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Modulation of electric field on persistent current of carbon nanotubes

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ABSTRACT

We use tight-binding model including curvature effects to study the effect of transverse electric field on the persistent currents of armchair and zigzag carbon nanotubes (ACNTs and ZCNTs) threaded by longitudinal magnetic field. With increasing field strength, ZCNTs could undergo zero-gap transitions, whereas metallic ACNTs are not affected. The current amplitude, without electric field, in a (m,m) ACNT is inversely proportional to m^2. However, for a $(m,0)$ ZCNT, it is determined by the modulus of m with respect to three. Electric field could enhance the current amplitude of an ACNT, but could not change its magnetism. As for a ZCNT, both electric-field-distorted electronic states and zero-gap transitions determine a change in magnetism that is pronouncedly related with nanotube's geometry.

1. Introduction

Quasi-one-dimensional carbon nanotubes (CNTs), first discovered by Iijima in 1991 [1], have attracted much attentions both theoretically and experimentally owing to their interesting physical properties and widely potential application in nanodevices. A single-walled carbon nanotube (SWCNT) can be considered as a rolled up monolayer graphene (MG). Therefore, its geometric structure could be described by two vectors specified in the unit cell of a MG. The first is the chiral vector $\mathbf{C}_h = m\mathbf{a}_1 + n\mathbf{a}_2$ in the circumferential direction and the second is the translational vector $\mathbf{T} = p\mathbf{a}_1 + q\mathbf{a}_2$ along the longitudinal direction. $\mathbf{a}_1$ and $\mathbf{a}_2$ are primitive lattice vectors of a MG. Due to $\mathbf{C}_h \cdot \mathbf{T} = 0$, the parameters (m,n) uniquely define the geometric structure of a CNT. The radius and chiral angle are $r = b\sqrt{m^2+mn+n^2}/2\pi$ and $\theta = \tan^{-1}[-\sqrt{3}n/(2m+n)]$, respectively. $b = 1.42$ Å is C–C bond length. (m,m) armchair carbon nanotubes (ACNTs) and $(m,0)$ zigzag carbon nanotubes (ZCNTs) belong to achiral systems. A (m,m) ACNT has $r = 3mb/2\pi$ and $\theta = -30°$. They are $r = \sqrt{3}mb/2\pi$ and $\theta = 0°$ for a $(m,0)$ ZCNT. The number of carbon atoms in a unit cell is $N_u = 4\sqrt{(p^2+pq+q^2)(m^2+mn+n^2)}/3$, and both the ACNT and ZCNT have the same $N_u = 4m$.

Each SWCNT can be a metal or a semiconductor depending on its radius and/or chirality [2–4]. The peculiar geometry-dependent electronic properties have been verified by scanning tunneling microscope. It is also known that mechanical deformation [5] and boron(nitrogen)-doping [6,7] can remarkably affect electronic properties of CNTs. Another effective way to modulate electronic structures of CNTs is to apply external fields, e.g., magnetic field and/or electric field. Magnetic field, due to the cylindrical symmetry of nanotubes, induces magnetic phase that would affect energy dispersions and energy gaps. Furthermore, electronic structures exhibit periodical Aharonov–Bohm (AB) oscillation [8]. The AB-effect is reflected in magnetoresistance [9], magnetooptical [10], and magnetic properties [11,12]. On the other hand, the carbon nanotube field-effect transistor is a promising candidate for future nanoelectronic devices [13]. The response of a CNT to external electric field is of interest for studying its future application. The band structure of a CNT can be effectively modulated if the transverse electric field strength is large enough to couple the neighboring subbands. While the magnitude of electric field reaches a critical field strength, a CNT could exhibits a zero-gap transition (ZGT), i.e., energy gap with a finite value approaching zero. The electric-field-dependent energy dispersion and ZGTs strongly affect transport and excitation properties of CNTs [14–16].

Persistent current (I_{pc}) in normal metal rings is created by the threaded magnetic flux and an intriguing phenomenon occurring in thermodynamic equilibrium. It is quantum-mechanical in nature and reflect the coherence of the wave functions. Persistent current in normal metal rings has been studied in theory [17,18] and experimental measurement [19,20]. In experiment, the variation of persistent current with magnetic flux displayed an AB-oscillation with a period of flux quantum (hc/e) and had an amplitude about nanoampere (nA). Similarly, a CNT with cylindrical symmetry, its occupied electronic states are modulated by varying magnetic fields leading to persistent current along nanotube's circumference. The current amplitude and magnetism are

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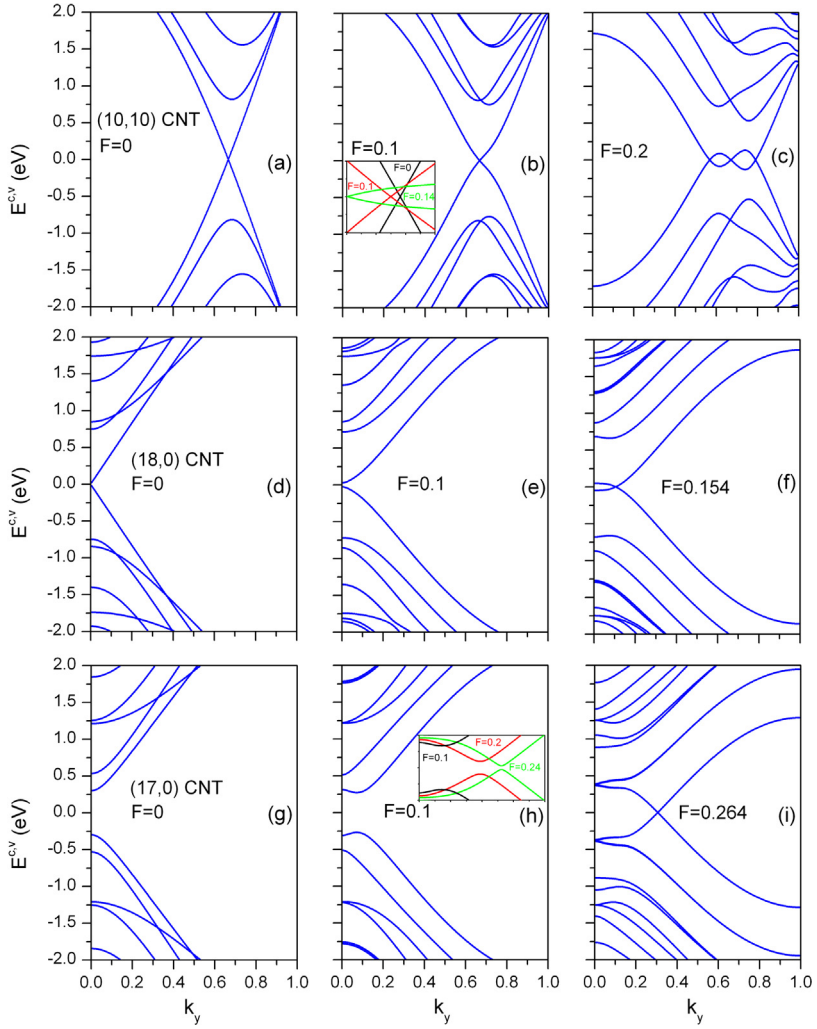

Fig. 1. The band structures of CNTs at various electric fields, (a)–(c) for a (10, 10) CNT, (d)–(f) for a (18, 0) CNT, and (g)–(i) for a (17, 0) CNT. The inset in Fig. 1(b) shows energy dispersions near the Fermi energy ($0.65 \leqslant k_y \leqslant 0.68$; $|E^{c,v}| \leqslant 0.05$ eV) for a (10,10) CNT at $F = 0$ (the dark lines), $F = 0.1$ (the red lines), and $F = 0.14$ (the green lines). As for a (17, 0) CNT, energy dispersions near the Fermi energy ($0 \leqslant k_y \leqslant 0.4$; $|E^{c,v}| \leqslant 0.4$ eV) are shown in the inset of Fig. 1(h) at $F = 0.1$ (the dark lines), $F = 0.2$ (the red lines), and $F = 0.24$ (the green lines). (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

pronouncedly associated with the magnitude and direction of magnetic field [11,12].

In this work, we use $2p_z$ orbital tight-binding model including curvature effect to study electronic structures of ACNTs and ZCNTs in the transverse electric field. Electric field strongly modulates energy dispersions and induces zero-gap transitions. Then, longitudinal magnetic field is further applied for studying persistent current. Our study shows that zero-gap transition could exhibit a special structure in persistent current and a change in magnetism. The electric-field-distorted energy dispersions could also affect nanotube's magnetism and enhance the current amplitude. Modulations of electric field on persistent current such as the amplitude, special structure, and magnetism are strongly dependent on geometric structure of CNTs.

2. The tight-binding model for electronic structures

In the tight-binding model, the hermitian Hamiltonian matrix is built from the subspace spanned by the N_u wave functions of $2p_z$ orbitals. Under electric and magnetic fields, the Hamiltonian with nearest-neighbor interactions is given by

$$H = \sum_i \epsilon_i a_i^+ a_i + \sum_{i,j} t_{ij} e^{i(2\pi/\phi_0)\int_i^j \mathbf{A}\cdot\mathbf{dr}} a_i^+ a_j, \tag{1}$$

where $\epsilon_i = Fr\cos\alpha_i$ is the on-site energy due to the electric field and α_i is the angle between the position vector of the ith atom and the transverse electric field $\mathbf{F}$ (unit eV/Å). t_{ij}s, the nearest-neighbor hopping integral, based on the curvature effect are, respectively, given by $\gamma_1 = \gamma_0(1 - b^2\sin^2\theta/8r^2)$, $\gamma_2 = \gamma_0[1 - b^2(\sin\theta + \sqrt{3}\cos\theta)^2/32r^2)]$, and $\gamma_3 = \gamma_0[1 - b^2(\sin\theta - \sqrt{3}\cos\theta)^2/32r^2)]$ [12]. $\gamma_0 = -2.66$ eV is the nearest-neighbor hopping integral without curvature effect. $\exp[i(2\pi/\phi_0)\int_i^j \mathbf{A}\cdot\mathbf{dr}]$ is the magnetic phase, where $\mathbf{A}$ is the vector potential and $\phi_0 = hc/e$ is the flux quantum. When the transverse electric field and the longitudinal magnetic field ($\mathbf{B}$) are applied, the longitudinal wave vector (k_y) is still a good quantum number. The first Brillouin zone has the range $-\pi/|\mathbf{T}| \leqslant k_y \leqslant \pi/|\mathbf{T}|$. For ACNTs and ZCNTs, the band structures could be calculated by diagonalizing the $4m \times 4m$ hermitian Hamiltonian matrix.

In this study, we concern that the modulation of electric field on I_{pc} of a CNT. Therefore, we first make a detailed comparison for electronic structures with and without electric field. In the absence of external field, the unit cell of a CNT contains two carbon atoms. Based on the tight-binding model, the Hamiltonian in Eq. (1) could be reduced to a 2×2 hermitian matrix. Electronic states and state energies are specified by the transverse (k_x) and longitudinal (k_y) wave vectors. The wave vector k_x, due to the transverse boundary condition, could be written as $k_x = J/r$ ($J = 1, 2, \ldots, N_u/2$). The