Multibands tunneling in AAA-stacked trilayer graphene

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ABSTRACT

We study the electronic transport through np and npn junctions for AAA-stacked trilayer graphene. Two kinds of gates are considered where the first is a single gate and the second is a double gate. After obtaining the solutions for the energy spectrum, we use the transfer matrix method to determine the three transmission probabilities for each individual cone \( \tau = 0, \pm 1 \). We show that the quasiparticles in AAA-stacked trilayer graphene are not only chiral but also labeled by an additional cone index \( \tau \). The obtained bands are composed of three Dirac cones that depend on the chirality indexes. We show that there is perfect transmission for normal or near normal incidence, which is a manifestation of the Klein tunneling effect. We analyze also the corresponding total conductance, which is defined as the sum of the conductance channels in each individual cone. Our results are numerically discussed and compared with those obtained for ABA- and ABC-stacked trilayer graphene.

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1. Introduction

During the last decade, the physics of single layer graphene and stacks of graphene layers has emerged as a fertile research area [1–3]. This is due to its unusual electronic properties, that may be useful in the design of new electronic devices [4–6]. Among them, we cite the linear dispersion relation of a single graphene layer, manifestation of the Klein tunneling [2,3], chiral parabolic bands in bilayers [7] and the possibility of confining charge to the surface in systems with a multilayer graphene [8]. Furthermore, it has been observed in different works [9–17] that the properties of multilayer graphene materials depend on their stacking order and the number of layers. Most of these works have been devoted to the few-layer graphene materials with Bernal (ABA) and rhombohedral (ABC) stacking order [18,19]. For the rhombohedral form, the Klein tunneling depends on the stacking order [20,21] and is absent for the Bernal stacking.

Recently a new stable multilayer graphene with AA-stacking order has been experimentally observed [22,23]. In such system, each sublattice in the top layer is located directly above the same one in the bottom layer. Due to this stacking order, the AA-stacked bilayer graphene (BLG) has a special low energy band structure. It is just the double copy of single layer graphene bands shifted up/down by the interlayer coupling \( \gamma = 0.2 \) eV [24] and is also different from that corresponding to the AB-stacked BLG. Due to this special band structure, the AA-stacked BLG shows many interesting properties which are different from that of single layer and also have not been observed in other graphene-based materials [24–29].

There has been a growing interest in the study of the tunneling problem of charge carriers in trilayer graphene systems including ABA- and ABC-stacked trilayer graphene (TLG) [18,19]. In the present work, we consider the AAA-stacked TLG as...
schematically shown in Fig. 1 (a), which is composed of three single layers, each sublattice in a top layer is located directly above the same one in the bottom layer. The unit cell of an AAA-stacked layers consists of 6 inequivalent carbon atoms with two different atoms in each layer. We study the electronic transport through np and nnp junctions for AAA-stacked TLG where two kinds of gates will be considered such that the first causes an equal potential shift $V$ for all three layers and the second induces an interlayer potential difference $\delta$ between neighboring layers. We show that the quasiparticles in AAA-stacked TLG are not only chiral but also labeled by an additional cone index $\tau$. We obtain band structures that are composed of three Dirac cones and depending on the cone indexes and chirality indexes. Our theoretical model is based on the well established tight binding Hamiltonian [30]. The single and double gates act as a boundary for which we calculate the three transmission probabilities as a function of the angle of incidence and Fermi energy of the incident electron for different configurations of the device. Subsequently, we numerically evaluate the total conductance and underline the basic features of our system.

The rest of the paper is organized as follows. In section 2, we formulate our model by setting the Hamiltonian system used to describe AAA-stacked TLG. By using the direct method, we solve the $6 \times 6$ system of equations to determine the solutions of the energy spectrum in each layer ($\tau = -1, 0, 1$). Later on, we present the formalism, indicate the different propagating modes, define the four different cases for transmission for the six-band model and explain the three possible transmission probabilities. In section 3, using the transfer matrix at boundaries together with the incident, transmitted and reflected currents we end up with three transmission probabilities. Next, we numerically discuss the obtained transmissions for each individual cones ($\tau = 0, \pm 1$) for np and nnp junctions to underline the behavior of our system. In section 4, we show the numerical results for the conductance and investigate the contribution of each transmission channel. Finally, we conclude our work and emphasize our main results.

2. Tight binding formalism

We consider a system consisting of three layers of graphene having the AAA-stacking structure. The unit cell consists of six atoms labeled $A_1, B_1$ in the top layer, $A_2, B_2$ in the central layer and $A_3, B_3$ in the bottom layer as depicted in Fig. 1(a). Each carbon atom in the bottom (center) layer is located above the corresponding atom in the center (top) layer, respectively and they are bound by an interlayer coupling energy $\gamma = 0.2$ eV.

The Hamiltonian describing the system, in the nearest-neighbor tight-binding approximation [29], is given by

$$\mathcal{H} = \sum_\mathbf{q} \Psi_\mathbf{q}^\dagger \hat{H}(\mathbf{q}) \Psi_\mathbf{q}$$

and different quantities read as

$$\hat{H}(\mathbf{q}) = \begin{pmatrix}
0 & f^*(\mathbf{q}) & \gamma & 0 & 0 & 0 \\
f(\mathbf{q}) & 0 & 0 & \gamma & 0 & 0 \\
\gamma & 0 & 0 & f^*(\mathbf{q}) & \gamma & 0 \\
0 & \gamma & f(\mathbf{q}) & 0 & 0 & \gamma \\
0 & 0 & \gamma & f(\mathbf{q}) & 0 & \gamma \\
0 & 0 & 0 & \gamma & f(\mathbf{q}) & 0
\end{pmatrix}, \quad \Psi_\mathbf{q} = \begin{pmatrix}
a_{1\mathbf{q}} \\
b_{1\mathbf{q}} \\
a_{2\mathbf{q}} \\
b_{2\mathbf{q}} \\
a_{3\mathbf{q}} \\
b_{3\mathbf{q}}
\end{pmatrix},$$

where $a_{i\mathbf{q}}$ and $b_{i\mathbf{q}}$ are the annihilation (creation) operators with the momentum $\mathbf{q}$ of the electrons, respectively on the $A_i$ and $B_i$ sites, $i = 1, 2, 3$ indexes each of the three layers. Here we have $f(\mathbf{q}) = -\gamma_0 \sum_{j=1}^3 e^{i\mathbf{q} \cdot \mathbf{d}_j}$ with $\gamma_0$ is the intralayer hopping energy, $\mathbf{d}_j$ are vectors connecting each carbon atom to its in-plane nearest neighbors and $\mathbf{q} = (qx, qy)$ is the two dimensional momentum. By transforming the Hamiltonian into the $\mathbf{p}$ space, we can write the low energy Hamiltonian as

![Fig. 1. (a): Schematic representation of the lattice structure of the AAA-stacked trilayer graphene with (A,B) atoms within the same layer and $\gamma$ is the interlayer hopping energy. (b): Diagram for the np junction of height $V_{np}(x)$. (c): Diagram for the nnp junction of height $V_{nnp}(x)$ and width $d$.](image)
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