Electronic superlattices in corrugated graphene

A. Isacsson,1 L. M. Jonsson,1 J. M. Kinaret,1 and M. Jonsson2,3

1Department of Applied Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden
2Department of Physics, Göteborg University, SE-412 96 Göteborg, Sweden
3School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, Scotland, UK

We theoretically investigate electron transport through corrugated graphene ribbons and show how the ribbon curvature leads to an electronic superlattice with a period set by the corrugation wave length. Transport through the ribbon depends sensitively on the superlattice band structure which, in turn, strongly depends on the geometry of the deformed sheet. In particular, we find that for ribbon widths where the transverse level separation is comparable to the the band edge energy, a strong current switching occurs as function of an applied backgate voltage. Thus, artificially corrugated graphene sheets or ribbons can be used for the study of Dirac fermions in periodic potentials. Furthermore, this provides an additional design paradigm for graphene-based electronics.

A single layer of graphite, known as graphene, was for the first time studied experimentally in 2004 [1]. This started a massive interest in graphene, mainly because it is a 2D gapless semiconductor with massless “relativistic” quasiparticles [2, 3, 4, 5, 6, 7, 8]. An unusual integer quantum Hall effect [9] and a predicted minimal conductivity $\sigma = 4e^2/(h\pi)$ are among the manifestations of the linear energy dispersion in the vicinity of the Fermi energy. In addition to being a tool for studying fundamental properties of graphene, this is also of interest for device applications (e.g. transistors, lenses and NEMS resonators [10, 11, 12, 13]).

Proposed graphene-based devices typically rely on external electrostatic gates for controlling the electronic transport. In this Letter, however, we show that the effective potential induced in a graphene ribbon placed on a corrugated substrate, can strongly alter the transport properties. This effective potential is determined by the local curvature [14] of the ribbon and introduces an additional design degree of freedom of interest for both fundamental studies of graphene and graphene-based electronic devices. For illustration, we focus here on periodically modulated surfaces — superlattices — and show how the corresponding band structure can be readily probed by conductance measurements.

We consider a single graphene ribbon placed on a corrugated surface and biased by a small applied DC voltage as shown in Fig. 1. In the tight binding description the ribbon is described by

$$\hat{H}_{\text{TB}} = \sum_{\langle i,j \rangle} t_{ij} a_i^\dagger b_j + \sum_{\langle \langle i,j \rangle \rangle} t_{ij}' \left( a_i^\dagger a_j + b_i^\dagger b_j \right) + \text{h.c.} \quad (1)$$

Here $\langle i,j \rangle$ denote nearest neighbors ($a$ and $b$ atoms) and $\langle \langle i,j \rangle \rangle$ next nearest neighbors. When the ribbon is deformed, the matrix elements $t$ and $t'$ change. Thus, if $t_{ij} = V_{pp\sigma}$ describes hopping between atoms $i$ and $j$ on a flat graphene sheet, we find [14, 15] that for a deformed sheet $t_{ij}'^{(t)}$ is replaced by

$$t_{ij}'^{(t)} = \frac{u_{ij}^2}{d_{ij}} \left[ (V_{pp\sigma} - V_{pp\sigma}) (\mathbf{n}_i \cdot \mathbf{d}_{ij}) (\mathbf{n}_j \cdot \mathbf{d}_{ij}) + V_{pp\sigma} d_{ij}^2 \mathbf{n}_i \cdot \mathbf{n}_j \right].$$

Here $\mathbf{u}_{ij}$ is the vector connecting atoms $i$ and $j$ in the undeformed lattice while $\mathbf{d}_{ij}$ is the corresponding vector after deformation. The surface normals are denoted by $\mathbf{n}_{i,j}$. While a general deformation involves both bending and stretching, we will here restrict our attention to pure bending deformations in one direction, i.e. $z = h(x)$ (see Fig. 1). We write the new matrix elements $\hat{t}_{ij}'^{(t)} = t_{ij}'^{(t)} + \delta_{ij}'$, and to second order in $\partial^2 h$ we find

$$\delta_{ij}' = \frac{(\partial^2 h)^2 (u_{ij} \cdot \hat{x})^4}{2u_{ij}^2} \left[ \left( \frac{u_{ij}^2}{(n_{ij} \cdot \hat{x})^2} - \frac{2}{3} \right) V_{pp\sigma} + \frac{1}{2} V_{pp\sigma} \right].$$

Figure 1: Schematic illustration of the graphene ribbon system investigated in this paper. The DC-biased ribbon of width $W$ rests on a corrugated substrate surface of length $L$ and height profile $h(x, y)$.

We note that this expression is similar but not identical to the one in Ref. [14]. Inserting the new matrix elements in Eq. (1) and expanding around the Fermi points $\mathbf{K}$ and $\mathbf{K}'$, results in an effective Hamiltonian with two new terms $A_{\text{eff}}$ and $\Phi_{\text{eff}}$ which are of order $a_0^2 (\partial^2 h)^2$ ($a_0 = 1.42$ Å is the lattice constant). For electrons near the $\mathbf{K}$ point the Hamiltonian is

$$\hat{H}_{\text{eff}} = \hbar v_F \hat{\sigma} \cdot \left[ -i \nabla + \mathbf{A}_{\text{eff}}(\mathbf{x}) + \epsilon V_G + \Phi_{\text{eff}}(\mathbf{x}) \right]. \quad (2)$$

Here $\hat{\sigma} = \hat{x} \sigma_x + \hat{y} \sigma_y$ and $\sigma_{x,y}$ are Pauli matrices, $v_F = 10^6$ m/s is the Fermi velocity, and $\epsilon V_G$ can be produced by the action of a back-gate.

Unless time reversal symmetry is broken, e.g. by a magnetic field, the effective vector potential $A_{\text{eff}}(\mathbf{x})$ at the $\mathbf{K}$-point, and its time reversed counterpart at the $\mathbf{K}'$-point, only contribute to second order in $a_0^2 (\partial^2 h)^2$ and
will be ignored in what follows. The second new term corresponds to an effective potential, which for graphene bent along the “armchair” direction is

$$\Phi_{\text{eff}}(x) = \frac{27}{4} a_0^2 (\partial_x^2 \phi) \left( \frac{3}{8} V_{pp\sigma} - \frac{1}{6} V_{ppn} \right).$$

In addition, because of the vanishing of the first order matrix element of $A_{\text{eff}}(x)$, a third new term corresponding to a local variation in Fermi-velocity should be considered. However, for long wavelengths, $k_0 \lesssim 1$, this term can be shown to be much smaller than the effective potential $\Phi_{\text{eff}}$.

The form of the effective potential is simplified if we take the shape of the ribbon to be $h(x, y) = A \sin(n \pi x/L)$. This approximation captures the qualitative behavior of a general periodic potential and results in the expression

$$\Phi_{\text{eff}}(x) = E_0 (A/a_0)^2 (k_a a_0)^4 (1 - \cos k_a x), \quad (3)$$

where $k_a = 2n \pi / L$ and $E_0 \approx 0.22$ eV. Note that $\Phi_{\text{eff}}(x)$ is positive definite (repulsive), and its strength varies rapidly with $k_a$. Because of this, large amplitudes $A/a_0 \gg 1$ are necessary. Hence, it is important that Eq. (3) is transformed to a coordinate system $s = s(x)$ that follows the graphene ribbon. The relation between $s(x)$ and $x$ is

$$s(x) = \frac{L}{\pi n} \sqrt{1 + A^2 E} \left( \frac{n \pi x}{L} - \sqrt{\frac{A^2}{1 + A^2}} \right),$$

where $E$ is the elliptic integral of the second kind and $\tilde{A} = n \pi A / L$. The total length of the graphene sheet is then $s(L)$. For simplicity we will from here on write $x$ rather than $s(x)$ for the coordinate along the sheet.

For narrow graphene nano-ribbons the choice of transverse electronic boundary conditions is of great importance. They depend on the configuration of carbon atoms along the edge as well as the ribbon width. In this Letter, we use boundary conditions for a metallic armchair edge. The wave vector quantization in the transverse direction ($y$) gives $k_y = n \pi / W$. In the absence of fields the wave functions satisfy the Dirac equation

$$-i \hbar v_F \begin{bmatrix} \nabla & \sigma \cdot 0 \\ 0 & \nabla \cdot \sigma^* \end{bmatrix} e^{ikx \phi^{\pm}_n(k, y)} = \epsilon_n^{\pm} e^{ikx \phi_n^{\pm}(k, y)},$$

with $\epsilon_n^{\pm} = \pm \hbar v_F \sqrt{k^2 + k^2_n}$. For $n > 0$ the eigenspinors are

$$\phi^{\pm}_n(k, y) = e^{ik_n y} \begin{bmatrix} 1 \\ \pm e^{i \phi_{n+1}(k)} \\ \pm e^{i \phi_{n}(k)} \\ \pm e^{i \phi_{n+1}(k)} \end{bmatrix},$$

which are two-fold degenerate and for $n = 0$ they are

$$\phi^0_n(k, y) = [1, \pm \text{sgn}(k), 1, \pm \text{sgn}(k)]^T,$
Figure 3: (Color online) Conductivity ($\sigma = GL/W$) for a graphene sheet of length $L = 1 \mu m$ with a periodic potential $V_0 \sin(2\pi x/\lambda)$ ($V_0 \sim 2.5$ meV, $\lambda = 100$ nm) as a function of gate voltage and sheet width $W$. The pseudo gaps at $V_G = 0.02$ eV and $V_G = 0.04$ eV shown in Fig. 2 correspond to local minima in the conductivity. The inset shows the conductivity along the white dashed line ($W = 1 \mu m$) corresponding to the band diagram in Fig. 2. The thick line represents an average over nearby gate voltages, which removes the Fabry-Perot interferences (see text). The non-averaged data is shown as the thin (blue) line.

$V_G$ [meV] $V$ [meV]

Figure 4: Effective potential along a graphene sheet of a shape defined by $h(x) = A \sin(2\pi x/\lambda)$; $A = 20$ nm, $\lambda = 20$ nm. is an effect which increases with mass \(^{[20]}\). Here we consider one-dimensional motion along the graphene ribbon in bands corresponding to quantized transverse momenta $k_n$. In the effective equation for the longitudinal motion, Eq. (4), these transverse momenta produce a mass term that is zero for $n = 0$ and finite and increasing with $n$ for $n > 0$.

The band structure in Fig. 2 can be probed by transport measurements. To demonstrate this we adopt a Landauer approach together with a transfer matrix method and calculate the transmission probabilities assuming coherent and ballistic transport. The conductance is then found from $G \sim (4e^2/h) \sum t_n$ where $t_n$ is the transmission probability for channel $n$ and the sum over $n$ runs over all channels. The transmission probabilities $t_n$ are obtained from the transfer matrices $T_n = \prod_{m=1}^{N} T_n^{(m)}$ \(^{[21]}\). Here the interval $0 < x < s(L)$ is divided into $N$ steps each having a constant potential $V_m = V(x_m)$, $x_m = ms(L)/N$. The transfer matrices between slices are found from the requirement that the wave functions be continuous everywhere (current conservation). The reservoirs on the left and right sides are taken to be infinitely wide graphene strips. As will be seen, this gives rise to a Fabry-Perot like interference pattern in the conductance, due to reflections at the reservoir-ribbon interfaces, as the back gate voltage is varied. These fluctuations are expected to smear out at finite temperatures and in the presence of impurities. As pointed out in Ref. \(^{[22]}\) it is in general not allowed (as in the case of a 2DEG) to introduce a general adiabatic widening of the strip to remove these fluctuations. Such a widening will introduce a changing structure of the transverse boundary conditions and a detailed description of the edge geometry is necessary.

The conductivity of a finite system of length $L = 1 \mu m$ is shown as a function of gate voltage and strip width in Fig. 3. For widths $W > L \gg \lambda$ the conductivity does not change appreciably as the the ribbon becomes wider whereas for narrow strips strong alteration of the conductivity occurs. The inset shows the conductivity for parameters corresponding to Fig. 2. The conductivity minima agree with the predicted pseudo gaps from the infinite structure in Fig. 2.

Now we consider a finite length graphene ribbon placed on a corrugated substrate. We will specifically consider narrow strips where the transverse energy level spacing $\Delta E_n \sim h\nu_F/W$ is of the same order as the band edge energy, i.e. $\lambda \sim W$. For illustration we chose a ribbon placed on a sinusoidally shaped substrate, $h(x) = A \sin(2\pi x/\lambda)$ with $A = 20$ nm and $\lambda = 20$ nm. This leads to an effective potential (see Fig. 3) of the order of 10 meV with an effective wavelength of the order of 80 nm (consistent with the assumption $ka_0 < 1$). Choosing a width of $W = 100$ nm thus puts us in the desired regime. Figure 5 shows the conductance of a graphene ribbon with $L = 1 \mu m$ as a function of the back-gate voltage (thick blue solid curve) calculated using the transfer matrix method described above. The conductance of a flat ribbon of equivalent length $s(L)$ is also shown for comparison (red dashed curve). Both curves have been averaged over nearby points to remove spurious interferences arising from the abrupt boundary conditions. Non-averaged data for the corrugated sheet is shown as the thin (blue) line.

A comparison of the conductances of flat and corrugated graphene sheets shown in Fig. 5 reveals two distinct features. Firstly, there is an asymmetry in the conductance of a corrugated sheet with respect to positive and negative back-gate voltages because the average effective potential $\Phi_{\text{eff}}$ is strictly positive. This results in a total shift $\Delta V_G = \Phi_{\text{eff}}$ as well as in changes in the detailed structure. Secondly, the effect of corrugation is clearly seen to strongly alter the conductance due to conductance channels being switched on and off. This can be traced to the band structure for an infinite system with corresponding parameters shown in the right panel of Fig. 5 (N.B. the unaffected $n = 0$ band has been omitted).
Finally, we have also considered short graphene ribbons where $L \sim W \sim \lambda$. Figure 5 shows the conductance of a ribbon with $s(L) = 160$ nm and therefore only two potential maxima (double barrier). Again, comparing with a flat system of equal length we find that the overall features in the conductance change in the same qualitative ways as described above. In this case, however, one should be careful not to confuse structure in the conductance due to the Fabry-Perot like interferences on the one hand with structure due to resonant tunneling on the other. In this case both effects are of similar importance.

In conclusion, we have shown that placing graphene on an artificially corrugated surface produces an effective local potential for the graphene electrons. This potential, which is related to the local curvature, can be tailored to significantly alter the transport properties of graphene. Specifically we have considered the effect on the electrical conductance of periodic potentials and showed how the band structure manifest itself in graphene nano-ribbons. Such a relation between transport properties and geometrical configurations may add to the number of design degrees of freedom available for constructing graphene based electronic devices. It may also provide an alternative transduction mechanism in graphene based NEMS.

We are grateful for stimulating discussions with Leonid Gorelik. Funding was provided by the Swedish Foundation for Strategic Research (SSF).

Figure 5: (Color online) Conductance of a graphene ribbon as a function of gate voltage (left panel). The conductance of a ribbon placed on a corrugated surface (thick blue solid curve) is asymmetric with respect to the sign of the gate voltage in contrast to when the surface is flat (red dashed curve). The origin of this asymmetry is that the curvature-induced potential is not symmetric. Focusing on positive gate bias we can identify points (A-G) in the conductance curve, corresponding to switching on and off conductance in specific channels. The corresponding band edges for an infinite ribbon are shown in the right panel. For negative $V_G$ similar features appear in the conductance (not labelled).

Figure 6: (Color online) Conductance of a short metallic ribbon with (solid, black) and without (dashed, red) corrugation.

* Electronic address: andreas.isacsson@chalmers.se

[1] K. S. Novoselov et al., Science 306, 666 (2004).
[2] A. K. Geim and K. S. Novoselov, Nat. Mater. 6, 183 (2007).
[3] M. Katsnelson and K. Novoselov, Solid State Commun. 143, 3 (2007).
[4] K. Nomura and A. H. MacDonald, Phys. Rev. Lett. 98, 076602 (2007).
[5] K. S. Novoselov et al., Nature 438, 197 (2005).
[6] J. Tworzydlo, B. Trauzettel, M. Titov, A. Rycerz, and C. W. J. Beenakker, Phys. Rev. Lett. 96, 246802 (2006).
[7] Y. Zhang, Y.-W. Tan, H. L. Stormer, and P. Kim, Nature 438, 202 (2005).
[8] A. L. Vasquez de Parga et al., arXiv:cond-mat/0709.0360, (2007).
[9] V. P. Gusynin and S. G. Sharapov, Phys. Rev. Lett. 95, 146801 (2005).
[10] J. S. Bunch et al., Science 315, 490 (2007).
[11] Z. Xu, Q.-S. Zheng, and G. Chen, Appl. Phys. Lett. 90, 223115 (2007).
[12] V. V. Cheianov and V. I. Fal’ko, Phys. Rev. B 74, 041403 (2006).
[13] V. V. Cheianov, V. Fal’ko, and B. L. Altshuler, Science 315, 1252 (2007).
[14] A. H. Castro-Neto and E.-A. Kim arXiv:cond-mat/0702562,(2007).
[15] More detailed derivations and results for other boundary conditions will be given elsewhere.
[16] W. A. Harrison, Elementary Electronic Structure (World Scientific, Singapore, 2004), revised ed.
[17] L. Brey and H. A. Fertig, Phys. Rev. B 73, 235411 (2006).
[18] C. L. Roy, B. Mendez, and F. Dominguez-Adame, J. Phys. A 27, 3539 (1994).
[19] B. F. Samsonov, A. A. Pecheritsin, E. O. Pozdeeva, and M. L. Glasser, Eur. J. Phys. 24, 435 (2003).
[20] A. Calogeracos, N. Dombey, Contemp. Phys. 40, 313 (1999).
[21] S. Datta, Electronic transport in mesoscopic systems (Cambridge University Press, Cambridge, 1995).
[22] M. Katsnelson, Eur. Phys. J. B 57, 225 (2007).