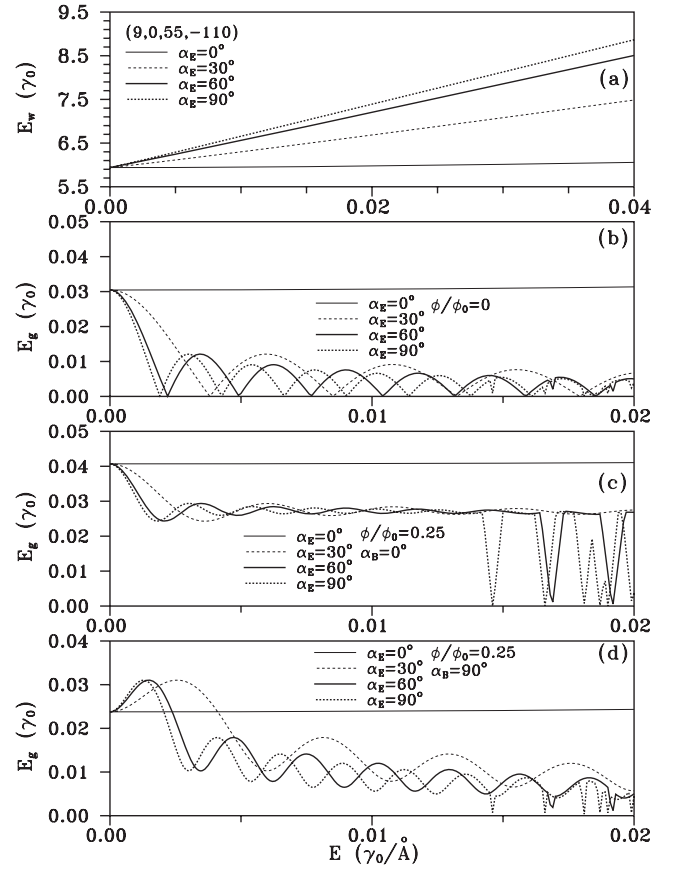


Fig. 4. Same plot as Fig. 3, but shown for the (9,0,55,−110) toroid.

bare electron mass. The Zeeman splitting and the parallel magnetic field might make ZGT's happen more frequently [Fig. 3(c)]. The similar energy-gap modulations could also be found in zigzag carbon tori, e.g., energy gap of the (9,0,55,−110) zigzag toroid in Figs. 4(b)–4(d). At $\mathbf{B} = 0$ and $\alpha_E \neq 0^\circ$, Fig. 4(b) shows that energy gap has stronger dependence on the electric field than that in armchair tori. However, the ZGT's hardly survive in the magnetic field for the weak electric field, mainly owing to the widened energy gap at $E = 0$ [Figs. 4(c) and 4(d)]. It is worth noting that the contribution of the zero-gap transition mainly comes from the orbital magnetization. But the Zeeman energy, at sufficiently large magnetic fields, could increase the times of ZGT-occurrence. The predicted energy gaps could be test by the transport measurements.¹¹⁾

The above-mentioned features of electronic states are directly reflected in density of states (DOS). The low-energy DOS of the (5,5,100,−100) armchair toroid is shown in Figs. 5(a)–5(d). DOS exhibits many delta-function-like symmetric peaks because of the zero-dimensional discrete states. The height of peak corresponds to the state degeneracy. The double degeneracy remains unchanged in the presence of the parallel electric field, as shown in Fig. 5(a). The sufficiently large electric field only changes the state energies (the light dashed curve at $E = 0.05 \gamma_0/\text{\AA}$). The number of the prominent peaks grows in the increasing of α_E [Figs. 5(b)–5(d)]. This result clearly illustrates that a lot of discrete states are grouped into the low-energy region. The peak height could be reduced to half as α_E or E increases. For example, a lot of singlet states exist at $E = 0.05 \gamma_0/\text{\AA}$

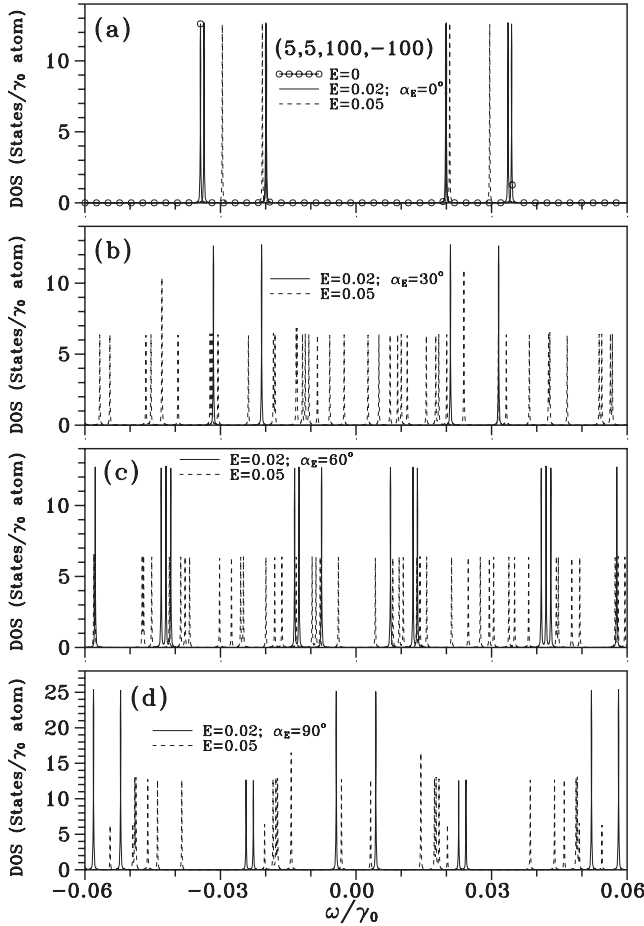


Fig. 5. The density of states of the (5,5,100,-100) toroid at $E = 0.02 \gamma_0/\text{\AA}$ and $E = 0.05 \gamma_0/\text{\AA}$ for (a) $\alpha_E = 0^\circ$, (b) $\alpha_E = 30^\circ$, (c) $\alpha_E = 60^\circ$, (d) $\alpha_E = 90^\circ$. The zero-field result is also shown in (a) for comparison.

[Fig. 5(d)]. It might also have fourfold-degeneracy states, e.g., DOS at $E = 0.02 \gamma_0/\text{\AA}$ and $\alpha_E = 90^\circ$ [Fig. 5(d)]. Such states come from the higher energy states at $E = 0$, as shown in Fig. 1(a). That is to say, the perpendicular electric field could make the higher energy states approach to the Fermi level. The magnitude and the direction of the electric field play a similar role on the low-energy DOS of the (9,0,55,-110) zigzag toroid, such as the increase in the peak number and the reduction of the peak height with the increasing E or α_E [Figs. 6(a)–6(d)].

The mixing effects of $\mathbf{E}$ and $\mathbf{B}$ on the density of states deserve a closer investigation. The field directions of $\mathbf{E}$ and $\mathbf{B}$ are assumed to be parallel or perpendicular to each other. Armchair tori quite differ from zigzag tori in state degeneracy. For the former, (I) the double degeneracy at $\alpha_E = 0^\circ$ is destroyed by the parallel magnetic field [solid lines in Fig. 7(a)], (II) the double degeneracy at $\alpha_E = 0^\circ$ remains unchanged for the perpendicular magnetic field [dashed lines in Fig. 7(a)], (III) the double degeneracy at $\alpha_E = 90^\circ$ is destroyed for the parallel magnetic field, or the fourfold degeneracy keeps the same for the parallel magnetic field [solid lines in Fig. 7(b)], and (IV) the perpendicular magnetic field does not affect the double degeneracy and the fourfold degeneracy at $\alpha_E = 90^\circ$ [dashed lines in Fig. 7(b)]. As to the latter, (I) the fourfold degeneracy at $\alpha_E = 0^\circ$ is changed into the double degeneracy by the parallel magnetic

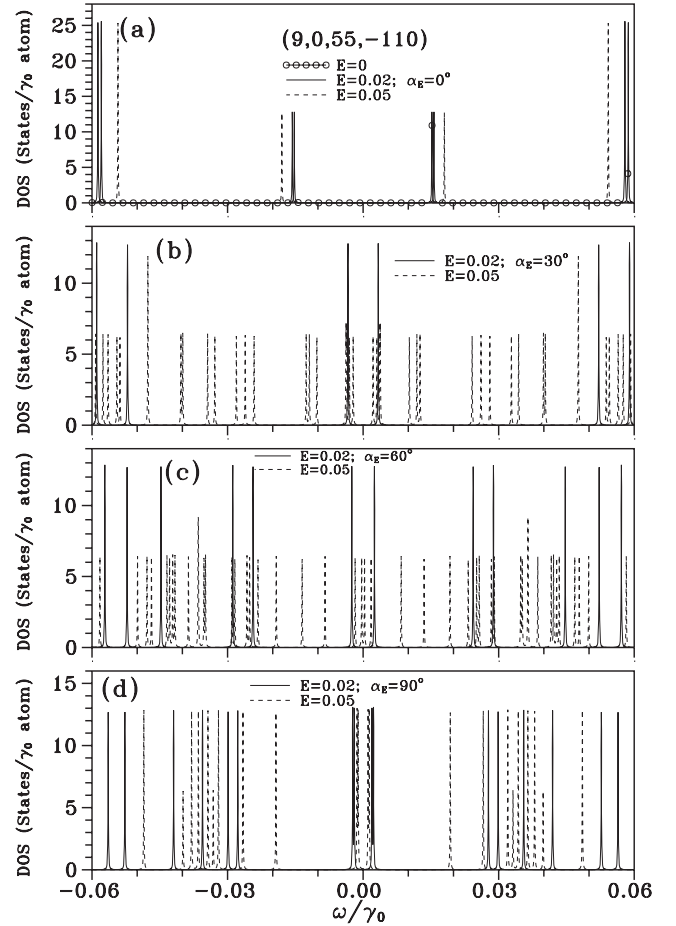


Fig. 6. Same plot as Fig. 5, but shown for the (9,0,55,-110) toroid.

field [solid lines in Fig. 7(c)]. The double degeneracy exists in other cases [Figs. 7(c)–7(d)]; that is, zigzag tori exhibit the double degeneracy for four kinds of cases. (II) The perpendicular magnetic field [dashed lines in Fig. 7(c)] or the perpendicular electric field [Fig. 7(d)] could also lead to the destruction of state degeneracy.

4. Conclusion

In this work, we have studied electronic properties of carbon tori in the presence of electric and magnetic fields. Electronic states, energy gaps, and density of states strongly depend on the direction and the magnitude of the external fields, and the geometric structure. The electric field leads to the broadening of the π -electron energy width, more low- and extreme-energy states, the strong modulation of energy gap, the state crossing, and the destruction of state degeneracy. The zero-gap transition happens more frequently when the electric field deviates from the symmetric axis, or its magnitude is sufficiently large. The modulation of electronic states is largely enhanced by the magnetic field. The predicted electronic properties could be verified by the transport measurements.

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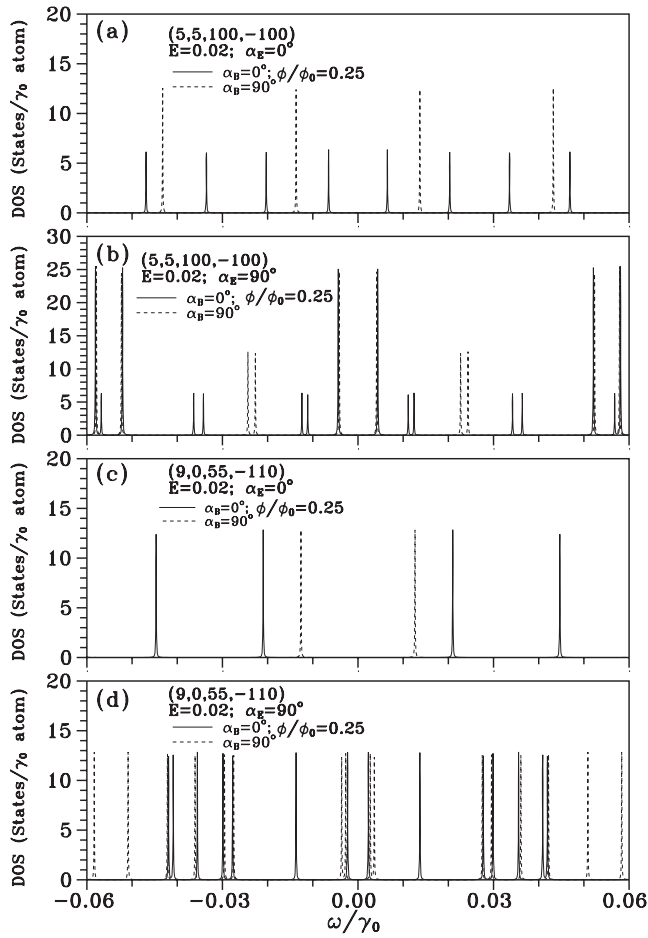


Fig. 7. The density of states of the (5, 5, 100, -100) toroid in the absence of the Zeeman splitting at $E = 0.02 \gamma_0/\text{\AA}$, $\phi = 0.25 \phi_0$, and (a) ($\alpha_E = 0^\circ$, $\alpha_B = 0^\circ$, and $\alpha_B = 90^\circ$), (b) ($\alpha_E = 90^\circ$, $\alpha_B = 0^\circ$, and $\alpha_B = 90^\circ$). (c) and (d) are same plots as (a) and (b) but for the (9, 0, 55, -110) toroid.

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- 1) S. Iijima: *Nature* **354** (1991) 56.
- 2) R. Saito, M. Fujita, G. Dresselhaus and M. S. Dresselhaus: *Appl. Phys. Lett.* **60** (1992) 2204.
- 3) N. Hamada, S. I. Sawada and A. Oshiyama: *Phys. Rev. Lett.* **68** (1992) 1579.
- 4) J. W. Mintmire, B. I. Dunlap and C. T. White: *Phys. Rev. Lett.* **68** (1992) 631.
- 5) C. L. Kane and E. J. Mele: *Phys. Rev. Lett.* **78** (1997) 1932.
- 6) K. Tanaka, K. Okahara, M. Okada and T. Yamabe: *Chem. Phys. Lett.* **191** (1992) 469.
- 7) H. Ajiki and T. Ando: *J. Phys. Soc. Jpn.* **65** (1996) 505.
- 8) F. L. Shyu, C. P. Chang, R. B. Chen and M. F. Lin: *J. Phys. Soc. Jpn.* **72** (2003) 454.
- 9) T. Ando: *J. Phys. Soc. Jpn.* **74** (2005) 777.
- 10) X. Zhou, H. Chen and O. Y. Zhong: *J. Phys.: Condens. Matter* **13** (2001) L635.
- 11) Y. H. Kim and K. J. Chang: *Phys. Rev. B* **64** (2001) 153404.
- 12) J. O'keeffe, C. Wei and K. Cho: *Appl. Phys. Lett.* **80** (2002) 676.
- 13) J. Liu, H. Dai, J. H. Hafner, D. T. Colbert, R. E. Smalley, S. J. Tan and C. Dekker: *Nature* **385** (1997) 780.
- 14) M. F. Lin, R. B. Chen and F. L. Shyu: *Solid State Commun.* **107** (1998) 227.
- 15) D. H. Oh, J. M. Park and K. S. Kim: *Phys. Rev. B* **62** (2000) 1600.
- 16) S. A. Bovin, L. F. Chibotaru and A. Ceulemans: *J. Mol. Catal. A* **166** (2001) 47.
- 17) M. F. Lin and D. S. Chuu: *J. Phys. Soc. Jpn.* **67** (1998) 259.
- 18) M. F. Lin and D. S. Chuu: *Phys. Rev. B* **57** (1998) 6731.
- 19) M. F. Lin: *J. Phys. Soc. Jpn.* **67** (1998) 1094.
- 20) R. C. Haddon: *Nature* **388** (1997) 31.
- 21) A. A. Odintsov, W. Smit and H. Yoshioka: *Europhys. Lett.* **45** (1999) 598.
- 22) S. Latil, S. Roche and A. Rubio: *Phys. Rev. B* **67** (2003) 165420.
- 23) C. C. Tsai, F. L. Shyu, C. W. Chiu, C. P. Chang, R. B. Chen and M. F. Lin: *Phys. Rev. B* **70** (2004) 075411.
- 24) F. L. Shyu, C. C. Tsai, C. P. Chang, R. B. Chen and M. F. Lin: *Carbon* **42** (2004) 2879.
- 25) M. F. Lin: *Phys. Rev. B* **58** (1998) 3629.
- 26) M. F. Lin: *J. Phys. Soc. Jpn.* **67** (1998) 2218.
- 27) F. L. Shyu: *Phys. Rev. B* **72** (2005) 045424.
- 28) H. R. Shea, R. Martel and Ph. Avouris: *Phys. Rev. Lett.* **84** (2000) 4441.
- 29) H. Watanabe, C. Manabe, T. Shigematsu and M. Shimizu: *Appl. Phys. Lett.* **78** (2001) 2928.
- 30) S. Roche, G. Dresselhaus, M. S. Dresselhaus and R. Saito: *Phys. Rev. B* **62** (2000) 16092.