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Magnetic response of carbon nanotori: the importance of curvature and disorder

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Abstract

Taking into account both curvature and disorder, we study the magnetic moments of carbon nanotori in the presence of magnetic field B (perpendicular to the torus plane). Due to the intrinsic curvature effect, energy gaps of about 10 meV are obtained in those primary metallic carbon nanotori, which result in a novel magnetic response, depending on its chirality. An armchair carbon nanotorus exhibits a diamagnetic response in the vicinity of zero magnetic field, while the primary metallic zigzag nanotorus presents a much weaker paramagnetic response. This result differs substantially from previous predictions. In the weak-magnetic-field regime, it is found that the low-temperature magnetic moments show up the periodic Aharonov–Bohm (AB) oscillation, with period $\Delta B \approx \phi_0/S$, $\phi_0 = h/e$ being the quantum flux, S the area enclosed by the torus, while at high temperature, the AB oscillation is destroyed because of the loss of phase coherence. A phase transition from diamagnetic to paramagnetic is observed by increasing the disorder strength.

1. Introduction

The possibilities of utilizing the Aharonov–Bohm (AB) effect in future nanotechnology has stimulated much interest in nanoscopic quantum rings [1]. Recently, there have been reports on the observation of ring-shaped carbon nanostructures (carbon nanotori) [2]. Theoretically, it can be formed by joining the two ends of conventional carbon nanotubes, similar to a mesoscopic ring. Due to its special geometry and the controllable size, a carbon nanotorus would be an ideal nanometer-scale electromagnetic element in future circuits, and considerable work [3–10] has been devoted to the physical properties of this novel carbon nanostructure since its discovery. This new type of quantum ring offers remarkable opportunities to observe and exploit new phenomena.

The magnetic moments in quantum rings as well as in carbon nanostructures have become an important issue [11], since they are thought to play an important role in the magnetic properties of these systems. As regards carbon nanotori, the persistent current and the induced magnetic moments in this ring structure have been the subject of intense research during recent years [5–7]. For example, the metallic carbon nanotori was expected to possess paramagnetic persistent current near zero flux [7], while giant paramagnetic moments were claimed to exist in metallic carbon nanotori due to the interplay between the toroidal geometry and the ballistic motion of the π electrons in the metallic nanotubes [5]. The magnetic response of a carbon nanotorus would depend on its electronic structure. However, some important factors, such as the effects of curvature and disorder, were neglected in these calculations of electronic structure and the nature of the metallicity or the presence of a gap is crucial for the determination of the magnetic response of this system. Moreover, our previous calculation demonstrates that the curvature induced energy gap may be present in a primary metallic carbon nanotorus, such as $(5, 5, p = 3 \times \text{integer})$, representing a torus formed from a finite length $(5, 5)$ carbon nanotube consisting of p (multiple of 3) unit cells [10]. From this point of view, it is worthwhile clarifying whether this intrinsic curvature has significant effect on the magnetic moments of carbon nanotori. To our knowledge, the theoretical study of the magnetic moments has performed so far only considering its variation with temperature at a given low magnetic field B for these small sized carbon nanotori [5], which are about two

orders of magnitude smaller than that observed experimentally. Additionally, the effect of disorder should also be important for the magnetic response of carbon nanotori.

Taking into account the effect of curvature, in this paper we investigate the induced magnetic moments as a function of B, temperature and disorder strength for a large sized torus under an applied magnetic field (with the field perpendicular to the torus plane). As is known for mesoscopic rings, there have been some disagreements between theory and experiment, such as the magnitude and the sign of persistent currents [12]. Here, we also expect our exploration can shed light on these open questions.

This paper is organized as follows. In section 2, we give a brief description for the tight-binding model used in this paper. The results of simulation and analysis are presented in section 3. The main results are finally summarized in the conclusions of section 4.

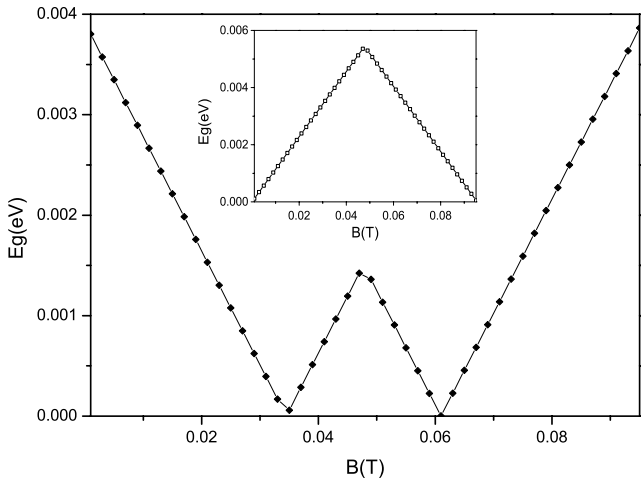

Figure 1. The dependence of the energy gap on magnetic field B for (5, 5, 3000), and the inset is the case without the curvature effect.

2. Method

A carbon nanotorus can be formed by bending around a single nanotube and connecting its two ends. In this paper, we take the index (n, m, p) to define a carbon nanotorus, formed from a finite length single wall carbon nanotube (n, m) containing p unit cells. The number of atoms in an unit cell of (n, m, p) is equal to that corresponding to (n, m). For instance, the achiral type of carbon nanotorus $(n, n, p)/(n, 0, p)$ contains $4np$ atoms, with $4n$ atoms in each unit cell.

The electronic structure is calculated based on the single-orbital nearest-neighbor tight-binding Hamiltonian. Based on the London approximation, the hopping between site i and site j is modified by a phase factor due to the presence of magnetic field,

$$H_{ij} = H_{ij}^0 \exp\left[\mathrm{i}\,(2\pi/\phi_0)\int_i^j \mathbf{A}\,(\mathbf{r})\cdot \mathrm{d}\mathbf{r}\right], \qquad (1)$$

where H_{ij}^0 is the hopping amplitude for zero field, $\phi_0 = h/e$ the flux quantum, and $\mathbf{A}(\mathbf{r})$ the vector potential [5, 13]. The effect of curvature enters the hopping amplitude via $H_{ij}^0 \longrightarrow H_{ij}^0(r_{ij}^0/r_{ij})^2$, where r_{ij}^0 and r_{ij} are bond lengths without and with deformation, respectively [14]. Since the uniform magnetic field B is perpendicular to the torus plane, the rotational symmetry is hence preserved. Assuming nearest-neighbor hopping and one orbital per site, the energy spectrum can be obtained by diagonalizing the matrix,

$$\mathrm{e}^{-\mathrm{i}\alpha} H_{1,2}^{+}\,(B) + H_{1,1}\,(B) + \mathrm{e}^{\mathrm{i}\alpha} H_{1,2}\,(B)\,, \qquad (2)$$

with $H_{1,1}$ and $H_{1,2}$ representing the Hamiltonian matrix of one unit cell and the coupling matrix between two neighboring unit cells, respectively, and $\alpha = j \times 2\pi/p$ is the phase difference between wavefunctions of two neighboring unit cells, where $j = 1, 2, \ldots, p$ [10, 15]. The magnetic moment of a nanotorus is then determined by

$$M(B, T) = -\,(\partial F(B, T)/\partial B)_T\,, \qquad (3)$$

where $F = -kT\sum_n \ln\{1 + \exp[(\mu - E_n)/kT]\} + N\mu$, is the free energy. Here E_n denotes the eigenenergy of the nanotorus in an applied field B and μ the chemical potential of the N-electron system. Without considering the effects of curvature and disorder, we have reproduced the results of [5] by using equation (3). Since the measurable magnetic moments only exist in carbon nanotori with zero or very small gap ('metallic'), in the following calculations we focus on these 'metallic' nanotori.

3. Results and discussion

First, the magnetic field dependent electronic structure of carbon nanotori is investigated. Figure 1 presents the energy gap as a function of B for a typical armchair carbon nanotorus (5, 5, 3000). The most notable thing is that due to the curvature effect, a narrow-gap E_g of about 3.8 meV appears around zero field, differing from the previous predictions of $E_g = 0$ [5–7, 9]. In [5], the authors argue that the curvature effect should not affect the metallicity of armchair carbon nanotori. However, the n-fold rotational symmetry in an (n, n) carbon nanotube is broken in the case of an (n, n, p) torus. Analogous with the armchair nanotube bundles, this n-fold rotational symmetry broken off a carbon nanotorus can lead to a pseudogap at E_F by considering the curvature effect [16, 17]. For comparison, the inset of figure 1 shows the result obtained when the curvature effect is neglected. In the weak-magnetic-field limit, the B-dependent electronic structure would exhibit the periodical AB oscillations, with a period $\Delta B \approx \phi_0/S$, where ϕ_0 is the quantum flux (h/e), S the area enclosed by the torus. The energy gap curve shown in figure 1 is symmetrical about axis $B = \Delta B/2$. Without considering the curvature effect, the energy gap increases linearly with magnetic field until E_g reaches its maximum value at $B = \Delta B/2$, while considering the curvature effect, it follows the 'W' like pattern, with two minimum points (corresponding to semiconductor–metal transition) at the two sides of $B = \Delta B/2$. Since the magnetic field is weak, the Zeeman effect is thus neglected in our calculation. In figures 2(a) and (b), we further illustrate the ten energy levels near the

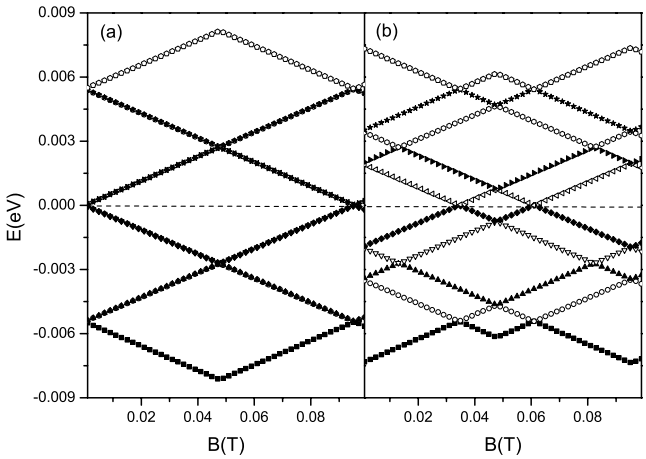

Figure 2. Ten energy levels near the Fermi level as a function of B for (5, 5, 3000). (a) and (b) corresponding to the cases without and with considering the curvature effect, respectively.

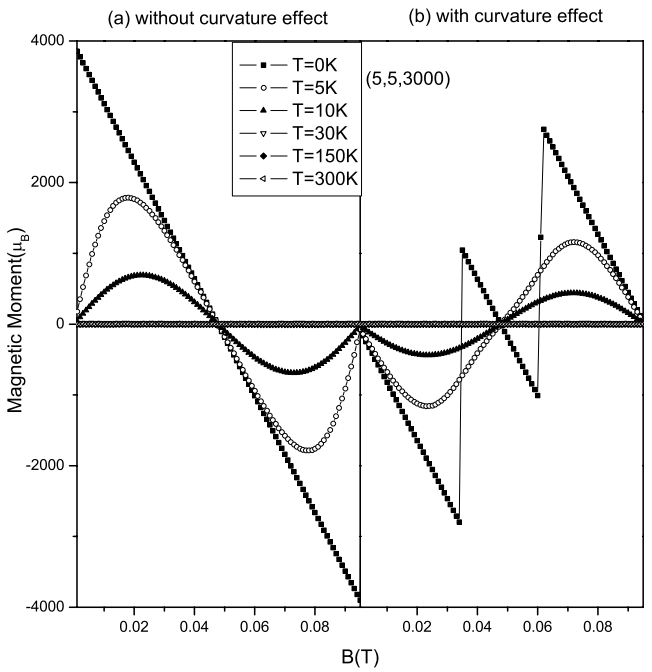

Figure 3. Temperature dependence of magnetic moment for (5, 5, 3000). (a) and (b) correspond to the cases without and with considering the curvature effect, respectively.

Fermi level without and with considering the curvature effect, respectively. As is shown, the curvature effect breaks level degeneracies. The B-dependent evolution of the discrete levels demonstrates that several crossings between eigenstates are driven by increasing magnetic field. Since the curvature effect changes the electronic structure dramatically, one can expect that the induced magnetic moments would exhibit distinctly different character compared with that without considering the curvature effect.

Finite temperature will affect the magnetic moment through two different mechanisms. The first is to mix contributions of states both below and above the Fermi level, resulting in a reduction of magnetic moments. The second is to reduce the phase coherence length L_ϕ. For $L_\phi < L$ (the circumference of torus), the magnetic moment vanishes exponentially. In order to illustrate the temperature dependence, we calculated the magnetic moments at different temperatures. In figure 3, we show the magnetic moments of (5, 5, 3000) as a function of magnetic field for different temperatures. The results without and with the curvature effect being considered are given in figures 3(a) and (b), respectively. At $T = 0$ K, as can be seen, the magnetic moments in both cases exhibit the characteristics of AB type periodicity, antisymmetry, linear B dependence and the special jump structures. However, there are three remarkable differences between the two cases at zero temperature. First, the magnetic moments show the opposite sign in the vicinity of zero field, i.e. figure 3(b) exhibits diamagnetic moment while figure 3(a) presents the giant paramagnetic moment. This is one of the most important results in this paper. We predict that at zero temperature, all of the armchair carbon nanotori would exhibit the diamagnetic moments near zero field due to the curvature effect, other than the corresponding predictions of [5]. This result can be extended to the persistent current induced by the magnetic flux, i.e. diamagnetic persistent current in the vicinity of zero flux, which might be contrary to that reported in [7]. The diamagnetic response has also been found in other armchair tori with different sizes. For instance, the $E_g(B = 0)$ for (5, 5, 3120) is about 0.579 meV, and the calculated $M(B = 0.001\ \text{T}, T = 0\ \text{K})$ is $-92.16\ \mu_B$; while for (5, 5, 9000), $E_g(B = 0)$ is about 0.293 meV, and $M(B = 5 \times 10^{-4}\ \text{T}, T = 0\ \text{K})$ is $-1109.45\ \mu_B$. Second, the special jump structures are different. These jumps are closely related to B leading to semiconductor–metal transitions or vice versa. Third, the magnitude of M is reduced obviously (by nearly about 25%) in the case with the curvature effect. This reduction can be ascribed to the localization induced by the curvature effect. Recently, puzzling behaviors have been observed for averaged persistent currents in diffusive normal-metal or semiconducting rings, i.e. experiments clearly indicate a sign of diamagnetism in the vicinity of zero field [12], which is contrary to the paramagnetism predicted from the existing theory [18]. Here, we would like to give a possible explanation of the intrinsic curvature effect giving rise to this diamagnetism. When increasing the temperature, as is shown (figure 3), the amplitude of AB oscillation declines rapidly. For relatively low temperatures, e.g. $T \leqslant 10$ K, the jump structures would be replaced by the peak structures, owing to the thermal broadening. Periodicity of the AB oscillation is preserved at low temperature. However, in the case of higher temperatures, for example, at $T = 150$ K, magnetic moments oscillate around zero randomly, with a very small magnitude about 0.4 μ_B, which can be ascribed to the loss of phase coherence.

As for 'metallic' zigzag carbon nanotori, in figure 4 we only give the results of typical $(9, 0, 300)$ considering the curvature effect. In analogy with armchair tori, the B-dependent M and E_g (the inset of figure 4) show the AB oscillation at low temperatures. However, there are two major distinctions in contrast with the armchair nanotori. First,

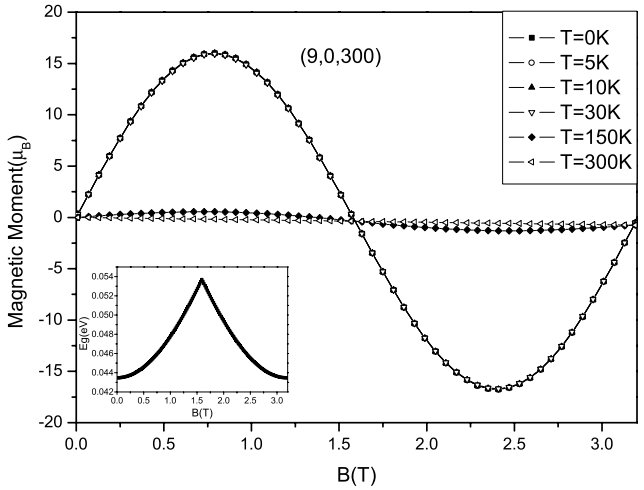

Figure 4. The temperature dependence of the magnetic moment for (9, 0, 300), and the inset is the corresponding dependence of E_g on B.

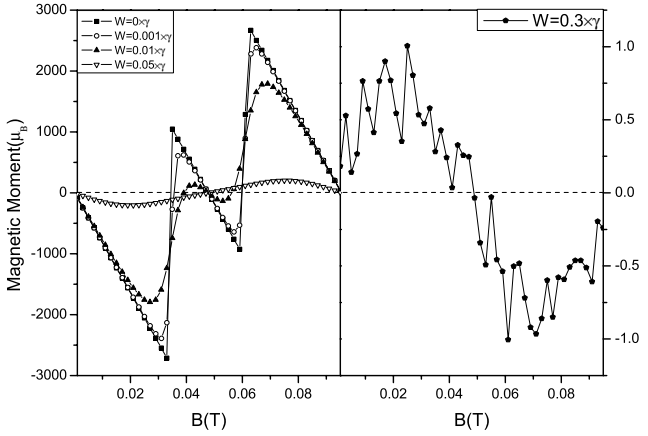

Figure 5. Magnetic moment of (5, 5, 3000) as a function of B for different disorder strengths at zero temperature. Left panel shows the case of $W = 0 \times \gamma, 0.001 \times \gamma, 0.01 \times \gamma, 0.05 \times \gamma$. Right panel corresponds to a relatively large disorder strength $W = 0.3 \times \gamma$.

near zero field, the metallic zigzag nanotorus exhibits the paramagnetic response with its magnetic moment being much weaker than the case without the curvature effect. For example, the (9, 0, 300) torus possesses a small magnetic moment of 0.32 μ_B at $T = 0$ K, $B = 0.01$ T, while 678.0 μ_B when neglecting the curvature effect. This weak paramagnetic response in 'metallic' zigzag carbon nanotori can be ascribed to their specific electronic structure. When taking into account the curvature effect, $E_g(B = 0) = 43.47$ meV, and is enhanced by the nonzero field (see inset of figure 4). This field enhanced E_g was also confirmed by Lin *et al* [17]. Second, in comparison with armchair nanotori, magnetic moments in 'metallic' zigzag nanotori only keep AB oscillations in those with relatively small radii. For instance, when considering the curvature effect, the magnetic moment in (9, 0, 2000) presents a small random oscillation around zero even at $T = 0$ K due to the loss of phase coherence (since the effective length of the path is larger than L_ϕ). In comparison with armchair tori, we owe these differences to their specific atomic structures. Similar results can be expected in 'metallic' chiral nanotori. These AB type periodical magnetic moments originate from the persistent current induced by the magnetic flux, while the diamagnetism or paramagnetism is determined by their specific electronic structure. Here, we give a brief comparison between our results and that of [5]. Without considering the curvature effect, the metallic carbon nanotori present large paramagnetic moments in the vicinity of zero magnetic field, while with the curvature effect considered in our calculation, the magnetic moments of these primary metallic carbon nanotori could exhibit a diamagnetic or paramagnetic response, depending on their chirality. Therefore, we can conclude that curvatures have a remarkable effect on the magnetic moments of carbon nanotori.

We now turn to exploring the disorder effect on the magnetic moments of carbon nanotori. Here, the disorder is simulated by a random modulation of the on-site energies, since this so-called Anderson-type random potential has allowed a reasonable interpretation of experiment [19]. For simplicity, here the disorder is assumed to be distributed identically in each supercell consisting of ten unit cells. Although this approximation is somewhat idealized compared with the realistic case, the results can give a qualitative description for the disorder effect. The range of the on-site energy fluctuation is $[-W, W]$, with W the disorder strength. Following the procedure as described in section 2, we calculated the magnetic moments of (5, 5, 3000) for different disorder strengths. In figure 5, we illustrate the W-dependent magnetic moments of (5, 5, 3000) at zero temperature. It is found that the effects of disorder and temperature on $M(B)$ are very similar, i.e. disorder can reduce the amplitude of the AB oscillation or even destroy the AB oscillation. For these relatively small disorder strengths, such as $W < 0.05 \times \gamma$, the AB oscillation is preserved (see the left panel of figure 5), while for large W, e.g. $0.4 \times \gamma$ (not shown), AB periodicity is destroyed (here γ is set to be 3.0 eV). This character can be understood by the fact that the localization length L_ξ is generally reduced by increasing the disorder strength and in the strong disorder regime, the amplitude of magnetic moment should decrease exponentially with L/L_ξ, with L being the circumference of a torus [20]. Another interesting phenomenon is that there may exist a disorder strength which can make a phase transition of magnetic response from diamagnetic to paramagnetic. In our simulation, we found that a disorder strength $W = 0.3 \times \gamma$ makes nanotorus (5, 5, 3000) exhibit a weak paramagnetic response in the vicinity of zero field (see right panel of figure 5). Therefore, with increasing disorder strength, there may appear a phase transition from diamagnetic to paramagnetic. Finally, we provide a comparison between our results (considering the disorder effect) and that of [5] (without considering the disorder effect) to complete our discussion of the disorder effect. In our case when we considered the disorder effect, both the magnitude and the sign of magnetic moments were changed. Thus the giant paramagnetic moments in [5] may not be expected when considering the disorder effect.

4. Conclusion

In conclusion, we have studied the magnetic moments in 'metallic' carbon nanotori (with very small gap) as a function of magnetic field and temperature. It is found that both the curvature and the disorder have significant effects on the magnetic moment of a carbon nanotorus. The results show that the behavior of the magnetic moments in carbon nanotori has the following features: (1) in the low-temperature limit, the pure armchair nanotori exhibit a diamagnetic response in the vicinity of zero magnetic field due to the curvature effect, while these pure 'metallic' zigzag nanotori present a weak paramagnetic response; (2) both curvature effect and high temperature decrease the amplitude of the Aharonov–Bohm oscillation; (3) the disorder reduces the amplitude of the AB oscillation and smoothes the jump structure in the M–B dependence; and with increasing disorder strength, there may appear a phase transition from diamagnetic to paramagnetic; (4) strong disorder strength as well as high temperature would destroy the AB oscillation, in which case the $M(B)$ is generally very small, and oscillates from a diamagnetic moment to a paramagnetic moment and vice versa. Future experiments could be used to test the results presented in this paper.

Acknowledgments

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