Mechanical manipulations on electronic transport of graphene nanoribbons

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Abstract
We study the effects of uniaxial strains on the transport properties of graphene nanoribbons (GNRs) connected with two metallic leads in heterojunctions, using the transfer matrix method. Two typical GNRs with zigzag and armchair boundaries are considered and the tension is applied either parallel or perpendicular to the ribbon axis. It turns out that the electron–hole symmetry is missing in the gate voltage dependence of the conductance data of the armchair GNRs, while it persists in the zigzag ribbons under any strains. For an armchair GNR with a vertical tension applied, a sharp drop of conductance is found near the critical value of the strain inducing a quantum phase transition, which allows one to determine the critical strain accurately via measuring the conductance. In the zigzag ribbon, there exists a range of gate voltage around zero, where the conductance is insensitive to the small horizontal strains. The band structures and low-energy properties are calculated to elucidate the mechanism on the strain effects in GNRs. We expect that our results can be useful in developing graphene-based strain sensors.

Keywords: transport through graphene, strain effect, graphene nanoribbon

(Some figures may appear in colour only in the online journal)

1. Introduction

Graphene has attracted widespread interest both theoretically and experimentally since its discovery in 2004, because of its unique properties and promising applications [1–3]. Recently, there have been many studies on its mechanical deformation [4, 5] and the corresponding effects on the Raman spectroscopy [6], since strain is inevitable for the fabrication of graphene on substrate. Unlike the conventional materials, graphene has a tough mechanical property and could sustain elastic deformation up to 15 ~ 20% [7, 8]. There are two typical ways to control the strain in graphene samples [6, 7]. One way is using the substrate with an array of holes with diameter ranging from 1 µm to 1.5 µm. When a free-standing monolayer graphene is transferred onto it, a nonlinear strain–stress relation is observed by nanoindentation in the atomic force microscope [7], which has been verified theoretically [8]. The other one is by exerting tension on the substrate to control the strain on the graphene [6, 9, 10]. Graphene ripples on polydimethylsiloxane(PDMS) substrate can afford a reversible structural deformation under tensile strains as large as 20 ~ 30% [11].

At atomic scale, the C–C bond length is changed by the strain, as are the hopping integrals and the band structure of graphene. To open a band gap in graphene, one requires a uniaxial strain in excess of 20%, which is beyond the range of elastic deformation [12]. In contrast, a much smaller uniaxial strain can control (close or open) the band gap in narrow armchair graphene nanoribbons(AGNRs), while the zigzag graphene nanoribbons(ZGNRs) are quite robust against gap opening for small strain [13–15].

In recent years, the field of graphene-based strain sensors has developed rapidly, since it is feasible to mediate electronic properties of graphene by applying tensions. In a sample
of graphene from chemical vapor deposition, the resistance remains around 7.5 KΩ under strain less than 2.47% applied along the electronic transport direction, and increases rapidly to 25 KΩ under 5% strain [9]. This is because the ripples in graphene do not disappear until the strain exceeds 2.47%. The strain dependent transport properties enable graphene to have potential applications in the fields of the displays, robotics, fatigue detection, body monitoring and so forth. For instance, graphene-based strain sensors on transparent gloves can measure the magnitudes and directions of the principal strains on the glove induced by the motion of fingers [10].

Previous theoretical investigations on the transport properties of strained graphene nanoribbons [16–22] mostly deal with small-scale GNRs with a width of about several nanometers using homojunction contacts, while one may encounter more complicated situations in practice, e.g. heterojunction contacts and wider GNRs in the fabrication of GNR-based nanodevices. In this paper, we utilize a transfer matrix method [23] to study the transport properties of both narrow and wide GNRs under the strain, which are in particular connected to two metallic leads with heterojunctions. The width of graphene can reach the order of microns by means of the transfer matrix method [23]. A tight binding model is taken to describe the low energy physics for both π-electrons of graphene and metallic electrons in two leads. The effects of strains on the hopping integral of C–C bonds in graphene are elucidated in section 2. The band structures of AGNRs and ZGNRs for various sizes under different strains are presented in section 3. In section 4, we show the effects of strains on the transport properties of both AGNRs and ZGNRs. The edge effects on the conductance are discussed in section 5. We note that strain only affects the band structure of graphene, while the electronic transport of strained graphene in this paper essentially embodies the combined effects of strains and the heterojunctions composed of graphene and metallic contacts.

2. Model and method

2.1. Strained graphenes

To investigate the influence of uniaxial strain on the electronic transport properties of GNRs, we connect it with semi-infinite quantum wires, which are characterized by the square lattices, as illustrated in figure 1. Each interface between the GNR and a lead is a heterojunction. For AGNRs in figure 1(a), the interface is a ring consisting of five atoms, which eventually breaks the electron–hole (e–h) symmetry of the system, while for ZGNRs in figure 1(b), each ring at two interfaces contains four or six atoms which retains the e–h symmetry since the tight binding model involves only the nearest neighbor hopping in this paper. This is revealed by the dependence of conductance on gate voltages, as shown later. The uniaxial tension is only applied to the GNRs leading to the deformation of C–C bonds in an anistropic way.

The strain–stress relation for graphene is given in [12]. We quote those relevant results here for our further discussions.

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this direction are $S$ and $-vS$, respectively, with the Poisson’s ratio $v = 0.165$ [24]. In the lattice coordinate system the strain tensor reads
\[
\epsilon = S \begin{pmatrix}
\cos^2 \theta - v \sin^2 \theta & (1 + v) \cos \theta \sin \theta \\
(1 + v) \cos \theta \sin \theta & \sin^2 \theta - v \cos^2 \theta
\end{pmatrix}.
\]
(1)

For any vector $\vec{l}_0$ in the undeformed graphene plane, it is straightforward to obtain its deformed counterpart to the leading order by the transformation
\[
\vec{l} = (1 + \epsilon)\vec{l}_0.
\]
(2)

The hopping amplitude $t_i$ with $i = 1, 2, 3$ as defined in figure 1 is determined by the corresponding bond length $\delta_i$ via the following formula [12]
\[
t_i = t_0 e^{-3.37(\frac{\delta_i}{\delta_0} - 1)},
\]
(3)

with $t_0 = 2.6$ eV and $a = 1.42$ Å for the undeformed graphene. The bond length $\delta_i$ under the strain can be calculated by equations (1) and (2). Without loss of generality, we focus on two cases with $\theta = 0$ and $\pi/2$ as follows.

- For $\theta = 0$ shown in figure 1(c),
\[
\delta_1 = \delta_3 = (1 + \frac{1}{2} S - \frac{3}{4} vS) a, \quad \delta_2 = (1 + S) a.
\]

All three bond lengths increase as $S$ increases and the $t_i$s subsequently decrease for all $i = 1, 2, 3$. However, $\delta_2$ increases faster than $\delta_1$ and $\delta_3$. Therefore, we have $t_1 = t_3 > t_2$ as long as $S > 0$.

- For $\theta = \pi/2$ shown in figure 1(d),
\[
\delta_1 = \delta_3 = (1 + \frac{3}{4} S - \frac{1}{4} vS) a, \quad \delta_2 = (1 - vS) a.
\]

In this case, we also have $\delta_1 = \delta_3$ and $t_1 = t_3$. As $S$ increases, $\delta_1$, $\delta_3$ increases, while $\delta_2$ decreases. It turns out that $t_1$ and $t_3$ decrease and $t_2$ increases with increasing $S > 0$.

For ZGNRs, the lattice coordinate system is rotated by $\pi/2$ from that of AGNRs. Therefore, the strain effect on the hopping amplitudes for ZGNRs with $\theta = 0$ (or $\pi/2$) is identical to that for AGNRs with $\theta = \pi/2$ (or 0). The hopping amplitudes $t_i$s as functions of $S$ are plotted for AGNRs in figure 2(a), in the unit of $t_0$, which is set as one in the following discussions.

### 2.2. Tight-binding model and transfer matrix method

The $\pi$-electrons of carbon atoms are responsible for the low energy physics of graphene which can be described by the tight binding model on the honeycomb lattice
\[
\hat{H} = \sum_{(ij,j')} t_{ij,j'} c_{ij}^\dagger c_{j'}, + V_g \sum_{ij} c_{ij}^\dagger c_{ij},
\]
(4)

where a pair of integers $ij$ indicates the lattice position $\vec{R}_{ij} = x_i \vec{e}_x + y_i \vec{e}_y$ and $c_{ij}^\dagger$ ($c_{ij}$) is the corresponding electron annihilation(creation) operator. The summation is over the nearest neighbors indicated by $(\cdot,\cdot)$ and $t_{ij,j'}$ is the hopping amplitude which takes the value of $t_1$, $t_2$ or $t_3$ depending on the relative position $\vec{R}_{ij} = \vec{R}_{ij'}$. The spin indices of electrons are omitted simply for convenience. $V_g$ is the gate voltage which is applied only to the GNRs, not on the leads. In our simulation, we consider a simplified case with $V_g$ changing abruptly at the interfaces between the GNR and the leads. In fact, this simplification is reasonable for small $V_g$. For large $V_g$, there may exist a junction between the leads and GNR with finite width of several atoms. This situation would not be considered here, since it only incurs further unnecessary complexities as far as the strain effects are concerned.

The left and right electrodes are also described by the Hamiltonian in equation (4) with $V_g = 0$, but the lattice vectors $\vec{R}_{ij}$ describe a rectangular lattice instead of the hexagonal one. All the hopping integrals in the leads are fixed as $t_0$, despite that the vertical lattice constants may not be uniform in the leads connected to ZGNRs, as shown in figure 1(b). We also assume the leads are unaffected by the strain in our numerical simulation. This idealized setup mimics a normal-metal/GNR heterojunction, by which we shall demonstrate the strain effects on the transport through GNRs.

The single-particle eigenstate with energy $E$ can be expressed as $\hat{\psi}^\dagger(E) = \sum_{ij} \alpha_{ij} c_{ij}^\dagger$, which satisfies $[\hat{\psi}(E), \hat{H}] = E \hat{\psi}(E)$, leading to
\[
(E - V_g)\alpha_{ij} = \sum_{(j,j')} t_{ij,j'} \alpha_{j'},
\]
(5)

The wavefunctions of the electrons can be represented in terms of two numbers $k_x$ and $k_y$, where $k_x$ describes the plane wave traveling along the $x$ direction and $k_y$ is quantized as $k_{y,n} = n\pi/(M + 1)$ with $n = 1, 2, \ldots, M$ due to the open boundary condition imposed in the $y$ direction, to characterize different channels. The corresponding eigenenergy reads
\[
E = 2t_0 (\cos k_{y,n} + \cos k_{x,n}),
\]
(6)

which determines the wave number $k_{x,n}$ in $n$-th channel for the given Fermi energy $E$. Note that since the hopping amplitudes of all the bonds are given, the lattice constant is not needed anymore and one can simply use dimensionless wave numbers $k_{x,n}$ and $k_{y,n}$ to label the quantum states.

If we assume the electrons are incident from the left, the wavefunctions in the left and right electrodes can be written as [23, 25]
\[
\alpha_{ij}^L = \sum_{n} \left( \eta_{n} e^{i k_{x,n} x_{i}} + \eta_{n}^{*} e^{-i k_{x,n} x_{i}} \right) \sin(k_{y,n} y_{j}),
\]
\[
\alpha_{ij}^R = \sum_{n} \left( \eta_{n} e^{i k_{x,n} x_{i}} - \eta_{n}^{*} e^{-i k_{x,n} x_{i}} \right) \sin(k_{y,n} y_{j}),
\]
(7)

where $t_{n,n}$ and $r_{n,n}$ are the transmission and reflection amplitudes from $n$-th to $n$’-th channel, respectively. Current conservation requires $\sum_{n} |\eta_{n,n'}|^2 + |r_{n,n'}|^2 = 1$ for each $n$ with $\eta_{n,n'} = |\sin(k_{y,n})|/|\sin(k_{y,n'})|$. In order to calculate the transmission coefficients $t_{n,n'}$, we adopt the transfer matrix method developed in [23] and then we can designate $\alpha_{ij}$ for the
$M$ coefficients with column index $j$, which satisfies the matrix equation

$$\begin{pmatrix} \alpha_j \\ \alpha_{j+1} \end{pmatrix} = \chi_j \begin{pmatrix} \alpha_{j-1} \\ \alpha_j \end{pmatrix},$$  

(8)

where $\chi_j$ is the $2M \times 2M$ transfer matrix as a function of Fermi energy $E$, gate voltage $V_g$, and the hopping amplitudes $t_i$. By acting on the transfer matrices consecutively, the coefficients in the left and right interfaces are connected in the following form

$$\begin{pmatrix} \alpha_N \\ \alpha_{N+1} \end{pmatrix} = \chi_N \chi_{N-1} \cdots \chi_2 \chi_1 \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}.$$  

(9)

Combining equations (7) and (9) one can obtain the transmission and reflection coefficients $t_{n,n}$ and $r_{n,n}$. In order to investigate the transport properties of the large scale GNRs, we actually utilize the renormalized transfer matrix method as described in [26]. It is straightforward to calculate the conductance by employing the Landauer–Büttiker formula

$$G = \frac{2e^2}{h} \sum_{n,n+1} \eta_{n,n} |t_{n,n}|^2,$$  

(10)

where the factor 2 is a consequence of the spin degeneracy.

### 3. Band structure of strained graphene nanoribbons

In this section, we study the band structure and low energy excitations of GNRs under strain by solving the tight binding model equation (4) with the hopping amplitudes given by equation (3). For convenience, we impose the periodic boundary condition along $x$-axis and the open boundary condition along $y$-axis and the energy $E$ is taken in units of $t_0$ in the following discussions. We also assume the horizontal lattice spacing to be unit so that $k_x$ is always in the interval $[0, 2\pi]$, although it changes as the tension is applied.

#### 3.1. Strained AGNRs

The spectra of AGNRs are plotted in figures 2(b)–(f) as functions of $k_x$ with $N = 100$ and $M = 100$ for different strains. The unstrained data is given in figure 2(b) which is precisely gapless at $k_x = 0$. In the presence of strains, the spectrum changes upon the direction of the applied tension. When the tension is applied horizontally to AGNRs, the spectra in figures 2(c) and (e) are similar to the unstrained case, except that the uniaxial strain may open a small gap at $k_x = 0$. This gap is proportional to $M^{-1}$ and becomes almost invisible for $M = 100$, which results from the combined effect of the finite ribbon widths and the strains. When the tension is applied vertically, i.e., $\theta = \pi/2$, the spectrum in figure 2(d) with strain $S = 0.15$ shows a tiny gap, which is also proportional to $M^{-1}$ with the same origin of that for $\theta = 0$. For $S = 0.3$, another type of gap opens at $k_x = 0$ as shown in figure 2(f), which is induced entirely by the strain [12] and can survive the thermodynamic limit unlike the previous gaps. In fact there is a critical strain $S$ separating the two different gaps, as discussed in detail later.

Figures 2(g) and (h) show the density of states (DOS) $\rho(E)$ for AGNRs under different strains for $\theta = 0$ and $\pi/2$, respectively. The band width is $D = 2t_1 + t_2$ plus a negligible dependence on the ribbon width, which obviously shrinks as $S$ increases for both $\theta = 0$ and $\theta = \pi/2$, although $t_1(t_3 = t_1)$ and $t_2$ behave very differently as functions of $S$ in figure 2(a). When $\theta = 0$, $t_1$ and $t_2$ are decreasing functions of $S$ so is the band width. When the strain increases for $\theta = \pi/2$, $t_2$ increases, but it is the decreasing $t_1$ that dominates the strain dependence of the band width. Besides the shrinking band width, there are no other common features in the DOS for both cases with $\theta = 0$ and $\theta = \pi/2$. For the unstrained ribbons, there are two peaks of DOS located at $\pm t_0$. Each of them splits into double peaks if the tension is applied horizontally, which locate at $\pm t_2$ and $\pm (2t_1 - t_2)$, as seen in figure 2(g). When the tension is applied vertically, the peaks at $E = \pm (2t_1 - t_2)$, except two shoulders emerging at $\pm 0.5t_0$ for $S = 0.1$ as a remnant of the peaks. For other strains in figure 2(h), even the shoulders cannot be seen. When the strain $S = 0.3$, the DOS vanishes in the energy range $[-0.205, 0.205]$ implying a gap of 0.409($t_0$) opens.

Now we turn to the dependence of energy gaps at $k_x = 0$ on the ribbon widths and strains. For the unstrained AGNRs, the gap is zero for $\text{mod}(M, 3) = 1$ and inversely proportional to $M$ for $\text{mod}(M, 3) = 0, 2$, which coincides with previous studies using the first-principle calculation [27] and the tight binding model [23, 28]. This feature is manifested in figures 3(a)–(d) for $M = 10, 11, 12, 49$ and 100 with a fixed ribbon length $N = 100$.

When the tension is applied horizontally with different ribbon widths, the band gaps oscillate with the strains in similar zigzag patterns, but with different ‘phases’ according to different values of $\text{mod}(M, 3)$, as shown in figure 3(a). The oscillatory amplitude is inversely proportional to $M$ and barely changes with $S$ and the oscillatory frequency increases with $M$, but decreases with $S$ as shown in figure 3(c).

For $\theta = \pi/2$, as shown in figures 3(b) and (d), the band gap behaves significantly differently from that for $\theta = 0$. The oscillation only happens for $S < S_c$. In this region, the oscillatory amplitude decreases with both $M$ and $S$, while the frequency increases with both $M$ and $S$. The band gaps for both $\theta = 0$ and $\theta = \pi/2$ result from the combined effects of the strains and the finite ribbon widths. Actually, they are almost invisible in figure 3(e) for $M$ as large as 1000. The essential difference occurs for $S > S_c$, where a gap opens for the $\theta = \pi/2$ with a dominant linear dependence on $S - S_c$ in the thermodynamic limit. This is demonstrated with the finite-$M$ scaling for different values of $S$ in figure 3(f).

In fact, for AGNRs with vertical strains, the gap opening implies a quantum phase transition occurring at $S = S_c$ from a Fermi liquid to a dimerized solid phase. As shown in figure 2(a), $t_2$ increases and $t_1$ decreases with increasing $S$ for $\theta = \pi/2$, which eventually leads to the dimerized $t_2$-bonds with an energy gap $\Delta = 2|t_2 - 2t_1|$ opening. The
critical strain $S_c = 0.235$ can be determined by solving the equation $\Delta(S) = 0$, or equivalently $t_2(S) = 2t_1(S)$ [12]. It is then understandable that the gaps of AGNRs with finite widths diminish to zero as $S$ approaches $S_c$ from the left, since a quantum phase transition occurs there. For $\theta = 0$, all $t_i$ decrease with $S$ monotonically and $t_2$ decreases even faster, hence there is no phase transition at all.

3.2. Strained ZGNRs

In this subsection, we discuss the band structure of ZGNRs with the periodical boundary condition in $x$ direction and open boundary condition in the $y$ direction. Figure 4(a) is the band structure of unstrained ZGNRs, which shows a midgap flat band corresponding to the edge states [29] localized in the

![Figure 2](image-url)

Figure 2. (a) shows the strain dependence of the three hopping amplitudes. (b)–(f) are the band structures of AGNRs with $N = M = 100$ under various strains. (g) and (h) are the density of states $\rho(E)$ of AGNRs with $M = 100$ and $N = 1600$ for the tensions along $x$ and $y$ axis, respectively.
upper and lower zigzag boundaries. The flat band exists in a finite region of momentum \([k_x, 2\pi - k_x]\) with \(k_x = 2\pi/3\) for the unstrained ribbon determined by the convergent condition for the wavefunction of the edge states \(2 \cos(k_x/2) \leq 1\) [29].

When the tension is applied, apart from those effects on the valence and conduction bands, the region of the momentum for the flat band is also affected by strain, as seen in figure 4. For the horizontal strain of \(\theta = 0\), as shown in figures 4(c) and (e), \(k_x\) moves towards zero with increasing \(S\) until \(S = S_c\), after that \(k_x = 0\) and the flat band with zero energy extends over the whole Brillouin zone accompanied by the conduction and valence bands detached from each other. \(S_c\) is the same as that defined for AGNRs in the previous subsection which signals the dimerization of the \(t_2\)-bonds. In contrast, for the vertical strain of \(\theta = \pi/2\), \(k_x\) moves toward \(\pi\) with increasing \(S\) and the flat band shrinks into a single point with \(k_x = \pi\) in the large \(S\) limit as shown in figures 4(d) and (f).

In fact, the range of the momentum for the flat band is given by the convergent condition on the wave function, which requests \(|2t_1/t_2 \cos(k_x/2)| \leq 1\) leading to \(k_x = 2 \cos^{-1}(t_2/2t_1)\) [13]. We plot \(k_x\) and \(t_2/t_1\) as functions of strain \(S\) in figure 4(b). When \(\theta = 0\), \(t_2/(2t_1) \leq 1\) holds only for \(S \leq S_c = 0.235\), where \(k_x\) has a solution between 0 and \(\pi\). If \(S > S_c\), \(t_2/(2t_1) > 1\) and the convergent condition holds for all possible momentum \(k_x\), therefore, the flat band extends throughout the whole Brillouin zone. When \(\theta = \pi/2\), \(t_2/(2t_1) \leq 1\) is satisfied for any positive \(S\). In this case, \(k_x\) always has a solution between 0 and \(\pi\). We note that the flat band can shrink into a point with \(k_x = \pi\) if \(t_2 = 0\), which corresponds to the horizontal \(t_2\)-bonds broken and the ribbon becomes \(M\) independent carbon chains connecting the left and right electrodes.

The edge states are also revealed by the zero energy peak in the DOS shown in figures 4(g) and (h). As the tensile strain increases, the peak intensity is enhanced for \(\theta = 0\), while it is suppressed for \(\theta = \pi/2\). This coincides with previous analysis for the region of momentum allowed for the edge states. Similar to the AGNRs, the band width \(D = 2t_1 + t_2\) with a minor correction proportional to \(M^{-1}\), which also shrinks with increasing \(S\). In fact, except for the additional zero energy peaks, the characteristics of \(\rho(E)\) for ZGNRs under the uniaxial strains with \(\theta = 0\) (or \(\theta = \pi/2\)) are quite similar to those for AGNRs with \(\theta = \pi/2\) (or \(\theta = 0\)), including the positions of the shoulders for \(S = 0.1\) and of double peaks, since the lattice coordinates of ZGNRs can be obtained from those of AGNRs rotated by \(\pi/2\).
4. Transport properties of graphene nanoribbons

The interplay between the strain and the finite size effect leads to the fine-tuning of the band structures of GNRs as presented in the previous section. This allows GNRs to be considered as a promising candidate for mechanically controllable electronic nano-devices. In this section, we use the transfer matrix method described in section 2.2 to explore in detail the transport properties of strained GNRs with various sizes and gate voltages as well. The transport properties essentially depend on both the band structures of GNRs and two leads. Transport results discussed in this section are expected to bring...
some insights into the designation of GNR-based nano-devices for experimentalists.

4.1. Conductance of strained AGNRs

We first discuss the conductance $G$ of neutral GNRs, i.e., the gate voltage $V_g = 0$. As discussed in section 3.1, the band gaps oscillate with the strains and ribbon widths, which signals one sort of the metal-semiconductor transition \[16, 18\]. This results in that the conductances in figure 5 also oscillate accordingly, where the conductance peaks are precisely located at the gapless points of figure 3.

Figures 5(a) and (b) show the conductances for the narrow ribbons with $M \leq N$. When $M$ is small enough, say $M = 10$, all the maxima of $G$ equal $2e^2/h$, which implies that only one effective conducting channel is maximally opened due to the strong confinement in the $y$ direction. As the ribbon width increases from 10 to 400, as shown in figures 5(a)–(d), more and more channels are involved in the electronic transport, leading to the enhancement of the conductance.
In fact $G$ is almost linear in $M$ for AGNRs with fixed lengths, which is reflected by the universal strain dependence of $G/M$ in figures 5(e) and (f). Besides the ribbon width, the hopping amplitude $t_2$ also has a positive correlation with the conductance. As one can see in an extreme situation as indicated by the geometry of AGNRs in figure 1, that if $t_2=0$, the electronic transport would be completely shut down. At the same time $t_2$ is controlled by the strain, which monotonically decreases for $\theta=0$ and increases for $\theta=\pi/2$ when $S$ increases, as shown in figure 2(a). This explains the strikingly different strain dependence of the conductance in figure 5(c) for $\theta=0$ and in figure 5(d) for $\theta=\pi/2$ (with $S<S_c$), respectively. Figures 5(a)–(f) also indicate that the conductance oscillation is greatly suppressed in wider ribbons. For the ribbons with the same size, the oscillation is obviously more violent under horizontal strain than under vertical.

It is interesting to note that when $\theta=\pi/2$, the conductance of AGNRs vanishes completely in the region $S>S_c$ for any widths. This is because a gap is opened in this region mainly by the uniaxial strain, on which the ribbon width has little effect. In fact there is a quantum phase transition occurring at the critical strain $S_c$, as we have discussed in section 3.1. Correspondingly, we find a $\lambda$-like in the strain dependence of the conductance in figures 5(d) and (f). The sudden drop of the conductance is expected to be useful in the identification of the tension-driven phase transition, as well as the determination of the critical strain accurately via electronic measurements.

To further understand the electronic transport features of AGNRs, we plot the transmission probability $T_k(\kappa)\equiv\sum_{\kappa'}\eta_{\kappa',\kappa'}|t_{\kappa',\kappa}|^2$ [23] under different circumstances as functions of $\kappa$ in figure 5(g) for $\theta=0$ and figure 5(h) for $\theta=\pi/2$. One can see then $T_k$ has a spike at the momentum $k_s$, which is exactly the onset momentum of the flat band in the spectra of ZGNRs with the same strain, as seen in figure 4. In fact, the interface between each lead and the AGNR has a zigzag pattern, where localized states might exist similar to the edge states in ZGNRs. As long as $k_s$ is close enough to $k_z$, the localization length is comparable to the ribbon length [29–31]. Therefore, the corresponding quantum states extend from the left lead to the right one, giving the major contributions to the conductances. For $\theta=0$, the peak position $k_s$ moves from $2\pi/3$ towards $\pi$ and the peak height decreases with increasing $S$. However, when $\theta=\pi/2$, $k_s$ moves towards zero and the height increases slightly as $S$ increases, until $S=S_c$. After that, the peak position shifts backward and the height drops rapidly when $S>S_c$. For $S=0$, the analytic $T_k$ obtained in [23] gives rise to $G/N=M=4e^2/3h$ at $V_g=0$ as $N,M\to\infty$ and $M/N\gg1$. This finite value is the maximal value for $\theta=0$ and all $S$, but the minimal value for $\theta=\pi/2$ and $S<S_c$.

Figure 6 with $M=N=100$ shows the overall features of the conductance as a function of the gate voltage for AGNRs. One can see that the conductance is not symmetric with respect to $V_g=0$, revealing an e–h asymmetry, which has been observed in many experiments [1–3]. This is a direct consequence of using ordinary metallic leads [23]. It is well-known that a tight binding model on a bipartite lattice with only nearest neighbor hopping is e–h symmetric. In the present system, the interface between each lead and the AGNR consists of five-atom rings, which cannot be bipartite well-known that a tight binding model on a bipartite lattice with only nearest neighbor hopping is e–h symmetric. In the present system, the interface between each lead and the AGNR consists of five-atom rings, which cannot be bipartite.
Figure 7. The conductance of AGNRs for the vertical strain $S = 0.3 > S_c$ with various lengths $N$ and widths $M$. The size parameters: (a) $M = 100$ and $N = 400, 800$ and $1600$; and (b) $N = 500$ and $M = 100, 300$ and $500$. Inset in (b): the conductance scaled by the width $M$.

Figure 8. The conductance of ZGNRs as a function of the gate voltage $V_g$ under various strains: (a) and (c) for $\theta = 0$; (b) and (d) for $\theta = \pi/2$. The size parameters: (a) and (b) for $N = 100$ and $M = 101$; (c) and (d) for $N = 100$ and $M = 901$.

the armchair edges, since there is no impurity and disorder in the present system. The edges reflection of AGNRs can be suppressed relatively by increasing the width, as demonstrated in figures 6(c) and (d) with $M = 1000$, especially for small gate voltage and strains. The remaining fluctuations in figures 6(c) and (d) should be attributed essentially to the scattering on the lead-ribbon interfaces.

In figure 6(a) for $\theta = 0$, the conductance curves are rather smooth for $V_g < 0$ and show a cusp at $V_g = 2t_1 - t_2 > 0$ corresponding to the higher energy peak of $\rho(E)$ in figure 2(g) and move outwards as $S$ increases. However, the lower energy peak of $\rho(E)$ at $E = t_1$ shows no evidence in the conductance curves. When $\theta = 0$, the conductances are suppressed by increasing $S$ for all $V_g$, as observed in previous studies [9, 10]. As a contrast, when $\theta = \pi/2$, the conductance in figure 6(b) shows a more complicated $V_g$-dependence, which reflects the significant differences between the strain dependences of the band structures in the two cases. When $S$ increases but is still smaller than $S_c$, we find the conductance dome in the negative energy region, an abrupt increase for $0 < V_g < 2t_1 - t_2$, a gentle slope for $2t_1 - t_2 < V_g < t_2$ and finally a decreasing region for $V_g > t_2$. Although the hopping amplitudes $t_i$ shift with $S$, we can still claim that, $G$ is an increasing function of $S$ for small $V_g$ and a decreasing function for large $V_g$. When $S > S_c$, a gap $\Delta$ opens and $G$ vanishes for $V_g > \Delta$ and is suppressed by increasing $S$ for any $V_g > \Delta$ as can be seen in figures 6(b) and (d).

Figures 7(a) and (b) show more details on $G$ for $S = 0.3$ and $-0.5t_0 < V_g < 0.5t_0$. The conductance is zero for
−0.2t_0 < V_g < 0.2t_0, which indicates Δ = 0.4t_0 for S = 0.3 in consistency with that from the direct calculation given in figure 3(e). Figure 7(a) also implies that as N ≥ 400 the conductance barely changes with increasing N due to the ballistic transport. Figure 7(b) shows the dependence of the conductance on M and its inset reveals the universal behavior of renormalized conductance G/M.

4.2. Conductance of strained ZGNRs

Figures 8(a)–(d) display the conductance of the ZGNRs as a function of V_g with various S and M for fixed N = 100. In particular, figures 8(a) and (b) with M = 101 show the overall features of G in the full range of the band width, while figures 8(c) and (d) with a larger M = 901 demonstrate less conductance fluctuations for |V_g| ≤ 1.0. The conductance data obviously shows the e–h symmetry, unlike the AGNRs case. This is because the whole system is still bipartite since those rings on the interfaces between the leads and ZGNR contain either four or six atoms, as seen in Figure 1(b), in contrast to the non-bipartite five-atom rings on the interfaces in the system of AGNRs. It thus seems that all the features of the conductance are essentially consistent with the DOS for ZGNRs in figure 4. It is also remarkable that the conductance is a constant around G_0(G_0 ≡ 2e^2/h) or vanishingly small at zero gate voltage in the large N and M limit and the flat band is apparently not involved in electronic transport, even at V_g = 0. This feature is unchanged under the strains and we will discuss it later.

In figure 8(a) for θ = 0, two sharp peaks of the conductance for each different strain correspond to the peaks of ρ(E) at E = ±t_2 in figure 4(g), which move outwards when the strain increases. It is interesting to note that in figures 8(a) and (c) the conductance for S = 0.1 is almost identical to that for S = 0 in the region |V_g| < 0.5t_0. In fact this phenomena emerges for any given strain S < S_0 = 0.235 and the overlapping region between G(S) and G(0) is given by |V_g| < 2t_1 − t_2 which is obviously strain dependent. In other words, given a small V_g, the relation |V_g| = 2t_1 − t_2 gives rise to a threshold of strain, below which the measured conductance barely changes with respect to S. Despite this identical region, figure 8(a) for θ = 0 also indicates that the conductance is reduced with increasing S if the gate voltage is fixed. Figures 8(b) and (d) show the conductance for θ = π/2, where we find a cross point of the conductance curves under different strains. For convenience we denote the corresponding gate voltage as V_g^C which is around 1.5t_0. The strain enhances the conductance for |V_g| < V_g^C and suppresses it otherwise.

To interpret the difference of the conductances between θ = 0 and θ = π/2, we recall that the hopping integrals t_1,s have different strain dependence, as seen in figure 2(a). When the strain increases for θ = 0, t_2 increases, while t_1,3 decreases. However, t_1,3 effectively favors the horizontal electronic transport, while t_2 may cause the formation of the dimers for vertical bonds which hinders the electrons from moving freely. Therefore, the conductance is reduced by increasing the strain for given V_g. However, for θ = π/2, both t_1,3 and t_2 decrease, but t_2 drops faster. As a consequence, the ribbon tends to form M metallic chains with a weak interchain coupling. The conductance is then enhanced with an upper limit MG_0 as t_2 → 0 for small V_g. Since more and more channels below V_g^C are fully filled due to the reduction of the hopping amplitudes t_1,3, they do not contribute to the conductance for large gate voltage. It turns out that there are two turning points ±V_g^C in figure 8(b) and opposite strain dependences of the conductance are found for |V_g| < V_g^C and for |V_g| > V_g^C, respectively.

For ZGNRs, the topology of structure not only protects the e–h symmetry of the electronic transport but also stimulates the analysis of more general features of the conductance in a whole range of t_2/t_1, which might be beyond the values given by the relations equation (3). In principle, one has actually two limits: t_2/t_1 ≫ 1 and t_2/t_1 ≪ 1. For the former case, the system possesses an ordered and insulating ground state consisting of dimerized t_2-bonds, which already emerges actually with a zero conductance at t_2/t_1 ≳ 2.9 for M = 101 and N ≳ M as demonstrated in figures 9(a) and (b). When t_2/t_1 ≪ 1, the honeycomb lattice becomes M weakly coupled metallic (zigzag) chains and the conductance reaches its maximal value MG_0, as seen in figure 9(a), where the conductance is shown.
as a function of $t_2/t_1$ for $N = 100$ with $M = 101, 201$ and 401. One can see that $G$ is enhanced by decreasing $t_2/t_1$ and indeed proportional to $M$ as being well renormalized by $M$ for $t_2/t_1 \ll 0.05$ in the inset. Figure 9(b) shows that the conductance is also reduced by increasing the length of ribbons, implying a non-ballistic transport. In addition, the conductance fluctuations around $G_0$ show up for $t_2/t_1 \geq 0.1$.

Figure 10 shows an even–odd $M$ effect on $G$ for ZGNRs, which is relevant for either experiments or designing nano-devices with narrow and short ribbons. This effect diminishes for sufficiently wide and long ribbons so that our above discussions for figures 8 and 9 are given just for odd but sufficiently large $M$. For $S = 0$ and $V_g = 0$, one finds that the conductance of narrow ZGNRs shows two different scaling behaviors according to the parity of $M$ as $N \to \infty$ [32, 33].

The conductance is a constant around $G_0$ for odd $M$ to indicate metallic nature, while $G \sim N^{-2}$ for even $M$ to present a semiconducting feature [30]. In the presence of strains, one can still find two types of scaling behaviors for the conductance at $V_g = 0$, as shown in figures 10(a) and (b). When $M$ is odd, the conductance changes a little with both $N$ and $S$. When $M$ is even, although the conductance decreases in a power law $N^{-2}$, $G$ is suppressed for $\theta = 0$ and enhanced for $\theta = \pi/2$ with increasing $S$ if $N$ is fixed.

5. Edge effects

In realistic situations, there may exist passivation and spin polarization on the ribbon edges, which affect the band structure of narrow ribbons [28]\(^6\). One can expect that the edge effects diminish when the width of ribbons becomes sufficiently large, since the hopping integrals should be effectively modified for those sites near the edge. On the contrary, the strain can affect all the carbon–carbon bonds in the ribbon. It turns out that the effect of strain dominates over that of the edge relaxation on the band structures of AGNRs, except for the edge states. In fact, as can be seen in figure 3, the band gaps of AGNRs oscillate with the strain and the oscillatory amplitude can be as large as $0.25t_0$ for ribbons with width $M = 10$, while the edge relaxation can only open a gap around $0.032t_0$ for the same ribbon according to the first-principle calculation given in [28]\(^7\).

Usually, the transport properties at finite $V_g$ are governed by the vast bulk electrons rather than those at the edges so that the edge relaxation has relatively small effect on the transport properties in wide graphene ribbons. Figure 11 shows the conductances as functions of $V_g$ for both pristine GNRs (black lines) and those with edge relaxation (red lines). The edge relaxation is simulated by tuning the hopping integral $t_e$ and on-site energies $\epsilon_{0e}$ at the edges. For AGNRs, we take $t_e = 1.12t_0$ as suggested in [38] and $\epsilon_{0e} = 0.3t_0$. According to the tight binding parameters of ZGNRs, as shown in [34], $t_e$ is close to $t_0$ and the difference between $\epsilon_{0e}$ and on-site energies of other carbon atoms reaches $0.259t_0$. Here we set $t_e = 1.05t_0$ and $\epsilon_{0e} = 0.3t_0$ for ZGNRs. The ribbon width is taken to be larger than 10 nm ($M > 42$). One can clearly see that the effect of edge relaxation on the electronic transport is negligible as anticipated.

Finally, we discuss the relevance of the edge spin polarization in the ZGNRs, which requires the introduction of Coulomb interaction into the flat edge band. The edge magnetic moments modify the midgap states near the zero energy [28]\(^9\) and affect the conducting channels localized on the edges. The magnitude of edge magnetic moments can also be reduced by thermal fluctuations at finite temperature. Therefore, it is reasonable to expect that their effects on the

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6 See footnote 5.
7 See footnote 5.
8 See footnote 5.
9 See footnote 5.
transport through ZGNRs should also be less important than the strain which affects all the bulk channels for the transport properties. For convenience, we are allowed to ignore the edge effects when we investigate the strain effects on the transport properties.

6. Summary and conclusions

In this article, we have investigated the electronic transport of graphene nanoribbons under various tensile strains with connections to the normal metallic leads. For this purpose, we first calculated the band structures of strained GNRs with both zigzag and armchair edges. The direction of the uniaxial tension, which is taken to be either parallel ($\theta = 0$) or perpendicular ($\theta = \pi/2$) to the ribbon axis, has a crucial effect on the band structure.

In the strained armchair GNRs with $\theta = 0$, the band gap oscillates with the strain in a zigzag pattern, leading to the transitions between metal and semiconductor. The oscillatory amplitude is almost unchanged as $S$ increases. This kind of band gap is mainly a finite width effect, since it vanishes as $M$ goes to infinity. If $\theta = \pi/2$, a similar oscillatory gap also appears, but only for the strains smaller than a critical value $S_c$. As $S$ approaches $S_c$, the oscillatory amplitude goes to zero, unlike the case for $\theta = 0$. Once $S > S_c$, the other kind of band gap opens which is linear in $S - S_c$ and hardly affected by the ribbon width. In fact as the strain with $\theta = \pi/2$ increases, a quantum phase transition is induced at $S = S_c$ to separate a liquid phase from a solid phase where the bonds perpendicular to the strain are dimerized.

In the zigzag GNRs, the most intriguing phenomenon is the appearance of the flat band in a region of momentum $[k_s, 2\pi - k_s]$. As the strain with $\theta = 0$ increases, $k_s$ decreases to zero until $S = S_c$, then the flat band extends throughout the full Brillouin zone and the conduction and valence bands are separated. In contrast, with increasing $S$, $k_s$ moves towards $\pi$ and the region of the flat band shrinks into a point for $\theta = \pi/2$.

Except for the flat band, most features on the strain-dependence of the band structures are well revealed by the behaviors of the conductance of GNRs. For example, the band gap oscillation results in the conductance oscillation at the zero gate voltage $V_g = 0$ as the strain varies. The peak in the plot of the conductance versus $V_g$ is compatible with that in the DOS plot. Note that not all the modes with energy $V_g$ contribute to the conductance, but only those satisfying the boundary conditions are responsible for the electronic transport, therefore, it is not necessary to have a one-to-one correspondence between the peaks of the conductance and those of the DOS. Furthermore, by measuring the strain dependence of the conductance of AGNRs at $V_g = 0$, one can also detect the quantum phase transition induced by the tension perpendicular to a C–C bond and determine the critical strain as well.

Since we connect the GNRs with square lattices as the metallic electrodes, it is worth mentioning the fundamental
effect of the topology of the heterojunctions on the conductance of GNRs. In particular, due to the non-bipartite feature of the electrode-AGNR interfaces, the conductance data of AGNRs is not e–h symmetric, while this kind of symmetry can still be found in that of ZGNRs, since the electrode-ZGNR interfaces do not break the bipartite structure of the whole system. This phenomenon has no counterpart in the band structures obtained with periodic boundary condition, yet it may be important for designing the nano-size devices.

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