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Insulator-semimetallic transition in quasi-1D charged impurity-infected armchair boron-nitride nanoribbons

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ABSTRACT

We address control of electronic phase transition in charged impurity-infected armchair-edged boron-nitride nanoribbons (ABNNRs) with the local variation of Fermi energy. In particular, the density of states of disordered ribbons produces the main features in the context of pretty simple tight-binding model and Green's functions approach. To this end, the Born approximation has been implemented to find the effect of π-band electron-impurity interactions. A modulation of the π-band depending on the impurity concentrations and scattering potentials leads to the phase transition from insulator to semimetallic. We present here a detailed physical meaning of this transition by studying the treatment of massive Dirac fermions. From our findings, it is found that the ribbon width plays a crucial role in determining the electronic phase of disordered ABNNRs. The obtained results in controllable gap engineering are useful for future experiments. Also, the observations in this study have also fueled interest in the electronic properties of other 2D materials.

1. Introduction

Two-dimensional (2D) graphene clearly has advantages over other carbon nanomaterials due to high electron mobility, massless relativistic Dirac fermions, and strong mechanical properties [1–3]. Graphene nanoribbons (GNRs) have been synthesized empirically by cutting exfoliated graphene [4] and attracted the attention of researchers owing to their unique properties, for instance, many different devices can be designed using graphene because of their excellent geometrics. In recent years, the electronic and magnetic properties of GNRs have been widely addressed theoretically in various fields [5–7].

Doping is one of the possible ways to improve the electronic properties of GNRs [8–11]. Yu et al. [9] have reported that the doping site is an important factor related to the electronic properties of nitrogen-doped GNRs. In Ref. [11], the authors studied the effect of boron doping on the electronic transport properties of GNRs and found that transition from metallic to the semiconductor in GNRs can occur when boron atoms substitute at nanoribbons edges. They also argued that the symmetry of spin-up and spin-down transmittance channel breaks by this substitution. In another study, which set out to determine the doping effect on electronic properties of GNRs, it has been shown that substitution of oxygen in edges of GNRs prevents the agglomeration of spin in its neighborhood and leads to semiconductor-metal transition at high density in zigzag nanoribbons [12].

Novoselov et al. [13] discovered the single-layered hexagonal boron-bnitride (h-BN) atomic crystals empirically. This new material has been used in many electronic devices owing to high thermal stability [14] and excellent electronic properties [15]. Similar to GNRs, BN nanoribbons (BNNRs) could be prepared empirically by cutting the 2D BN crystal, as schemed in Fig. 1(a). In contradiction with the GNRs, the zigzag-type BNNRs are metallic, while the armchair BNNRs are insulators, as shown in Fig. 1(b), separate of ribbon widths ($t \simeq 3$ eV [16]). More recent attention has focused on these new 2D materials [17–19]. The substitutional carbon doping of BN nanostructures has been exemplified in a report by Wei et al. [17]. The findings from this study have demonstrated carbon doping leads to electrical insulator-metal transition, specifically adjustable and possible to change electrical and magnetic properties of BN nanostructures. Furthermore, the preferential doping was found to occur at the sites more vulnerable to electron beam irradiation.

In this work, motivated by the discussion above, we employ a simple analytical procedure based on the Born approximation and **T** matrix to describe electronic phase transition from insulator to semimetallic in impurity-infected BNNRs using the tight-binding

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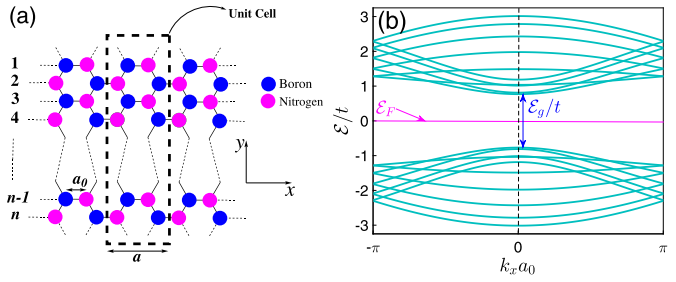

Fig. 1. (Color online) (a) Schematic view of an ABNNR with width $\sqrt{3}na_0$ ($a_0 \simeq 2.5$ Å denotes the interatomic distance between boron and nitrogen atoms) given by $2n$ atoms. The black bold dashed lines delimit the unit cells of the system and $a = 3a_0$ is the respective unit cell width. Periodic boundary conditions are also applied in the vertical direction. Furthermore, the band structure for the infinitely long BNNR in x-direction is plotted with (b) $n = 10$ width to show the insulating phase of BNNRs ($\mathcal{E}_F$ is the Fermi energy and $\mathcal{E}_g/t$ presents the normalized energy band gap).

model Hamiltonian and the Green's function method. The system is subjected to charged impurities in the whole finite ribbon randomly neglecting the location of substituted impurity. Furthermore, the kind of impurity atoms is not important in our study in contrast to other studies and only two impurity concentration and impurity scattering potential factors play key roles in phase transitions. In particular, we study the effects of impurity concentration, impurity scattering potential, and the ribbon width on the density of states (DOS) of ABNNRs.

The sequence adapted in this paper is as follows: In Sec. 2, we give details about the effective boron-nitride Hamiltonian model and Green's functions. In Sec. 3, we describe the electronic self-energies induced by impurities and DOS. We show the numerical results in Sec. 4 and finally our main conclusions are summarized in Sec. 5.

2. Theoretical Model and Green's functions

To proceed, we construct the following effective single-orbital nearest neighbor tight-binding model in the basis $\{|A\ \text{(Boron)}, k_x, k_y\rangle = \psi_A(k_x, k_y)$ and $|B\ \text{(Nitrogen)}, k_x, k_y\rangle = \psi_B(k_x, k_y)\}$, where well captures all the low-energy features of electronic states of nano boron-nitride ribbons. Here, we consider an ABNNR with translational symmetry along the x-axis, as shown in Fig. 1(a). Thus, the simple Hamiltonian can be written as

$$\hat{\mathcal{H}} = -\varepsilon_0^A \sum_i \hat{a}_i^\dagger \hat{a}_i - \varepsilon_0^B \sum_i \hat{b}_i^\dagger \hat{b}_i - t \sum_{\langle i,j \rangle} [\hat{a}_i^\dagger \hat{b}_j + \text{H.c.}], \tag{1}$$

where $\hat{c}_i(\hat{c}_i^\dagger)$ with $\hat{c} = \hat{a}$ or $\hat{b}$ implies the on-site annihilation (creation) operator for electrons at the i-th site of the honeycomb lattice in the sublattice A or B. The coefficient $t \simeq 3$ eV [16] is the hopping parameter between nearest neighbor atoms belonging two sublattices A and B. ε_0^A and ε_0^B are the on-site energies of two different sublattice atoms (boron and nitrogen), which $\varepsilon_0^A - \varepsilon_0^B = 4.5$ eV [20,21]. The H.c. in the third term stands for the Hermitian conjugate. According to Fig. 1(a), each index site i contains the unit cell that can be labeled with index m and sublattice A_l and B_l ($l \in [1, n]$). With the help of

$$\hat{c}^\dagger_{A(B),k_x,k_y} \propto \sum_m \sum_{l=1}^{n} e^{\mathrm{i}k_x x_m} \psi_{A(B)}(l, k_y) \hat{c}^\dagger_{A(B),l,m},$$

in operator form of suggested basis sets, one can obtain the electronic spectrum of the system [22]. In this relation, x_m denotes the position of m-th unit cell along the x-axis. Also, $\hat{c}^\dagger_{A(B),l,m}$ creates an electron in the p_z-orbit in the sublattice A (B) with position l along the width of ribbon (y-axis) on the m-th unit cell. In the work of Zheng et al. [22], the hard-wall boundary conditions allows us to choose

$$\psi_{A(B)}(l, k_y) = \sin\left(\frac{\sqrt{3}k_y a_0}{2} l\right),$$

with discretized wave-vector

$$k_y = \frac{2}{\sqrt{3}a_0} \frac{z\pi}{n+1}, \quad z = 1, 2, 3, \ldots n$$

Rewriting the Hamiltonian in terms of $\hat{c}^\dagger_{A(B),k_x,k_y}$ operators

$$\hat{\mathcal{H}} = \sum_{k_x,z,\nu=\pm} \mathcal{E}_\nu(k_x, z) \hat{c}^\dagger_{k_x,z,\nu} c_{k_x,z,\nu},$$

where

$$\hat{c}^\dagger_{k_x,z,\nu} = \frac{\sqrt{2}}{2}\left(\hat{c}^\dagger_{A,k_x,z} + \nu \sqrt{\frac{\phi^*(k_x,z)}{\phi(k_x,z)}} \hat{c}^\dagger_{B,k_x,z}\right),$$

the band energy dispersion is given by

$$\mathcal{E}_\nu(k_x, z) = \frac{\varepsilon_0^A + \varepsilon_0^B}{2} + \nu \sqrt{|\phi(k_x,z)|^2 + \left(\frac{\varepsilon_0^A - \varepsilon_0^B}{2}\right)^2}, \tag{2}$$

where $\phi(k_x, z) = -t[2e^{\mathrm{i}k_x a_0/2} \cos\left(\frac{\sqrt{3}k_y a_0}{2}\right) + e^{-\mathrm{i}k_x a_0}]$. The on-site energies $\varepsilon_0^A = 2.25$ eV and $\varepsilon_0^B = -2.32$ eV are taken into account individually [23]. The momentums (k_x, k_y) belong to the first Brillouin zone (FBZ) of BNNR structure. Since unit cell of BNNR includes $2n$ atoms, the Green's functions can be written as a $2n \times 2n$ matrix. In the Matsubara formalism [24], each element of the Green's function matrix and its Fourier transformation are defined by

$$\begin{aligned} G^0_{\alpha\beta}(k_x, \tau) &= -\langle \mathcal{T}_\tau [\hat{c}_{k_x,\alpha}(\tau) \hat{c}^\dagger_{k_x,\beta}(0)] \rangle, \\ G^0_{\alpha\beta}(k_x, \mathrm{i}\omega_\mathcal{F}) &= \int_0^{1/k_B T} e^{\mathrm{i}\omega_\mathcal{F}\tau} G_{\alpha\beta}(k, \tau) d\tau, \end{aligned} \tag{3}$$

where α, β refer to each sublattice atoms A and B and τ is the imaginary time. Also, $\omega_\mathcal{F} = (2\mathcal{F} + 1)\pi k_B T$ is the Fermionic Matsubara frequency. Therefore, elements $G^0_{\alpha\beta}(k_x, \mathrm{i}\omega_\mathcal{F})$ in the reciprocal-space can be easily calculated. Once a solution has been achieved, the DOS in order to study the electronic phase transition from insulator to semimetallic in BNNRs can be expressed in the following.

3. Electronic self-energy and DOS

Suppose that now we apply a electron-impurity interaction within the tight-binding model by addition of the local energy term, given by

$$\hat{\mathcal{H}}_{\text{e-i}} = \sum_{\mathbf{q}} \nu_i [\hat{a}^\dagger_{\mathbf{q}} \hat{a}_{\mathbf{q}} + \hat{b}^\dagger_{\mathbf{q}} \hat{b}_{\mathbf{q}}] \tag{4}$$

where the induced momentum $\mathbf{q}$ by impurities belongs to the FBZ. According to the Born approximation in the scattering theory and using $\mathbf{T}$ matrix [24,25], the electronic self-energy matrix elements of disordered BNNR system in the presence of finite but small density of impurity atoms, $n_i = N_i/N_c$, can be obtained as

$$\Sigma_{\alpha\beta}(\mathbf{q}, \mathrm{i}\omega_\mathcal{F}) = \frac{n_i \nu_i}{1 - \frac{\nu_i}{N_c} \sum_{k_x \in \text{FBZ}} G^0_{\alpha\beta}(k_x, \mathrm{i}\omega_\mathcal{F})} \tag{5}$$

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