The coupling of geometrical and electronic properties is a promising venue to engineer conduction properties in graphene. Confinement added to strain allows for interplay of different transport mechanisms with potential device applications. To investigate strain signatures on transport in confined geometries, we focus on graphene nanoribbons (GNR) with circularly symmetric deformations. In particular, we study GNR with an inhomogeneous, out of plane Gaussian deformation, connected to reservoirs. We observe an enhancement of the density of states in the deformed region, accompanied with a decrease in the conductance, signaling the presence of confined states. The local density of states exhibits a six-fold symmetric structure with an oscillating sub-lattice occupation asymmetry, that persist for a wide range of energy and model parameters.

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a nanoribbon with \( N_x (N_y) \) sites on the horizontal (vertical) direction, connected to infinite graphene leads (see Fig. 1) modeled by the tight-binding Hamiltonian:

\[
H = \sum_{<i,j>} t_{ij} c_i^\dagger c_j + \sum_{<i,k>} t_{0i} c_i^\dagger c_k + \sum_{<i,k,r>} t_{0i} c_i^\dagger c_k c_r, \tag{1}
\]

Here, the first term refers to the central (deformed) system, while the second and third terms describe the connection to the reservoirs, with the indices \( k, k_r \) running over the sites of the left and right leads. \( c_i^\dagger (c_i) \) is the creation (annihilation) field operator in the \( i \)-th site, \( t_{ij} \) is the nearest-neighbor hopping energy and we take \( t_0 = -2.8 \) eV as the hopping parameter in the absence of deformation. The strain introduced by the Gaussian deformation modifies \( t_{ij} \) as \( t_{ij} = t_0 \Delta_{ij} \) with \( \Delta_{ij} = e^{-\beta((x_i-x_j)^2+(y_i-y_j)^2)/\sigma^2} \).

The interatomic distance in unstrained graphene is \( a = 1.42 \) Å, and the coefficient \( \beta = \left( \frac{\partial \log t_0}{\partial \log a} \right)^{-1} = 3.37. \) The distance \( l_{ij} = \frac{1}{\sigma} (a^2 + \varepsilon_{xx} x_i^2 + \varepsilon_{yy} y_j^2 + 2 \varepsilon_{xy} x_i y_j) \) is given by the strain tensor \( \varepsilon_{\mu\nu} = \frac{1}{2} (\partial_\mu u_\nu + \partial_\nu u_\mu + \partial_\mu h \partial_\nu h) \), characterized by the in- and out-of-plane deformation, \( u_\nu \) and \( h \), respectively.\(^{22}\) The out-of-plane deformation,

\[
h (x_i, y_i) = Ae^{-\frac{(x_i-x_0)^2+(y_i-y_0)^2}{2\sigma^2}}, \tag{2}
\]

has center at \( [x_0; y_0] \) (we use \( x_0 = L/2, y_0 = W/2 \) for the center of the ribbon), and \( A \) and \( b \) describe its amplitude and width respectively. The hopping modification can be understood as a gauge field.\(^{22}\) For a Gaussian deformation this field has a three-fold spatial distribution with different profiles for zigzag and armchair crystal directions.\(^{23}\) Notice that the bump also produces a deformation potential, akin to a local chemical potential,\(^{23}\) whose effects have not been included in the results showed below. Consequences of its presence are discussed in detail in the Supplemental Materials where it is shown that due to its axial symmetry, it does not affect the main findings of this paper. Eq. 1 is used to obtain the retarded Green’s function by recursive methods. Self-energies \( \Sigma_{r,l} \) associated to the leads, are calculated by standard decimation methods. Finally, the conductance is calculated via the Landauer formula and Fisher-Lee relation.\(^{52}\)

**Conductance and DOS:** The conductance and DOS for strained ribbons with armchair (AGNR) and zigzag (ZGNR) terminations are shown in Fig. 2 for deformations with varying amplitude \( A \) and fixed width \( b \). In both cases the position of the deformation is at the center of one hexagonal cell. The data is shown for AGNR with \( L = 30.7 \) nm and \( W = 30.0 \) nm (288 \( \times \) 245 atomic sites) and for ZGNR with \( L = 27.4 \) nm and \( W = 25.8 \) nm (224 \( \times \) 244 atomic sites). Similar results were observed with different ribbon sizes and positions of the Gaussian center (within a radius of \( \sim 0.2 \) nm). For all panels, the dashed (black) lines correspond to results in the absence of the deformation and continuous (color online) lines to different values of \( A \).

Conductance results are shown in panels a) and b) for AGNR and ZGNR, respectively. Both ribbons are metallic and the conductance exhibits the standard stepwise behavior for the unstrained case (black dashed). For both terminations, the zero-plateau is not modified by the Gaussian deformation, in contrast with results obtained with uniaxial in-plane strained junctions.\(^{39}\) As \( A \) increases, the value of the conductance decreases for non-zero plateaus. Note that the conductance for ZGNR and AGNR ribbons exhibit different profiles. These differences may be caused by the distinct orientations of the pseudo magnetic field space distributions with respect to the position of the leads. These distributions are \( 90^\circ \) rotated with respect to each other resulting on different scattering cross sections as shown by perturbation theory calculations on the continuum model.\(^{40}\) A common feature for both ribbons is the appearance of pronounced minima at the step-to-step transition, which have been observed in other systems, and are associated with interband mixing favored by the presence of perturbation.\(^{51}\)

Lower panels c) and d) show results for the corresponding DOS. The DOS curve for ZGNR shows the peak at zero energy corresponding to edge states that remains largely unaffected by the deformations from 4% up to a level of 11% strain. As the deformation is turned on, for both terminations, sharp peaks appear at lower energies followed by local minima. These minima are followed by raising features precisely at the energy values corresponding to the van Hove singularities in the absence of deformation. Thus, peaks in the undeformed system shift spectral weight lower energy peaks. These new peaks—in contrast to the original ones— are symmetric, fact more evident for ZGNR (see for example the third peak). This effect is accompanied by a decrease in height of higher energy peaks and a slow smoothening of the DOS. Notice that states in the newly formed low-energy DOS peaks, (produced by inhomogeneous pseudomagnetic field), do not generate additional contributions to the conductance. This indicates an incipient localiza-
at the deformation region, in contrast with previous studies where extended regions with constant pseudo-magnetic field generate pseudo LLs available for tunnelling assisted transport.\cite{31,33,34,36}

Fig. 3 shows similar results for a deformation with constant amplitude \( A \) and variable width \( b \). For both ribbons terminations, an increase in the curvature of the deformation (decreasing the value of \( b \)) results in a deterioration of the conductance and confined states. We find that the energy of the newly confined level decreases quadratically with the aspect ratio \( \frac{A}{b} \), a result predicted in the continuum description (Dirac) by perturbation theory and confirmed by scattering calculations.\cite{32}

LDOS and Pseudo-Spin Polarization: Non-homogeneous strain has profound effects on the space distribution of the DOS. An analysis of the LDOS reveals a well-defined pattern with a 60° symmetry, i.e., the ‘petals’ of the ‘flower’ structure. Fig. 4 presents typical LDOS structures obtained for AGRN and ZGNR at energies marked by vertical lines in Fig. 2. We have confirmed that this structure persists for a wide energy range and deformation parameter values (not shown). Similar patterns have been obtained in models of closed systems.\cite{21,31,33,34,38}

Notice that the structures for ZGNR and AGRN are rotated 90° relative to each other, following the spatial distribution of the pseudo-magnetic field.\cite{33}

Fig. 4 shows a zoom-in of one particular structure, for a ZGNR. The undeformed graphene lattice is represented by up- and downside triangles (distinguishing sublattices). The black dot represents the maximum height of the Gaussian bump that is centered in a maximum symmetry position in the ribbon. The values for sublattice occupancy alternates from ‘petal’ to ‘petal’, signaling a characteristic sublattice asymmetry or pseudo spin polarization with 3-fold symmetry. Such structure could be linked to a geometrical description of the microscopic model as realized in Ref. \cite{23}. Similar effects, with chiral states within the zero LL, were obtained in models of Dirac fermions with magnetic field in bounded regions.\cite{24}

In panels b) and c) we show values of LDOS on each sublattice. Panel b) exhibits the largest occupancies (darker regions) at the bottom ’petals’, while the contrary occurs in panel c). Notice that zigzag boundaries naturally introduce a difference in sublattice occupancies due to the different sublattice terminations at the top and bottom edges. These differences, due to ‘edge states’, are predicted to be localized at the edges, however for finite systems the amplitude of edge states decays inside the ribbon.\cite{52} It is thus natural to interpret the ’dark regions’ breaking the three-petal symmetry as a consequence of edge states in ZGNR. To confirm these hypotheses we carried out calculations for AGRN that reveal the same alternate pattern for sublattice occupancy.\cite{18}

In these systems the whole ’flower’ structure possesses ’dark regions’ in the ’petals’ appearing closer to the contacts to reservoirs. Although the leads are modeled as perfect graphene lattices, the absence of the deformation in the reservoirs could create an effective boundary condition at the contact, thus representing potentially a zigzag boundary. The presence of these developing ’edge states’ at the contacts could enhance the sublattice occupancy in certain petals. Calculations carried out in larger AGRN with deformation amplitudes vanishing before reaching contact regions (thus eliminating a ’zigzag boundary’), show that the distribution of the highest occupied ’petals’
becomes energy dependent with a persistence asymmetry between petals. However this asymmetry decreases with increasing AGNR width, suggesting a strong dependence on the underlying LDOS for the undeformed system.

Further calculations reveal that pseudo spin polarization appears in a wide range of energies, and deformation parameters, indicating a robust effect, that persists in the presence of external magnetic fields. Note that this local breaking of sub lattice symmetry (local breaking of inversion symmetry) does not open a gap as evidenced by the finite conductance. Although several theory studies have predicted sublattice asymmetry features in the LDOS, these appear to have been overlooked in STM experimental studies since no explicit connection with centro-symmetric deformations have been made. Our results, showing a peculiar sequential pattern for sublattice occupation provide a possible test for the origin of the observed asymmetries that could be tested in current experimental settings.

Conclusions: In closing, we present the first study of conductance of strained ribbons with Gaussian deformations that produce inhomogeneous pseudo magnetic fields at every length scale. In this system there are no Landau levels available for transport but instead there are bound states that concentrate in the region where the pseudo magnetic field acquires its maximum value. We provide a real space description of the location and symmetry of these states, that exhibit a sublattice occupation alternation of 60°, associated with a local pseudo spin polarization in the continuum Dirac (low-energy) description. These results are largely independent of lattice orientation. All these effects are within reach of current experiments and open the exciting possibility to design deformations for desired electronic confinement.

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