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Effect of electric field on persistent current of boron nitride nanotubes

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ABSTRACT

We study the effect of transverse electric field on persistent currents of armchair and zigzag boron nitride nanotubes (ABNNTs and ZBNNTs) threaded by longitudinal magnetic field within the tight-binding model. In the absence of electric field, the persistent current of (m,m) ABNNTs has a weak amplitude decaying exponentially with nanotube's radius and shows paramagnetism. For $(m,0)$ ZBNNTs, the current amplitude and magnetism are determined by the modulus of m with respect to three. Electric field could enhance the current amplitude of both ZBNNTs and ABNNTs, but could not change the magnetism of ABNNTs. However, for ZBNNTs, electric field could further change the magnetism and the symmetry in the current–flux curves that is pronouncedly associated with nanotube's geometry.

1. Introduction

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 wide potential application in nanodevices. Based on the analogy in geometry between graphite and hexagonal boron nitride, the excellent physical properties with CNTs have also motivated scientists to synthesize boron nitride nanotubes (BNNTs). Shortly after the theoretical predictions in 1994 [2], BNNTs, next year, have been synthesized experimentally [3]. However, distinct from the peculiar electronic structure (metals or semiconductors) of CNTs depending sensitively on the diameter and the chirality, BNNTs are semiconductors with a wide band-gap ranging from 4 eV to 5 eV which is independent of their geometry [4].

Previous studies showed that the modulations of electronic structures of CNTs and BNNTs can be achieved by applying transverse electric field [5–7], leading to a reduction of energy gap and even a zero-gap transition (ZGT), i.e., energy gap with a finite value approaching zero. This is the so-called giant Stark effect which is further confirmed experimentally by bias-dependent scanning tunneling microscopy [8]. The band structures of a BNNT, through the Stark effect, can be modulated by coupling the neighboring subbands, resulting in a significant change in their electronic structures and optical properties [9–11]. This effect is more pronounced in BNNTs than in CNTs due to the strong ionicity of boron-nitride bonding.

While normal metal rings are threaded by magnetic flux, persistent current (I_{pc}) is created which is an intriguing phenomenon in thermodynamic equilibrium. It is quantum-mechanical in nature and reflects the coherence of the wave functions. Persistent current in normal metal rings has been studied in theory [12,13] and experimental measurement [14–16]. In experiment, the current–flux curve had a maximum amplitude about nano-Ampere (nA) and displayed an AB-oscillation with a period of flux quantum $\phi_0 = h/e$. 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 pronouncedly associated with the magnitude and direction of magnetic filed [17,18]. As for a cylindrical BNNT, its rigid energy gap is hardly changed by applied magnetic flux. Thus, the amplitude of persistent current is predicted to be much smaller than that of a CNT and weakly depends on geometric structures. It is believed that electric field could also significantly affect persistent current and magnetism, since energy dispersion of a BNNT could be easily modulated by electric field.

In this work, we use the $2p_z$ orbital tight-binding model to study electronic structures of ABNNTs and ZBNNTs in the transverse electric field. Electric field strongly modulates energy dispersions and induces zero-gap transitions. Longitudinal magnetic field is further applied for studying persistent current. Our study shows that the electric-field-distorted energy dispersions could effectively affect nanotube's magnetism and enhance the current amplitude. Modulations of electric field on persistent current such

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as the amplitude, special structure, and magnetism are strongly dependent on geometric structure of BNNTs.

2. The tight-binding model for electronic structures in external fields

A boron nitride nanotube can be considered as a rolled up monolayer hexagonal boron nitride (hBN). Therefore, its geometric structure could be described by two vectors specified in the unit cell of a hBN as well as in a monolayer graphene. 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 hBN. Due to $\mathbf{C}_h \cdot \mathbf{T} = 0$, the parameters (m,n) uniquely define the geometric structure of a BNNT. 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. $b = 1.45$ Å is B–N bond length. (m,m) armchair boron nitride nanotubes (ABNNTs) and $(m,0)$ zigzag boron nitride nanotubes (ZBNNTs) belong to achiral systems. A (m,m) ABNNT has $r = 3mb/2\pi$ and $\theta = -30^\circ$. They are $r = \sqrt{3}mb/2\pi$ and $\theta = 0^\circ$ for a $(m,0)$ ZBNNT. The number of atoms in a unit cell is $N_u = 4\sqrt{(p^2+pq+q^2)(m^2+mn+n^2)/3}$, and both the ABNNT and the ZBNNT have the same N_u $(=4m)$.

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

$$H = \sum_i \epsilon_i a_i^+ a_i + \gamma_0 \sum_{i,j} e^{i(2\pi/\phi_0)\int_i^j \mathbf{A}\cdot\mathbf{dr}} a_i^+ a_j, \tag{1}$$

where $\epsilon_i = E_i + Fr\cos\alpha_i$ is the on-site energy due to the $2p_z$ atomic orbital and the external electric field. α_i is the angle between the position vector of the ith atom and the transverse electric field $\mathbf{F}$ (unit eV/Å). $\gamma_0 = -2.92$ eV is the nearest-neighbor hopping integral. The $2p_z$ on-site energies of boron atom and nitrogen atom are $E_B = 4.78$ eV and $E_N = 0.48$ eV, respectively. a_i^+ (a_i) is the creation (annihilation) operator. $\exp[i(2\pi/\phi_0)\int_i^j \mathbf{A}\cdot\mathbf{dr}]$ is the magnetic phase, where $\mathbf{A}$ is the vector potential. 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 $-\pi/|\mathbf{T}| \le k_y \le \pi/|\mathbf{T}|$. For ABNNTs and ZBNNTs, the band structures could be calculated by diagonalizing the $4m \times 4m$ hermitian Hamiltonian matrix.

In the absence of external field, all BNNTs are wide-gap semiconductors but the energy dispersions are very different between ABNNTs and ZBNNTs. For the (8,8) ABNNT (Fig. 1(a)), conduction and valence bands are symmetric about the Fermi energy ($E_F = 2.63$ eV). The first (closest to E_F) and the last subbands are singlet states, while others are doubly degenerate. The band-edge states are located at $k_y = 2/3$ (unit $\pi/|\mathbf{T}|$). With increasing wave vector k_y, energy spacing is getting smaller and all subbands are merged together at $k_y = 1$. As for the (9,0) ZBNNT shown in Fig. 1(d), energy dispersions show similar band-symmetry and degeneracy, but the two singlet states correspond to the fifth and last subbands. In contrast to an ABNNT, the differences existing in band structures of a ZBNNT include (I) the band-edge states are at $k_y = 0$ and (II) all subbands, at $k_y = 1$, are merged into one doubly and four four-fold degenerate states.

While a BNNT is threaded by uniform magnetic field along the nanotube axis, the induced magnetic phase could change the band degeneracy, energy dispersion, energy spacing, and energy gap. For example, Fig. 1(b) shows that at magnetic flux $\phi = 0.25$ (unit ϕ_0), all degenerate states of an ABNNT are split into singlet states leading to the smaller energy spacing except for electronic states at $k_y = 1$. As for a ZBNNT in Fig. 1(e), the influence of magnetic field on band structures is also similar but all electronic states at $k_y = 1$ are doubly degenerate. With increasing magnetic flux, electronic structures at $\phi = \phi_0$ are restored to those at $\phi = 0$, i.e., the Ahanorov–Bohm (AB) oscillation. However, magnetic filed just slightly changes band-width and energy gap. According to our studies (not shown here), the maximum change in the magnitude of energy gap is about 0.08 eV which is much smaller than energy gap (~ 4.5 eV) at $\phi = 0$. Moreover, magneto-energy gap is weakly dependent on the nanotube's radius. Thus, other methods should be considered for significantly modulating energy dispersions of BNNTs.

In contrast to magnetic field, electric field, due to the strong ionicity of BNNTs, is expected to have significant effects on electronic structures. While the transverse electric field is applied, the rotational symmetry is broken such that the transverse momenta are no longer good quantum numbers. The neighboring subbands with nearly equivalent energy would be coupled and the coupling is getting stronger with increasing field strength that leads to a strongly k_y-dependent energy dispersion. Fig. 1(c) shows that for an ABNNT, at $F = 0.2$, the band-width and the energy spacing increase and the band degeneracy is broken at $k_y = 1$. However, the symmetry of conduction and valence subbands about the Fermi energy is unaltered. Band-edge states of conduction and valence subbands shift toward the Fermi energy causing an effective decrease in energy gap. As the increasing electric field reaches to a critical magnitude F_c, a zero-gap transition occurs. The modulation of electric field on energy gap is strongly related to the nanotube's radius. For example, the value of critical electric field of a (23,23) ABNNT is drastically reduced to $F_c \approx 0.15$, whereas it equals $F_c \approx 0.52$ for a (8,8) ABNNT. With increasing the magnitude of electric field and the nanotube's radius, the optical absorption frequency could extensively include the range from the ultraviolet to the visible light. As for a zigzag BNNT, Fig. 1(f) shows that the F-dependent electronic structure has a similar behavior. However, the symmetry between conduction and valence subbands about E_F is broken and the electronic states with $k_y = 1$ are all doubly degenerate. Therefore, the response of electronic structures to applied external fields is profoundly associated with nanotube's geometry that might be reflected in magnetic properties.

3. Modulation of electric field on persistent current

Persistent current is a variation of total energies $(E_t(F,\phi))$ of occupied electronic states with applied magnetic flux. For non-interacting electrons, I_{pc} at zero temperature is calculated by the following formula:

$$I_{pc}(F,\phi) = -\sum_{h=c,v;\sigma} \int_{1stBz} \frac{dk_y}{2\pi} \frac{\partial E^h(k_y,F,\phi;\sigma)}{\partial\phi}, \tag{2}$$

where $h = c(v)$ represents the conduction (valence) band and the summation only includes the occupied electronic states. The persistent current, without spin-B interaction, is a periodic function of ϕ with a fundamental period ϕ_0.

Before discussing persistent current, it is needed to understand the total energy difference of occupied electronic states with and without magnetic flux, which is denoted by $\Delta E_t(F,\phi) = E_t(F,\phi) - E_t(F,0)$. It could be considered as a measurement of sensitivity of electronic structures to applied external fields and also deeply related to magnetic properties. For a (m,m) ABNNT, $\Delta E_t(F=0,\phi)$ without F reveals negative value for all different ms and its ϕ-dependence becomes weaker with increasing m (radius), as shown in Fig. 2(a). The persistent current is proportional to the negative slope of $\Delta E_t(F=0,\phi) - \phi$ curve. Therefore, the $I_{pc} - \phi$ curve, in Fig. 2(b), is antisymmetric about $\phi = 0.5$. Moreover, the amplitude of I_{pc} exponentially decays with increasing m that is similar to the study in the