Resonant tunneling through S- and U-shaped graphene nanoribbons

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Abstract

We theoretically investigate resonant tunneling through S- and U-shaped nanostructured graphene nanoribbons. A rich structure of resonant tunneling peaks is found emanating from different quasi-bound states in the middle region. The tunneling current can be turned on and off by varying the Fermi energy. Tunability of resonant tunneling is realized by changing the width of the left and/or right leads and without the use of any external gates.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Graphene is a single layer of carbon atoms arranged in a hexagonal lattice that is the building block for graphite material. Recently, graphene samples have been fabricated experimentally by micro-mechanical cleavage of graphite [1]. This material has aroused increasing attention due to its novel transport properties that arise from its unique band structure: the conduction and valence bands meet conically at the two nonequivalent Dirac points, called the K and K\(^\prime\) valleys of the Brillouin zone, which show opposite chirality. Around the two Dirac points, the energy dispersion is linear in momentum space and is well described by the massless Dirac–Weyl equation. The unique energy dispersion leads to a number of unusual electronic transport properties in graphene such as integer quantum Hall effect at room temperature [2], finite minimal conductivity and special Andreev reflection [3, 4]. In graphene electrons can pass through potential barriers without any reflection, i.e. Klein tunneling, in contrast to conventional electrons that exhibit an exponentially decreasing transmission with increasing barrier height and/or width. Klein tunneling makes it impossible to confine the carriers in single-layer graphene using the electric gates that are often used in a conventional semiconductor two-dimensional electron gas (2DEG). Tunneling through single barriers [5] and double barriers [6] in graphene has been investigated theoretically. Recent theoretical work demonstrated that the magnetic barriers can be used to confine the massless Dirac fermion [7] and block the Klein tunneling and display a huge magnetoresistance [8, 9]. Klein tunneling leads to a poor rectification effect and the absence of resonant tunneling for normal incidence in graphene and limits the performance of graphene-based electronic devices.

In graphene nanoribbons (GNRs), the presence of edges can change the energy spectrum of the \(\pi\)-electrons dramatically. GNRs can be fabricated using conventional lithography and etching techniques [10, 11]. The electronic properties of a GNR depend very sensitively on the sizes and shape of the edges, i.e. zigzag- and armchair-edged GNR. The zigzag-edged graphene nanoribbons (ZGNRs) and armchair-edged graphene nanoribbons (AGNRs) exhibit very different band structures. The ZGNRs always have localized states appearing at the edge near the Dirac point and therefore exhibit metallic-like behavior. The AGNRs show alternating metallic-like and semiconductor-like features alternatively as the width of nanoribbons increases [12]. Such features are very different from a conventional semiconductor quantum wire and provide a unique way to tailor the transport properties of GNRs [13–18]. Recently it is found that a single electronic potential barrier can block the electron tunneling in the ZGNRs and confine electrons in between double barriers [14]. The magnetic transport and spatial distribution of currents was investigated for unipolar and bipolar ZGNRs [16]. These previous works have demonstrate that the resonant tunneling can be realized using an electric and/or magnetic barrier. Here, we will address the question whether it is possible...
to realize resonant tunneling using only the geometry of the graphene nanoribbons. We focus on the S- and U-shaped structures consisting of zigzag leads and armchair nanoribbons in between them, because the zigzag nanoribbon is always metallic, while the bandgap of an armchair nanoribbon depends sensitively on the width of the nanoribbon. This combination of zigzag and armchair nanoribbon could lead to interesting transport properties.

In this work, we theoretically investigate the transport property through U-shaped nanoribbon structures sandwiched by two semi-infinite ZGNRs, i.e. the geometry of the graphene nanoribbon in the absence of any external nanostructured electric gates. We will demonstrate resonant tunneling behavior through these graphene nanostructures whenever the AGNR in the middle part is metal-like or semiconductor-like. In those structures, the middle structure acts as a barrier between ZGNR leads, and an interesting resonant tunneling behavior can be seen with varying lengths of the middle part of the U-shaped ZGNR or AGNR.

This paper is organized as follows. In section 2, the theoretical model and calculational method are given. In section 3, we present the numerical results and our discussions. Finally we give our conclusion in section 4.

2. Model and calculation method

To describe the electron transport through the S- or U-like structure sandwiched by two semi-infinite ZGNRs leads, the tight-binding Hamiltonian is adopted:

\[ H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + \text{h.c.}) - t' \sum_{\langle \langle i,j \rangle \rangle} (c_i^\dagger c_j + \text{h.c.}) \]

where \( c_{i(j)}(c_{i(j)}^\dagger) \) creates (annihilates) an electron on site \( R_{i(j)} \), \( t \) is the nearest-neighbor (\( \langle i, j \rangle \)) hopping energy (\( t \approx 3.03 \text{ eV} \)) and \( t' \) is the next-nearest-neighbor (\( \langle \langle i, j \rangle \rangle \)) hopping energy [19]. The conductance of the system is evaluated using the Landauer–Büttiker formula [20]:

\[ G(E_F) = \frac{e^2}{\pi \hbar} \sum_{\mu} T_{\mu}(E_F), \quad T_{\mu}(E_F) = \sum_{\nu} |t_{\mu,\nu}(E_F)|^2, \]

where \( t_{\mu,\nu}(E_F) \) is the transmission coefficient from the \( \nu \)th channel in the left lead to the \( \mu \)th channel in the right lead at the Fermi energy \( E_F \) (as shown in figure 1), calculated by a recursive Green’s function method [21], which is given as

\[ G_S = \frac{1}{E - \tilde{H}} = \frac{1}{E - H_C - \Sigma_L - \Sigma_R}, \]

where \( E \) is the Fermi energy, \( \tilde{H} \) is the effective Hamiltonian that equals the sum of the Hamiltonian of the central rectangular ring, \( H_C \), and the self-energies of the semi-infinite leads in the left and right leads, \( \Sigma_L + \Sigma_R \). The key point of the recursion Green’s function method is that the middle conductor region is divided into many meshes, and consequently reduces the dimensionality of the Green’s function greatly. Therefore the computation of the conductance becomes more practical.

The Fermi energy \( E_F \) can be tuned experimentally through electric top- and/or back-gates [22]. In our calculations, all physical quantities are dimensionless, e.g. the energy \( E_F \) and the conductances are in units of \( t \) and \( e^2/(\pi \hbar) \), respectively.

For completeness, here we repeat the essential steps in Ando’s work [21] to obtain the recursive Green’s function \( G_S \). The equation of motion for an ideal lead can be written as

\[ (E - H_0)C_j + TC_{j-1} + T^T C_{j+1} = 0, \]

where \( H_0 \) is the Hamiltonian of a mesh in the ideal lead containing \( M \) lattice sites, \( C_j \) is a vector describing the amplitudes of the \( j \)th mesh, and \( T \) and \( T^T \) are the matrix blocks adjacent to \( H_0 \) in the total tight-binding Hamiltonian matrix. To obtain linearly solutions for equation (4), we first set \( C_j = \lambda^j C_0 \). Substituting this into equation (4) we have

\[ \lambda \cdot C_j = (T^T)^{-1}(H_0 - E)C_j - (T^T)^{-1}TC_{j-1}, \]

leads to the following eigenvalue problem:

\[ \lambda \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix} = \begin{pmatrix} (T^T)^{-1}(H_0 - E) & -(T^T)^{-1}T \\ 0 & 1 \end{pmatrix} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix}. \]

We get the eigenvalues and corresponding eigenvectors, including \( M \) right-going and \( M \) left-going waves. We define the matrix for the eigenvalues and eigenvectors:

\[ U(\pm) = (u_1(\pm), \ldots, u_M(\pm)); \]
Figure 2. (a) Schematic diagram of the double-bend graphene nanoribbon structure. (b) The band structure of the perfect armchair graphene nanoribbon (AGNR) with the same middle conductor width ($N_c$). (c) The conductance as a function of the Fermi energy through the double-bend structure. The black solid and red dashed lines correspond to the different conductor lengths $N_H = 80$ and 160, respectively, while the green line is for the perfect zigzag graphene nanoribbon. (d) and (e) show the density distributions of quasi-bound electron states marked by points A and B in (c) for $N_H = 80$ double-bend structure. $N_L = N_R = 20$ and $N_C = 8$.  

3. Results and discussions

First, we discuss the transport property through the double-bend (S-shaped) GNR structure as shown in figure 2(a) for reference purposes. Figure 2(c) shows the conductance as a function of the Fermi energy for different lengths of the AGNRs. There are the strong peaks in the conductance spectrum corresponding to the resonant tunneling process through the double-bend GNR structure. The underlying physics of such a resonant tunneling process is that there are quasi-bound states in the middle conductor region which consists of the armchair and zigzag nanoribbons. The resonant tunneling occurs when the Fermi energy is equal to the energies of the quasi-bound states. The quasi-bound states arise from the propagation of electrons back and forth in the armchair region between the zigzag leads. The conductance of the perfect ZGNR displays a step-like feature, which corresponds to the opening of the different channels as the Fermi energy increases (see the green line in figure 2(c)). Note that we did not introduce any external electric field and/or gate to generate the barrier in the middle part. Therefore, this feature arises from the geometry effect, i.e. the different edges of the ZGNR leads and the AGNR conductor. As the Fermi energy increases, more incident channels are opened, the effect of the edge state becomes weaker and the ratio between peaks and valleys of the conductance decreases (see the black and red lines in figure 2(c)). When the Fermi energy increases further and even becomes higher than the bottom of the second subband of the middle AGNR conductor (see the black vertical line in figure 2(c)).
the left lead corresponds to the different widths of the right lead for fixed width of the left lead \( N_L = 20 \). The blue vertical lines correspond to the bottom of the second and third subbands for the perfect ZGNR with the same width of the right lead \( N_R = 40 \).

In figure 2(b), the oscillation of the conductance becomes more significant. Figure 2(c) indicates that there are more tunneling peaks as the AGNR length increases. The incident electron can be completely reflected when the incident energy is less than the bottom of the second subband of the left ZGNR lead corresponding to the case of single mode incidence.

To obtain a clear physical picture, we plot the distribution of electron states at specific Fermi energies \( E_F \) corresponding to points A and B marked in figure 2(c). Figure 2 shows the density distribution of the quasi-bound state in the middle AGNR part that contributes to the resonant tunneling (see point A in figure 2(c)). The electrons mainly localize at the edges of the middle AGNR, at the corner between the AGNR and ZGNR leads, and on the edge of the AGNR. This quasi-bound state is quite different from the electron states of a perfect AGNR where no edge state appears due to the two different kinds of carbon atoms at the edges. But for the quasi-bound state the electron state strongly localizes at the edges and especially at one kind of carbon atom (see figures 2(d) and (e)). This special quasi-bound state in the middle part contributes predominantly to the resonant tunneling process. We also plot the density distribution of the quasi-bound state corresponding to the complete reflection case (see point B in figure 2(c)) in figure 2(e). For this case, the electron state localizes at the edge of the left semi-infinite ZGNR lead near the interface between the lead and the middle conductor. In this case, the AGNR conductor can be used as an electron reflector. For the usual graphene nanoribbon, there is no quasi-bound state in the middle region since no armchair nanoribbon is located in between the zigzag leads. Therefore we can only observe the step-like feature of the conductance which corresponds to the opening of the channels with higher energies (see the green line in figure 3(b)).

Next, we show how the width of the right lead affects the resonant tunneling behavior in figure 3. We fix the width of the left lead at \( N_L = 20 \) while tuning the width of the right lead. In figure 3, the black solid, the black dashed and the red dashed lines correspond to \( N_R = 20, 10 \) and 40, respectively. Figure 3(a) demonstrates that the magnitude of the tunneling peaks decreases whether the width of the right lead is wider or narrower than that of the left lead. Thus the electrons cannot be fully transmitted through the nanostructure. The perfect transmission only takes place when the right lead has the same width as the left lead. When the width of the right lead is narrower than that of the left lead (see the black dashed line in figure 3), the first tunneling peak is weakened heavily. When the Fermi energy increases, the magnitude and width of the tunneling peaks increase gradually. These increases are caused by the enhanced coupling between the quasi-bound states in the middle part and the leads. Comparing the case with equal widths of the left and right leads shown in figure 3(a), all tunneling peaks for the wider (narrower) right leads shift to higher (lower) energy and become sparse as the Fermi energy increases. For the wider right lead case, the conductance shows different features. For the Fermi energy below the bottom of the second subband in the right lead (see the first vertical green line), the variation of the magnitude of the tunneling peaks is similar to the case with the narrower right lead. When the Fermi energy is above the bottom of the second subband in the right lead, the magnitude of the tunneling peaks increases abruptly, even approaching 1, and becomes wider (see the red dashed peaks in figure 3(b)). Comparing the conductances through the middle AGNR with different lengths \( (N_R) \) in figure 3, we find that the tunneling peaks become dense as the length \( N_R \) increases. For longer AGNR \( (N_R = 160) \), the variation of the width of the right lead induces changes in the conductance similar to that of the shorter AGNR \( (N_R = 80) \).
one can see that the first kind of resonant peak near $E = 0.05t$ splits into two peaks due to the coupling between the two lowest localized states in the left and right AGNRs through the ZGNR bridge, i.e. the bonding and antibonding splitting. Therefore the resonant peaks split into two peaks and show an anticrossing behavior with increasing length of the ZGNR bridge that describes the coupling strength. The other resonant tunneling peaks are sharper and are located between the strong tunneling peaks mentioned above and vary as the length $N_{TC}$ increases (see figure 5(a)). Those peaks are the result of the resonant tunneling processes through the double barriers, since the corresponding quasi-bound states localize in the ZGNR bridge of the middle conductor. These quasi-bound states mainly distribute in the ZGNR bridge, especially at the two vertical edges of the ZGNR bridge (see figures 6(b) and (c)). In order to make the picture clear, we plot several fitting curves in figure 5(a) which are obtained from the fitting formalism $E = \hbar v_f/\lambda$. The quasi-bound states are caused by the interference of electron waves moving back and forth in the middle region and forming standing waves. The quantization conditions for the bound states are typically given by $n\lambda/2 = L_{TC}$, where $n$ is an integer and $L_{TC} = N_{TC}a$ is the length over which the bound state is formed. Its energy is given by $E = \hbar v_f/\lambda$. So this leads to $E = n\hbar v_f/2L_{TC}$, where $L_{TC}$ is proportional to $N_{TC}$. From these fitting curves we can understand the position of the tunneling peaks correspond to the energies of the quasi-bound states in the middle part. In a word, the fitting curves clearly indicate the quasi-bound states in the middle parts. The spatial distributions of the quasi-bound states show the antibonding (figure 6(b)) and bonding (figure 6(c)) states corresponding to the resonant tunneling peaks B and C marked in figure 6(a). This bonding and antibonding feature also explains why the positions of the resonant tunneling peaks B (C) decrease (increase) as the length $N_{TC}$ increases.

Finally, we investigate the effect of the widths of the right lead on the transport property. We fix the width of the left lead at $N_L = 20$ while tuning the width of the right lead. Figure 7(a) shows the contour plot of the conductance as a function of the Fermi energy $E_F$ and the length of the ZGNR bridge $N_{TC}$ for the width of the right lead $N_R = 10$. The figure shows that the first kind of tunneling peak disappears but the second kind of tunneling peak can still be observed, because the latter is a consequence of tunneling through the quasi-bound states localized in the middle bridge. The effect of the width of the lead on the second kind of tunneling process is much weaker than on the first kind of tunneling process. For the wider right lead $N_R = 40$ in figure 7(b), the situation is similar with $N_R = 10$. But when the Fermi energy is larger

Figure 5. (a) The contour plot of the conductance as a function of the length of the ZGNR ($N_{TC}$) and Fermi energy ($E_F$) for the U-shaped structure. $N_{L(R)} = 20$, $N_{LC} = N_{RC} = 8$ and $N_{RH} = N_{NH} = 80$. The red solid curves are obtained from the fitting formalism $E = \hbar v_f/\lambda$. (b) The conductance as a function of the Fermi energy for the double-bend (S-shaped) GNR structure. $N_{L(R)} = 20$, $N_C = 8$ and $N_H = 80$. The red line denotes the conductance as a function of the Fermi energy for the U-shaped structure at $N_{TC} = 42$.  

Figure 4. Schematic diagram of the U-shaped graphene nanoribbon structures which is composed of two double-bend nanoribbons. The width of the left (right) ZGNR lead is denoted by $N_{L(R)}$ in units of the number of hexagonal units. The width and length of the left (right) AGNR are denoted by $N_{LC}$ and $N_{RH}$, $N_L$ and $N_{TC}$ correspond to the width and length of the bridge GNR (the black frame) connecting the left AGNR and the right AGNR.
than the bottom of the second subband of the right lead, a strong tunneling process appears at $E_F \approx 0.08t$. With a wider or narrower right lead, the second kind of tunneling process displays similar behavior as the length ($N_{TC}$) of the bridge increases. The tunneling processes induced by the quasi-bound antibonding states results in tunneling peaks with an energy that is approximately $0.04t$ higher. Those peaks shift to lower energy as the length of the bridge $N_{TC}$ increases. In contrast, the opposite behavior occurs compared to those induced by the antibonding states, i.e. a blueshift.

4. Conclusions

In summary, we investigated theoretically the transport properties of carriers that move through S- and U-shaped graphene nanoribbons. We found that, as a function of the Fermi energy, the tunneling current can be turned on and off periodically, making this device suitable for transistor action. We demonstrated that resonant tunneling can be realized utilizing the geometrical effect of such bent GNR structures even in the absence of any nanostructured gates. The strong resonant tunneling processes arise from the quasi-bound states that localize at the middle part and can be clearly seen in the conductance spectra. The spectra exhibits rich structures coming from the different kind of quasi-bound states in the middle part. The resonant tunneling processes can be tuned by changing the Fermi energy and the width of the left and right leads. Our theoretical results demonstrate that resonant tunneling can be realized utilizing the geometry of the graphene nanoribbon without any nanostructured electric

Figure 6. (a)–(c) show the density distributions of the quasi-bound electron states corresponding to points A, B and C in figure 5 for the $N_{TC} = 44$ U-type structure.

Figure 7. The same as figure 5(a), but (a) and (b) are for $N_R = 10$ and 20, respectively. The red solid curves are obtained from the fitting formalism $E \sim 1/N_{TC}$. 
gates. We believe that our theoretical results are interesting both for the basic physics and for the potential application of electronic devices based on graphene nanoribbons.

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