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The electronic structure of a deformed chiral carbon nanotorus

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Abstract

The electronic structure as a function of the chirality and deformations for various carbon nanotori is theoretically investigated by the tight-binding method. It has been found that for the various metallic tori the deformation-dependent energy gap displays almost the same changing features versus the deformations, whereas for the various semiconducting tori the deformation-dependent energy gap does not show the distinctive regularity associated with the deformed parameters and geometric parameters, but if the deformed parameters have some particular values the energy gap would be narrowed and even approach zero, causing the semiconducting torus to be quasi-metallic. Under the circumstances of $\tan\alpha = 0$ and $\varepsilon_L = \varepsilon_J$, the electronic structure seems to be very insensitive to the existence of deformations.

1. Introduction

The carbon nanotorus, an important member of the families of carbon clusters, was theoretically suggested by Dunlap [1], followed by Itoh *et al* [2]. Its structure is considered as consisting of small sliced parts of nanotubes connected through pairs of pentagons and heptagons. Another structure of carbon nanotorus is formed through bending a carbon nanotube and connecting the two ends without introducing the pairs of pentagons and heptagons. Such a nanotube, of course, has to be of sufficiently long length. Up to now, a number of papers have been published devoted to synthesis study [3–6], experimental measurement [7–9] and theoretical

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calculation [10–19] of rings (or tori); their various properties such as negative magnetoresistance and weak electron–electron interaction in the low temperature regime [8], the unique atomic structure [11, 15–17], electronic structure and its magnetic field response [10–14, 18], deformed and defective effects of electronic structure [16–18], etc, have been investigated and revealed.

Most single-wall carbon nanotubes are experimentally found to be chiral in their atomic arrangement [19]; so are carbon nanotori as they are formed through bending carbon nanotubes. The realistic carbon tubes and nanotori are easily bent by the tip of an SPM, or crossing-over electrodes in experimental measurements, or as a result of growth, deposition, and processing; their geometric structure yields deformation, leading to modification of their electronic structure. Although the effect of axial and torsional strains on the electronic structure of chiral carbon nanotubes has been investigated by several authors [20–22], research on the electronic structure of the carbon torus are still limited only to simple achiral cases (armchair–zigzag and zigzag–armchair tori) with the deformations and defects taken into account or not [13, 16–18]. Therefore, the effects of chirality and deformations on the electronic structure for various chiral carbon nanotori remain unexplored.

In order to obtain a unified and profound understanding of the electronics of the carbon nanotorus, in this paper we try to investigate the electronic structure in the coherent regime with the emphasis on the effects of chirality and structural deformations, which are of uniform and elastic deformations. The calculations show that for the various metallic tori the deformation-dependent energy gap displays almost the same changing features versus the deformations, whereas for the various semiconducting tori the deformation-dependent energy gap does not show the distinctive regularity associated with the deformed parameters and geometric parameters, but if the deformed parameters have some particular values the energy gap would be narrowed and even approach zero, causing the semiconducting torus to be quasi-metallic. Under the circumstances of $\tan\alpha = 0$ and $\varepsilon_L = \varepsilon_J$, the electronic structure seems very insensitive to the existence of deformations.

2. The unified expression of electron energy states

The tight-binding model with one π electron per atom is adopted in our present work to study the electronic structure of the deformed chiral carbon nanotorus. The applied tight-binding Hamiltonian can be unified and written as [23–26]

$$H = \sum_l \varepsilon_l C_l^\dagger C_l - \sum_{l,\rho} \gamma_{l,l+\rho} \exp\left(\mathrm{i}\frac{e}{\hbar}\int_{\boldsymbol{R}_l}^{\boldsymbol{R}_{l+\rho}} \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{l}\right) C_l^\dagger C_{l+\rho}, \tag{1}$$

where $C_l^\dagger$ ($C_{l+\rho}$) is the creation operator (annihilator) of the electron. ρ is restricted to nearest-neighbour atoms and $\boldsymbol{A}$ is a vector potential of the magnetic field $\boldsymbol{B}$. In equation (1), the phase shift induced by an applied magnetic field is described by London theory [27]. Make the operator transformations expressed as follows:

$$C_l^\dagger = \frac{1}{\sqrt{N}}\sum_k \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_l} C_k^\dagger, \qquad C_{l+\rho} = \frac{1}{\sqrt{N}}\sum_k \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_l+\boldsymbol{R}_\rho)} C_k, \tag{2}$$

where N is the number of the primitive cell. All the transfer integrals $\gamma_{l,l+\rho}$ depend solely on the bond length of the graphite sheet [28, 29]. If the atomic position $\boldsymbol{R}_l$ (i.e. atom A in figure 1) is given, then we take $\boldsymbol{R}_{l+\rho} - \boldsymbol{R}_l = \boldsymbol{R}_\rho$ and $\gamma_{l,l+\rho} = \gamma_\rho$ for short; ρ corresponds to *three* nearest-neighbour atoms B shown in figure 1. For simplicity, the on-site energies ε_l is set to zero. When a uniform magnetic field $\boldsymbol{B}$ threads through the torus plane, the vector

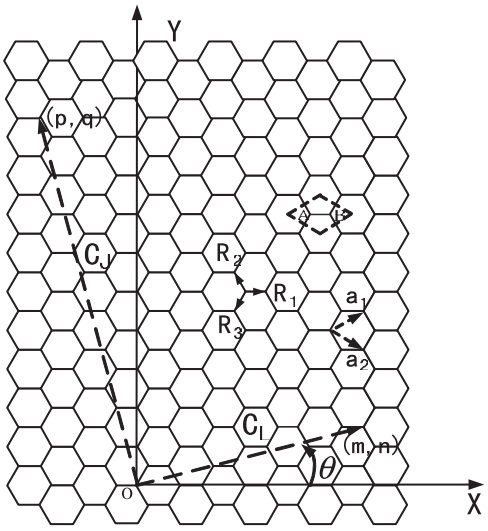

Figure 1. The unrolled honeycomb lattice of a graphite sheet. The transverse vector $\boldsymbol{C}_L = m\boldsymbol{a}_1 + n\boldsymbol{a}_2$ and the longitudinal vector $\boldsymbol{C}_J = p\boldsymbol{a}_1 + q\boldsymbol{a}_2$, respectively, correspond to tube and torus circumferences; $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the unit vectors of a graphite sheet. $\boldsymbol{R}_1$, $\boldsymbol{R}_2$ and $\boldsymbol{R}_3$ denote the vectors of bond length. θ is the chiral angle. The unit cell of the graphite sheet contains two inequivalent carbon atoms, A and B.

potential is chosen as $\boldsymbol{A} = \boldsymbol{B} \times \boldsymbol{r}/2$. If $\boldsymbol{r}$ is chosen as the vector $\boldsymbol{R}$ representing the centre to the surface of the torus, then $\boldsymbol{A}$ is unrelated to $\boldsymbol{l}$. Thus equation (1) can be rewritten as

$$H = -\sum_{k,\rho} \gamma_\rho \exp[\mathrm{i}(\boldsymbol{k} + 2\pi\boldsymbol{A}/\Phi_0) \cdot \boldsymbol{R}_\rho] C_k^\dagger C_k = \sum_k \varepsilon(\boldsymbol{k}) \hat{n}_k, \tag{3}$$

where $\Phi_0 = h/e$ is the flux quantum. The secular equation for the tight-binding model is [30, 31]

$$\det[H - ES] = 0, \tag{4}$$

with $H_{\mathrm{AA}} = 0$ ($H_{\mathrm{BB}} = 0$) and $H_{\mathrm{AB}} = \varepsilon(\boldsymbol{k})$ ($H_{\mathrm{BA}} = \varepsilon^*(\boldsymbol{k})$), taking $S_{\mathrm{AA}} = 1$ ($S_{\mathrm{BB}} = 1$) and $S_{\mathrm{AB}} = 0$ ($S_{\mathrm{BA}} = 0$) for simplicity [30, 31]. We have

$$\begin{vmatrix} -E(\boldsymbol{k}) & \varepsilon(\boldsymbol{k}) \\ \varepsilon^*(\boldsymbol{k}) & -E(\boldsymbol{k}) \end{vmatrix} = 0. \tag{5}$$

Solving equation (5), the energy dispersion relation for a π electron in such a system can be obtained as

$$\begin{aligned} E(\boldsymbol{k}) &= \pm\sqrt{|\varepsilon(\boldsymbol{k})|^2} \\ &= \pm\left\{\sum_{\rho=1}^{3} \gamma_\rho^2 + 2\gamma_1\gamma_2 \cos[(\boldsymbol{k} + 2\pi\boldsymbol{A}/\Phi_0) \cdot \boldsymbol{a}_2] + 2\gamma_1\gamma_3 \cos[(\boldsymbol{k} + 2\pi\boldsymbol{A}/\Phi_0) \cdot \boldsymbol{a}_1]\right. \\ &\quad \left. + 2\gamma_2\gamma_3 \cos[(\boldsymbol{k} + 2\pi\boldsymbol{A}/\Phi_0) \cdot (\boldsymbol{a}_1 - \boldsymbol{a}_2)]\right\}^{\frac{1}{2}}, \end{aligned} \tag{6}$$

where $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the unit vectors of a graphite sheet (see figure 1). It is necessary to point out that in equation (6) the periodical boundary conditions for a carbon nanotorus have not been considered yet.

A single carbon nanotorus may be described as a long rolled-up graphite sheet bent around in the form of a torus (see figure 1). The transverse vector $\boldsymbol{C}_L = m\boldsymbol{a}_1 + n\boldsymbol{a}_2$ and the longitudinal vector $\boldsymbol{C}_J = p\boldsymbol{a}_1 + q\boldsymbol{a}_2$, respectively, correspond to tube and torus circumferences; m, n, p and q are integral numbers and satisfy $(2m+n)p + (m+2n)q = 0$ and $|\boldsymbol{C}_J| \gg |\boldsymbol{C}_L|$. Therefore, a carbon nanotorus is uniquely defined as (m, n, p, q). In the case of a deformed graphite sheet, we use ε_L and ε_J to denote the strains due to tension or compression along the directions of $\hat{\boldsymbol{C}}_L$ and $\hat{\boldsymbol{C}}_J$, respectively. Here $\hat{\boldsymbol{C}}_L$ and $\hat{\boldsymbol{C}}_J$ are the unit vectors of $\boldsymbol{C}_L$ and $\boldsymbol{C}_J$, which are related to the fixed coordinate system (X, Y) with $\hat{\boldsymbol{C}}_L = \cos\theta\hat{\boldsymbol{i}} + \sin\theta\hat{\boldsymbol{j}}$ and $\hat{\boldsymbol{C}}_J = -\sin\theta\hat{\boldsymbol{i}} + \cos\theta\hat{\boldsymbol{j}}$. The torsion deformation is assumed to appear only around the straight tubular axis ($\|\boldsymbol{C}_J$) before bending carbon nanotubes to form a torus and α represents the shear strain. Within the context of continuum mechanics, the simultaneous occurrence of the deformations causes the change of the arbitrary lattice vector, $\boldsymbol{R}_l = R_{lL}\hat{\boldsymbol{C}}_L + R_{lJ}\hat{\boldsymbol{C}}_J$, corresponding to the position of carbon atoms of a graphite sheet and becoming

$$R_{lJ} \to (1+\varepsilon_J)R_{lJ}, \tag{7a}$$

$$R_{lL} \to (1+\varepsilon_L)R_{lL} + R_{lJ}\tan\alpha. \tag{7b}$$

For the deformed graphite sheet, the unit vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ can be written in the coordinate system (X, Y) of figure 1 as

$$\begin{aligned}\boldsymbol{a}_2(\varepsilon_L, \varepsilon_J, \tan\alpha) &= A(\varepsilon_L, \varepsilon_J, \tan\alpha)\hat{\boldsymbol{i}} + B(\varepsilon_L, \varepsilon_J, \tan\alpha)\hat{\boldsymbol{j}} \\ &= a[\cos(30+\theta)\cos\theta(1+\varepsilon_L) - \sin(30+\theta)\cos\theta(1+\varepsilon_J)\tan\alpha \\ &\quad + \sin(30+\theta)(1+\varepsilon_J)\sin\theta]\hat{\boldsymbol{i}} \\ &\quad + a[-\sin(30+\theta)(1+\varepsilon_J)\cos\theta + \cos(30+\theta)\sin\theta(1+\varepsilon_L) \\ &\quad - \sin(30+\theta)\sin\theta(1+\varepsilon_J)\tan\alpha]\hat{\boldsymbol{j}},\end{aligned} \tag{8a}$$

$$\begin{aligned}\boldsymbol{a}_1(\varepsilon_L, \varepsilon_J, \tan\alpha) &= C(\varepsilon_L, \varepsilon_J, \tan\alpha)\hat{\boldsymbol{i}} + D(\varepsilon_L, \varepsilon_J, \tan\alpha)\hat{\boldsymbol{j}} \\ &= a[\cos(30-\theta)\cos\theta(1+\varepsilon_L) + \sin(30-\theta)\cos\theta(1+\varepsilon_J)\tan\alpha \\ &\quad - \sin(30-\theta)(1+\varepsilon_J)\sin\theta]\hat{\boldsymbol{i}} \\ &\quad + a[\sin(30-\theta)(1+\varepsilon_J)\cos\theta + \cos(30-\theta)\sin\theta(1+\varepsilon_L) \\ &\quad + \sin(30-\theta)\sin\theta(1+\varepsilon_J)\tan\alpha]\hat{\boldsymbol{j}},\end{aligned} \tag{8b}$$

where A and C (B and D) are, respectively, the X-axis (Y-axis) components of $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ in a fixed coordinate system (X, Y) after deformations occur. All of them are complicated functions of ε_L, ε_J and $\tan\alpha$.

When a finite graphite sheet, whether deformation occurs or not, is rolled up to form a carbon nanotorus, the periodical boundary conditions of both the transverse and the longitudinal directions must be considered. At low temperature, if the electronic phase coherence in this structure is preserved on a length scale comparable to or larger than the torus dimension, then this nanotorus remains fully described by the eigenfunction of its Hamiltonian. Assuming a homogenous magnetic field $\boldsymbol{B}$ is applied to thread through the torus plane, that is, the potential vector $\boldsymbol{A}$ is chosen to run parallel with the longitudinal direction ($\|\boldsymbol{C}_J$), and using the periodical boundary conditions, $\Psi(\boldsymbol{r}) = \Psi(\boldsymbol{r}+\boldsymbol{C}_i)$ ($i = L, J$), where $\Psi(\boldsymbol{r})$ is the electron's Bloch function, we get

$$k_x + 2\pi\frac{A_x}{\Phi_0} = \frac{2\pi}{pn-qm}\left[\frac{pD+qB}{AD-CB}L - \frac{mD+nB}{AD-CB}(J + \Phi/\Phi_0)\right], \tag{9a}$$

$$k_y + 2\pi\frac{A_y}{\Phi_0} = \frac{2\pi}{pn-qm}\left[\frac{mC+nA}{AD-CB}(J + \Phi/\Phi_0) - \frac{pC+qA}{AD-CB}L\right], \tag{9b}$$

where L and J are integrals serving as the electronic state index and Φ is the magnetic flux enclosed in the torus. Obviously, the wavevectors with the discrete allowed values are

complicated functions of the geometric parameters (m, n, p, q) and the deformed parameters $(\varepsilon_L, \varepsilon_J, \tan\alpha)$ contained in A, B, C and D, which are defined in equations (8*a*) and (8*b*). Equations (9*a*) and (9*b*) are in combination with equations (8*a*) and (8*b*) and hence we obtain

$$(\boldsymbol{k} + 2\pi \boldsymbol{A}/\Phi_0) \cdot \boldsymbol{a}_2 = \frac{2\pi}{pn - qm}(pL - m(J + \Phi/\Phi_0)), \tag{10a}$$

$$(\boldsymbol{k} + 2\pi \boldsymbol{A}/\Phi_0) \cdot \boldsymbol{a}_1 = \frac{2\pi}{pn - qm}(-qL + n(J + \Phi/\Phi_0)). \tag{10b}$$

Substituting equations (10*a*) and (10*b*) into equation (6) and taking the spin-B interaction energy (the Zeeman splitting) $E(\sigma)$ into account, then the unified expression of π-electron energy states for the carbon nanotorus as a function of chirality and deformation with magnetic flux threading through the torus plane is given by

$$\begin{aligned} E^{(L,J)}(\Phi, \varepsilon_L, \varepsilon_J, \tan\alpha, \sigma) &= E^{(L,J)}(\Phi, \varepsilon_L, \varepsilon_J, \tan\alpha) + E(\sigma) \\ &= \pm\left\{\sum_{\rho=1}^{3}\gamma_\rho^2 + 2\gamma_1\gamma_2\cos\left[\frac{2\pi}{pn - qm}(pL - m(J + \Phi/\Phi_0))\right]\right. \\ &\quad + 2\gamma_1\gamma_3\cos\left[\frac{2\pi}{pn - qm}(-qL + n(J + \Phi/\Phi_0))\right] \\ &\quad \left. + 2\gamma_2\gamma_3\cos\left[\frac{2\pi}{pn - qm}(-(p + q)L + (m + n)(J + \Phi/\Phi_0))\right]\right\}^{1/2} \\ &\quad + \hbar^2 g\sigma/m^* R^2(\Phi/\Phi_0), \end{aligned} \tag{11}$$

where the + (−) sign in front of the square root denotes the antibonding states (the bonding states); the g factor is taken to be the same as that ($\approx$2) of the pure graphite; $\sigma = \pm 1/2$ is the electron spin and m^* is the bare electron mass [32]. It is very interesting to note that the electronic energy states of such a complicated deformed nanotorus system can be described through a surprisingly simple expression and it is affected only by deformation through the transfer integrals γ_j, not through $(\boldsymbol{k} + 2\pi \boldsymbol{A}/\Phi_0) \cdot \boldsymbol{a}_i$ $(i = 1, 2)$ contained in equation (6), although both $(\boldsymbol{k} + 2\pi \boldsymbol{A}/\Phi_0)$ and $\boldsymbol{a}_i$ are complicated functions of the deformed parameters $(\varepsilon_L, \varepsilon_J, \tan\alpha)$ as stated above. This is an unexpected result. Furthermore, seeing $E^{(L,J)}(\Phi/\Phi_0, \varepsilon_L, \varepsilon_J, \tan\alpha) = E^{(L,J-1)}(\Phi/\Phi_0 + 1, \varepsilon_L, \varepsilon_J, \tan\alpha)$, this means that $E^{(L,J)}(\Phi/\Phi_0, \varepsilon_L, \varepsilon_J, \tan\alpha)$ is a periodical function of the magnetic flux Φ with a period Φ_0 as a result of the AB effect.

From the result of $(\boldsymbol{k}+2\pi \boldsymbol{A}/\Phi_0)\cdot\boldsymbol{a}_i$ $(i = 1, 2)$ being independent of the strain parameters in carbon nanotorus, one may conclude that the electronic phase factor $(\boldsymbol{k} + 2\pi \boldsymbol{A}/\Phi_0) \cdot \boldsymbol{R}_\rho$ in equation (3) remains unchanged under the deformation and it means the geometric deformation does not change the electronic phase coherence. For a deformed structure, the transfer integrals γ_ρ have been suggested to have the simple relation with the bond length as $\gamma_\rho = \gamma_0(R_0/R_\rho)^2$ [28, 29], where γ_0 (=2.66 eV) and R_0 (=0.142 nm) are the transfer integral and bond length of an undeformed structure, respectively, and R_ρ is the bond length after deformations occur and is calculated by $R_\rho = \sqrt{R_{\rho L}^2 + R_{\rho J}^2}$ for the graphite sheet, where the formula of $R_{\rho L}$ and $R_{\rho J}$ can be derived from the deformed configuration as

$$R_{1L} = \lambda[\sqrt{3}(m + n)(1 + \varepsilon_L) + (n - m)\tan\alpha], \qquad R_{1J} = \lambda(n - m)(1 + \varepsilon_J), \tag{12a}$$

$$R_{2L} = \lambda[-\sqrt{3}n(1 + \varepsilon_L) + (2m + n)\tan\alpha], \qquad R_{2J} = \lambda(2m + n)(1 + \varepsilon_J), \tag{12b}$$

$$R_{3L} = \lambda[-\sqrt{3}m(1 + \varepsilon_L) + (m + 2n)\tan\alpha], \qquad R_{3J} = \lambda(m + 2n)(1 + \varepsilon_J), \tag{12c}$$

where $\lambda = a/6\sqrt{3(m^2 + n^2 + nm)}$ with the lattice constant $a = 0.248$ nm of a graphite sheet.

In equation (11), $L = 1, 2, \ldots, N_m$, and $J = 1, 2, \ldots, N_p$, where N_m (N_p) is obtained as a function of m and n (p and q) as

$$N_m = \begin{cases} \dfrac{2(m^2+n^2+mn)}{d_1} & (m-n \neq 3d_1 i) \\ \dfrac{2(m^2+n^2+nm)}{3d_1} & (m-n = 3d_1 i), \end{cases} \tag{13a}$$

$$N_p = \begin{cases} \dfrac{2(p^2+q^2+pq)}{d_2} & (p-q \neq 3d_2 i) \\ \dfrac{2(p^2+q^2+pq)}{3d_2} & (p-q = 3d_2 i), \end{cases} \tag{13b}$$

where i is an integral, and d_2 (d_1) is the greatest common divisor of p and q (m and n).

The tori can be classified as metal (type I), semiconductor (type I) or insulator (type III) depending entirely on the gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) in the proximity of the Fermi level. In the case without deformations and magnetic field, using equation (9) we deduce a simple rule, i.e., the geometric parameters of the chiral metallic carbon nanotori satisfy $m - n = 3i$ and $p - q = 3i$ (i is an integral), the chiral semiconductor tori satisfy $m - n = 3i$ and $p - q \neq 3i$ and the chiral insulator tori satisfy $m - n \neq 3i$ and $p - q = 3i$. We may also verify that the tori with $m - n \neq 3i$ and $p - q \neq 3i$ do not exist.

Here, we would like to emphasize that the assumed carbon nanotube bent to construct a torus is of sufficiently long length and large size that the effects of both inhomogeneous strain along the circumference of the torus and rehybridization of the π–σ orbital are neglected.

From equation (11) and in the case of neglecting the spin-B interaction, it is very easy to obtain the results in the previous works by us and other researchers for the particular simple situation [13, 14, 33].

(1) Setting $\tan\alpha = 0$ and assuming the deformation is originated only from curvature and bending of a graphite sheet for the formation of a carbon nanotorus inducing the transfer integrals γ_ρ to deviate γ_0 [14], we can obtain $\gamma_1 = \gamma_3$ for an $(m, 0, -p, 2p)$ zigzag–armchair (ZA) torus and $\gamma_2 = \gamma_3$ for an $(m, m, -p, p)$ armchair–zigzag (AZ) torus from equations (12a), (12b) and (12c). Substituting these data into equation (11), we obtain

$$E^{(L,J)}(\Phi, \varepsilon_L, \varepsilon_J)_{\mathrm{ZA}} = \pm\left\{\gamma_1^2 + 4\gamma_1\gamma_2 \cos\left[\frac{\pi J}{m}\right]\cos\left[\frac{\pi}{p}(L + \Phi/\Phi_0)\right] + 4\gamma_2^2\cos^2\left[\frac{\pi J}{m}\right]\right\}^{\frac{1}{2}}, \tag{14a}$$

$$E^{(L,J)}(\Phi, \varepsilon_L, \varepsilon_J)_{\mathrm{AZ}} = \pm\left\{\gamma_1^2 + 4\gamma_1\gamma_2 \cos\left[\frac{\pi J}{m}\right]\cos\left[\frac{\pi}{p}(L + \Phi/\Phi_0)\right] + 4\gamma_2^2\cos^2\left[\frac{\pi}{p}(L + \Phi/\Phi_0)\right]\right\}^{\frac{1}{2}}, \tag{14b}$$

which are identical with equations (2b) and (2c) in [14].

(2) In the absence of the geometric deformation, namely, when $\varepsilon_L = \varepsilon_J = \tan\alpha = 0$, one can obtain $\gamma_\rho = \gamma_0$ from equations (12a), (12b) and (12c), then the generic expression of π-electron energy states for the carbon nanotorus as a function of the chirality and magnetic flux threading through the torus plane, but without deformations occurring, is deduced from equation (11) as follows:

$$E^{(L,J)}(\Phi) = \pm\gamma_0\left\{1 + 4\cos\left(\frac{\pi}{pn - qm}\left[(n-m)\left(J + \frac{\Phi}{\Phi_0}\right) - L(q-p)\right]\right)\right.$$

$$\times \cos\left(\frac{\pi}{pn-qm}\left[(p+q)L-(n+m)\left(J+\frac{\Phi}{\Phi_0}\right)\right]\right)$$
$$+4\cos^2\left(\frac{\pi}{pn-qm}\left[(p+q)L-(n+m)\left(J+\frac{\Phi}{\Phi_0}\right)\right]\right)\Bigg\}^{1/2}, \tag{15}$$

which is in agreement with our previous work [33]. The electron energy states in the undeformed case of an $(m, m, -p, p)$ AZ torus and an $(m, 0, -p, 2p)$ ZA torus can be deduced directly from equation (15) as

$$E^{(L,J)}(\Phi)_{\mathrm{ZA}} = \pm\gamma_0\left\{1+4\cos\left[\frac{\pi J}{m}\right]\cos\left[\frac{\pi}{p}\left(L+\frac{\Phi}{\Phi_0}\right)\right]+4\cos^2\left[\frac{\pi J}{m}\right]\right\}^{\frac{1}{2}}, \tag{16a}$$

$$E^{(L,J)}(\Phi)_{\mathrm{AZ}} = \pm\gamma_0\left\{1+4\cos\left[\frac{\pi J}{m}\right]\cos\left[\frac{\pi}{p}\left(L+\frac{\Phi}{\Phi_0}\right)\right]+4\cos^2\left[\frac{\pi}{p}\left(L+\frac{\Phi}{\Phi_0}\right)\right]\right\}^{\frac{1}{2}}, \tag{16b}$$

which are identical with equations (1*a*) and (1*b*) in [13].

3. The deformed and magnetic effects on the energy gap

Numerous calculations using equation (11) in the absence of the magnetic flux have been performed to explore the correlations between the deformation-dependent energy gap E_{g} and related parameters, such as deformed parameters (ε_L, ε_J, $\tan\alpha$), torus radius R, tube radius (torus width) r and chiral angle θ.

For the metallic carbon nanotorus, selecting the tori with the parameters (3, 3, −450, 450) ($r = 2.0$ Å, $R = 177.4$ Å, $\theta = 0°$), (6, 3, −400, 500) ($r = 3.12$ Å, $R = 180.6$ Å, $\theta = 10.9°$), (4, 1, −360, 540) ($r = 1.8$ Å, $R = 187$ Å, $\theta = 19.1°$), (9, 0, −260, 520) ($r = 3.55$ Å, $R = 177.5$ Å, $\theta = 30°$), (8, 2, −360, 540) ($r = 3.6$ Å, $R = 187.7$ Å, $\theta = 19.1°$) and (6, 3, −120, 360) ($r = 3.12$ Å, $R = 125.2$ Å, $\theta = 10.9°$) as examples, the changing properties of the deformation-dependent energy gap E_{g} can be concluded as follows.

(1) The energy gaps E_{g} for the various metallic nanotori have similar changing curves versus the deformed parameters (ε_L, ε_J, $\tan\alpha$) and depend strongly on the values of ε_L, ε_J and $\tan\alpha$. If only a kind of deformation (ε_L or ε_J or $\tan\alpha$) exists, then the energy gap changes more quickly and shows linear evolution with this kind of deformation increasing (see figures 2(a)–(c)).

(2) When $\tan\alpha = 0$ (without torsion deformation) and $\varepsilon_L = \varepsilon_J$, the metallic nanotorus retains metallic characteristics ($E_{\mathrm{g}} = 0$) in spite of tension deformation existing; this is because the tension deformation in this case does not change the hexagonal symmetry of the honeycomb lattice although the bond length varies from deformation. As long as we set $\tan\alpha \neq 0$, always $E_{\mathrm{g}} \neq 0$, its minimal value appears at the position of $\varepsilon_L = \varepsilon_J$ (see figure 2(b)). Even if ε_L and ε_J are larger values (i.e. $\varepsilon_L = 0.01$ and $\varepsilon_J = 0.011$ in figure 2(c)), but the difference between both is smaller, then the evolution of energy gap versus $\tan\alpha$ in this case is nearly the same as in the case of $\varepsilon_L = \varepsilon_J = 0$; this means the smaller the difference between ε_L and ε_J is, the smaller the energy gap is.

(3) The energy gap E_{g} depends weakly on the chiral angle θ. E_{g} increases slightly with the chiral angle θ, which means that the deformation has less effect on the metallic armchair-zigzag torus ($\theta = 0$). In addition, we find that E_{g} is independent of torus radius R and torus width r.

For the semiconducting carbon nanotorus, selecting the tori with the parameters (5, 2, −375, 500) ($r = 2.5$ Å, $R = 177.7$ Å, $\theta = 13.9°$), (4, 1, −340, 510) ($r = 1.8$ Å, $R = 177.7$ Å, $\theta = 19.1°$), (3, 3, −451, 451) ($r = 2.0$ Å, $R = 177.8$ Å, $\theta = 0°$), (4, 1, −400, 600) ($r = 1.8$ Å, $R = 208.6$ Å, $\theta = 19.1°$), and (8, 2, −400, 600) ($r = 3.6$ Å,

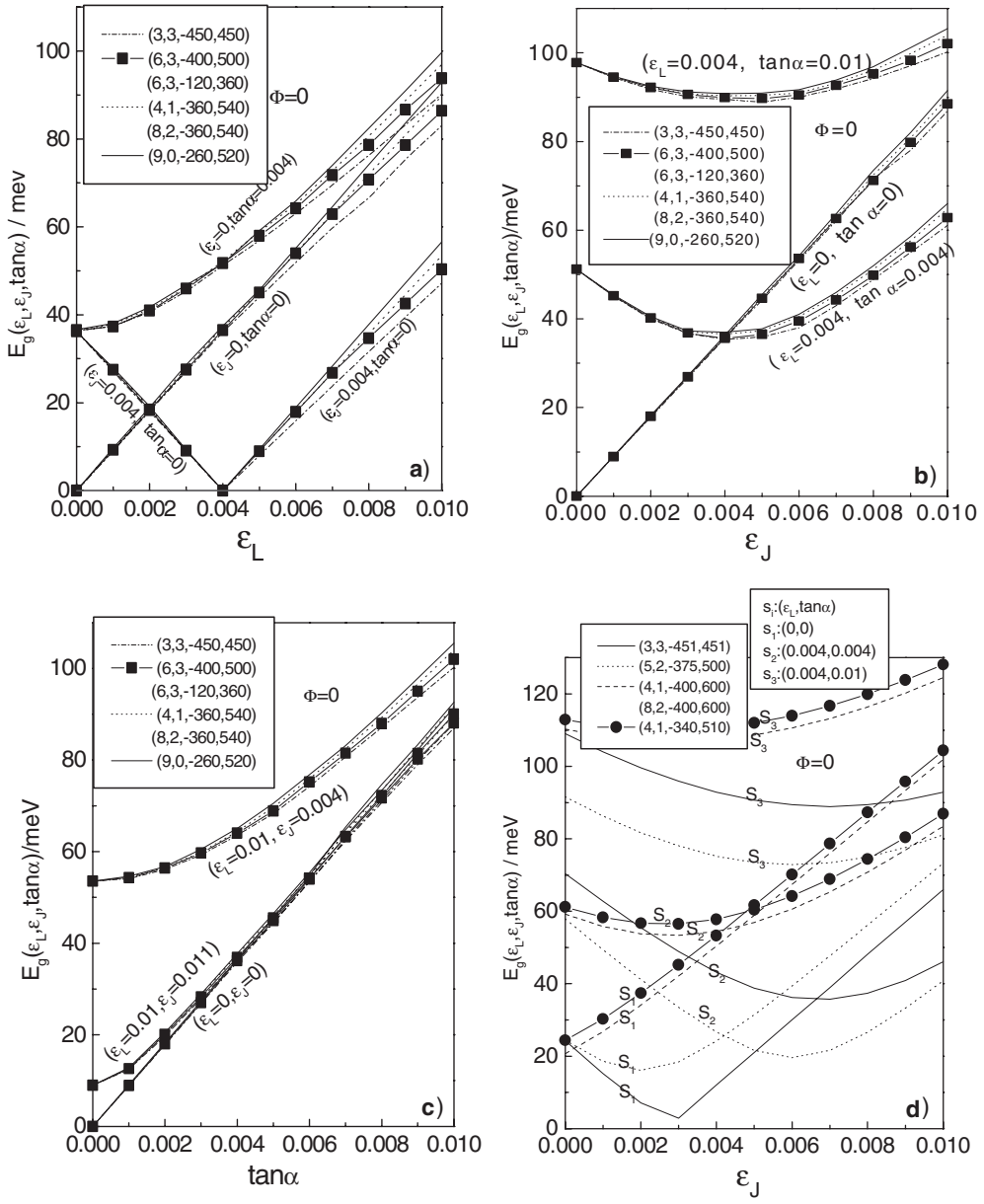

Figure 2. ((a)–(c)) The energy gaps E_g for various metallic (type I) tori; they strongly depend on deformations and weakly depend on their chirality, but have similar changing curves versus the deformed parameters (ε_L, ε_J, tan α), where ε_L and ε_J are the strains due to tension or compression along the directions of tube and torus circumferences, and α represents the shear strain. When tan $\alpha = 0$ and $\varepsilon_L = \varepsilon_J$, the metallic nanotorus retains its metallic characteristic. The smaller the difference between ε_L and ε_J is, the smaller the energy gap is. (d) The energy gaps E_g for various semiconducting (type II) tori; they strongly depend on deformations and chirality, but without the distinctive regularity. The smallest energy gap E_g may occur as the particular values of ε_L and ε_J are taken, and even approaches zero to cause the semiconducting torus to be quasi-metallic.

$R = 208.6$ Å, $\theta = 19.1°$) as examples, the changing properties of the deformation-dependent energy gap E_g, shown in figure 2(d), can be concluded as follows.

(1) The energy gap E_g shows a strong dependence on the magnitude of ε_L, ε_J and $\tan\alpha$, and increases or decreases without remarkable features as the deformation increases. In general, the greater the torsion is, the larger the energy gap is.

(2) Setting $\tan\alpha = 0$ and $\varepsilon_L = \varepsilon_J$, then E_g approaches a value smaller than that in the undeformed case, but the smallest energy gap E_g may occur as other particular values of ε_L and ε_J are taken, and even approaches zero, causing the semiconducting torus to be quasi-metallic. The simple linear relation for E_g with a kind of deformation parameter (ε_L or ε_J or $\tan\alpha$), which exists for the various deformed metallic tori, has not been found.

(3) The energy gap E_g is independent of torus width r and depends on the chiral angle θ and torus radius R, but without the distinctive regularity.

In the presence of flux, the energy gap of a torus varying with the deformations and flux is very complicated, but taking $\tan\alpha = 0$, $\varepsilon_L = \varepsilon_J = \varepsilon$ and $|C_J| \gg |C_L|$ and neglecting the spin-B interaction we can deduce the simple analytic expressions for the energy gap from equation (11). For the chiral metallic (type I) carbon nanotorus, the energy gap is given as

$$E_g(\Phi, \varepsilon, \tan\alpha = 0) = \begin{cases} \dfrac{2\sqrt{3}\pi(n+m)\gamma(\varepsilon)}{|pn-qm|}\dfrac{\Phi}{\Phi_0} & \left(0 \leqslant \Phi \leqslant \dfrac{\Phi_0}{2}\right) \\ \dfrac{2\sqrt{3}\pi(n+m)\gamma(\varepsilon)}{|pn-qm|}\left|1-\dfrac{\Phi}{\Phi_0}\right| & \left(\dfrac{\Phi_0}{2} \leqslant \Phi \leqslant \Phi_0\right). \end{cases} \tag{17a}$$

For the chiral semiconducting (type II) carbon nanotorus, the energy gap is given as

$$E_g(\Phi, \varepsilon, \tan\alpha = 0) = \begin{cases} \dfrac{2\sqrt{3}\pi(n+m)\gamma(\varepsilon)}{|pn-qm|}\left|\dfrac{1}{3}-\dfrac{\Phi}{\Phi_0}\right| & \left(0 \leqslant \Phi \leqslant \dfrac{\Phi_0}{2}\right) \\ \dfrac{2\sqrt{3}\pi(n+m)\gamma(\varepsilon)}{|pn-qm|}\left|\dfrac{2}{3}-\dfrac{\Phi}{\Phi_0}\right| & \left(\dfrac{\Phi_0}{2} \leqslant \Phi \leqslant \Phi_0\right) \end{cases} \tag{17b}$$

where m, n, p and q in energy gap expressions show the energy gap dependent on the chirality, radius R and width r of torus, but independent of torus width r just for the armchair–zigzag (AZ) and the zigzag–armchair (ZA) torus. Obviously, the energy gap is a linearly periodical function of the flux Φ threading through the torus plane, with a period Φ_0, and it is symmetric about $\Phi_0/2$. When the flux Φ varies, the type I and II tori exhibit properties of the continuous transitions from a metallic phase to a semiconducting phase or vice versa. The type I (II) tori are metallic at $\Phi_c = \mathrm{i}\Phi_0$ ($\Phi_c = (\mathrm{i} \pm 1/3)\Phi_0$). Furthermore, we may confirm that type III tori are very insensitive to the magnetic field and do not have a simple energy gap expression similar to equations (17*a*) and (17*b*) for type I and II tori, and the larger gap remains almost unchanged while the flux Φ varies.

4. Conclusion

Based on the tight-binding model, a concisely unified expression of π-electron energy states for the carbon nanotorus as a function of chirality and deformation with magnetic field vertical to the torus plane is obtained; the result shows that electron energy states are affected by deformation solely through the transfer integrals γ_ρ, not by the electronic phase factor. For the various deformed metallic tori their deformation-dependent energy gap E_g displays almost the same changing features with the deformed parameters (ε_L, ε_J, $\tan\alpha$) varying and strongly depends on the values of ε_L, ε_J and $\tan\alpha$, weakly depends on their chirality and is independent of torus radius R and torus width r, whereas for the various semiconducting tori their deformation-dependent energy gap does not show the distinctive regularity associated with the deformed parameters and geometric parameters, but if the deformed parameters have

some particular values the energy gap would be narrowed and even approach zero, causing the semiconducting torus to be quasi-metallic. Under the circumstances of $\tan\alpha = 0$ and $\varepsilon_L = \varepsilon_J$, the electronic structure seems to be very insensitive to the existence of deformations. The flux-dependent energy gap for the deformed chiral metallic torus or semiconducting torus in the case of $\tan\alpha = 0$, $\varepsilon_L = \varepsilon_J = \varepsilon$ and $|C_J| \gg |C_L|$ can be derived as an analytic expression.

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References

[1] Dunlap B I 1992 *Phys. Rev.* B **46** 1933
[2] Itoh S *et al* 1993 *Phys. Rev.* B **47** 1703
Itoh S *et al* 1993 *Phys. Rev.* B **47** 12908
[3] Sano M *et al* 2001 *Science* **293** 1299
[4] Liu J *et al* 1997 *Nature* **385** 780
[5] Martel R, Shea H R and Avouris P 1999 *Nature* **398** 299
Martel R, Shea H R and Avouris P 1999 *J. Phys. Chem.* B **103** 7551
[6] Ahlskog M *et al* 1999 *Chem. Phys. Lett.* **300** 202
[7] Terrones M *et al* 1996 *Phil. Trans. R. Soc.* A **354** 2025
[8] Shea H R, Martel R and Avouris P 2000 *Phys. Rev. Lett.* **84** 4441
[9] Watanabe H *et al* 2001 *Appl. Phys. Lett.* **78** 2928
[10] Haddon R C 1997 *Nature* **388** 31
[11] Kuzubov A A *et al* 2001 *Phys. Solid. State* **43** 1982
[12] Meunier V, Lambin Ph and Lucas A A 1998 *Phys. Rev.* B **57** 14886
[13] Lin M F and Chun D S 1998 *Phys. Rev.* B **57** 6731
[14] Lin M F 1998 *J. Phys. Soc. Japan* **67** 1094
[15] Oh D-H, Park J M and Kim K S 2000 *Phys. Rev.* B **62** 1600
[16] Liu L, Jayanthi C S and Wu S Y 2001 *Phys. Rev.* B **64** 033412
[17] Hod O, Rabani E and Baer R 2003 *Phys. Rev.* B **67** 195408
[18] Latge A, Rocha C G and Wanderley L A L 2003 *Phys. Rev.* B **67** 155413
[19] Iijima S and Ichihashi T 1993 *Nature* **363** 603
[20] Heyd R, Charlier A and McRae E 1997 *Phys. Rev.* B **55** 6820
[21] Yang L, Anantram M P, Han J and Lu J P 1999 *Phys. Rev.* B **60** 13874
[22] Yang L and Han J 2000 *Phys. Rev. Lett.* **85** 154
[23] Li Z Z 2002 *Solid State Theory* (Peking: Higher Education Press)
[24] Latil S *et al* 2003 *Phys. Rev.* B **67** 165420
[25] Roche S *et al* 1999 *Phys. Rev.* B **59** 5342
[26] Luttinger J M 1951 *Phys. Rev.* **84** 814
[27] Ceulemans A *et al* 1998 *Phys. Rev. Lett.* **80** 1861
[28] Froyan S *et al* 1979 *Phys. Rev.* B **20** 240
[29] Harrison W A 1989 *Electronic Structure and the Properties of Solids* (New York: Dover)
[30] Saito R, Dresselhaus G and Dresselhaus M S 1998 *Physical Properties of Carbon Nantubes* (London: Imperial College Press)
[31] Zhang Z *et al* 2001 *China J. At. Mol. Phys.* **18** 31
[32] Zhang Z *et al* 2002 *Phys. Rev.* B **66** 085405
[33] Zhang Z *et al* 2001 *Acta Phys. Sin.* **50** 1150