Conductance signatures of electron confinement induced by strained nanobubbles in graphene

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The effect of graphene nanobubbles on the transport properties of graphene nanoribbons is investigated using a combined molecular dynamics–tight-binding simulation scheme. We show that the conductance, density of states, and current density of zigzag or armchair graphene nanoribbons are modified by the presence of a nanobubble. In particular, we establish that low-energy electrons can be confined in the vicinity or within the nanobubbles by the delicate interplay between the pseudomagnetic field pattern created by the shape of the bubble, mode mixing, and substrate interaction. The coupling between the confined evanescent state and the propagating modes can be enhanced under different clamping and substrate conditions, leading to Fano resonances in the conductance traces.

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The fine control over nanofabrication techniques has not only increased the performance of existing electronic devices1, but has also allowed the emergence of concept devices based on the strictly quantum-mechanical properties of electrons. One such proposal is the incorporation of patterned ferromagnetic or superconducting films on two dimensional electron gas (2DEG) structures. Under the right conditions and design parameters, these can be tailored to provide non-homogeneous magnetic fields able to interact strongly with the underlying electrons in the ballistic transport regime2–5. Ideally, the spatial profile of such fields should be extremely sharp along the transport direction and homogeneous in the transverse direction, so that the resulting magnetic barrier might behave as an effective momentum filter, which is necessary to achieve control of the ballistic transmission4,5. In addition, strong and sharp barriers generally beget richer transmission characteristics, including the stabilization of confined states within the barrier5.

The same concept has been proposed following the advent of graphene as a versatile two-dimensional platform for nanoscale electronic devices, with local magnetic barriers being one of several proposed means to confine, guide, and control electron flow7–11. The need for robust and tunable confinement strategies is more fundamental in graphene electronic devices than in conventional semiconductors: on account of their massless Dirac character, charge carriers in graphene are vulnerable to the phenomenon of Klein tunneling, and cannot be adequately confined by standard electrostatic means, particularly in the ballistic regime.

However, even though the search towards achieving control of the electron flow in graphene remains one of the most active research areas when it comes to applications of graphene in the electronics industry, little progress has been made towards this concept of magnetic confinement. This is partly because of the size requirements that call for magnetic barriers that are much smaller than the electronic mean free path, and also because of the need to limit the spatial extent of the magnetic field within regions equally small, since it might be desirable to have portions of the system free of any magnetic fields.

Graphene, with its outstanding electronic and mechanical properties, offers a completely new approach towards this goal of local magnetic barriers that can, in principle, be modulated on scales of a few angstroms. Owing to the peculiar coupling of electrons and lattice deformations, it is possible to perturb the electrons in graphene in the same way they would react to an external magnetic field by purely mechanical means12,13. Several authors have envisaged the study of phenomena and applications predicted to happen in the presence of magnetic fields by purely mechanical means, exploring appropriately engineered strain configurations to achieve desired pseudomagnetic field (PMF) profiles14–16. The development of Landau quantization in the absence of magnetic fields is one such prediction17 that was recently confirmed in local tunneling spectroscopy experiments18,19. One possible application of this ability to create quasi-uniform PMFs over nm scales is the fabrication of pseudomagnetic quantum dots20 whose sharp resonant tunneling characteristics might provide a very sensitive strain detector.

The experiments of Levy18 and Lu19 with graphene nanobubbles affirm the potential of strain-engineering for effective manipulation of the electronic motion in graphene, and demonstrate the unique characteristics of this approach: (i) the ability to generate local PMFs with magnitudes that can easily exceed several 100s of
implemented a combined MD-TB simulation. Molecule-derived transport properties as accurately as possible, we tackled this in the same framework developed in reference 21, that combines molecular dynamics (MD) and tight-binding (TB) calculations. In this approach, the lattice deformation is determined fully atomistically for the prescribed substrate and loading conditions, and the relaxed atomic positions are used to build a TB description of the electron dynamics in the system. The aim is to reduce any bias in the description of the electronic system by capturing all the atomic-scale details of deformation and curvature, since they play an important role at these scales of less than 50 nm. Similar to what is observed for real magnetic barriers\(^6\) or Gaussian bump deformations\(^{22,23}\), the conductance of either zigzag (ZZ) or armchair (AC) graphene nanoribbons (GNR) develops marked dips (anti-resonances) at the edge of each conductance plateau. We show that this is due to scattering of propagating modes into evanescent states confined in the nanobubble. The coupling between the confined evanescent state and the propagating modes can be enhanced under different clamping and substrate conditions, leading to Fano resonances\(^{24–26}\) in the conductance traces. Our calculations show that these signatures of electronic confinement in graphene nanobubbles are a robust effect, being observed irrespective of the orientation of the underlying graphene lattice, for different substrates, and for different bubble geometries.

I. MODEL AND METHODOLOGY

To reproduce the deformation of graphene and its derived transport properties as accurately as possible, we implemented a combined MD-TB simulation. Molecular dynamics provides the spatial location of the carbon atoms when graphene is subjected to gas pressure and a nanobulge forms through the substrate aperture. Once the coordinates of each atom are known, the nearest-neighbor TB parameters are calculated throughout the system and the TB Hamiltonian for the deformed system is built. This Hamiltonian constitutes the basis for the calculation of all the local spectral and transport properties. Electronic transport is addressed via the lattice representation of the non-equilibrium Green’s function (NEGF).

A. Molecular dynamics simulations

For an unbiased analysis of the local profile of deformations, the mechanical response of the system was simulated by MD with the Sandia-developed open source code LAMMPS\(^{28,29}\). The MD simulation system consisted of three subsystems: a graphene monolayer, a rigid substrate with a central aperture, and argon gas that was used to inflate graphene through the aperture to generate a nanobubble. An illustration of the system is shown in Fig. 1. The AIREBO potential\(^{30}\) was used to describe the C-C interactions. The dimension of the simulation box was \(20\times20\times8\text{ nm}^3\) and apertures of different shapes (viz. triangle, rectangle, square, pentagon, hexagon, and circle) were “etched” in the center of the substrate to allow the graphene membrane to bulge downwards due to the gas pressure. In each simulation, the system was initially relaxed for 50 ps before slowly raising the pressure.

FIG. 1: (Color online) Illustration of a MD simulation cell conveying the strategy used to generate the graphene nanobubbles. An aperture (a circle in this case) is perforated on the chosen substrate (orange) on which rests a monolayer of graphene (gray). Argon gas is then pressurized against graphene which bulges through the aperture, with a deflection that is controlled by the gas pressure. For ease of visualization the gas molecules are not shown in the picture above. Visualization is performed using VMD\(^{27}\).
to the desired target by decreasing the volume of the gas chamber. Upon reaching the target pressure, the system was allowed to relax for 10 ps, after which deformed configurations were obtained by averaging the coordinates during equilibrium. Target pressures are determined to yield a deflection of 0.9 nm. All simulations in the presence of the gas were carried out at room temperature (300 K) using the Nose-Hoover thermostat\textsuperscript{31}.

Since a previous study established that the magnitudes and space dependence of the strain-induced PMFs can be very sensitive to the clamping conditions and substrate type,\textsuperscript{21} we considered three scenarios to analyze how these effects impact the transport signatures. In one case the MD simulations are done with clamped boundary conditions, i.e., an ideal system consisting only of Ar gas and graphene, and where all carbon atoms outside the aperture region were strictly fixed. This is to study the effect of aperture geometry without considering the substrate, and is similar to the approach used in previous work\textsuperscript{14,32,33}. In the second scenario, we included a 2 nm thick substrate of FCC Au (111) and its interaction with the graphene sheet is explicitly taken into account. The substrate-graphene and gas-graphene interactions were modeled by a standard 12-6 Lennard-Jones potential with interaction parameters $\epsilon_{C-Au}=0.02936$ eV, $\sigma_{C-Au}=2.9943$ Å\textsuperscript{34}, $\epsilon_{C-Ar}=0.0123$ eV, $\sigma_{C-Ar}=3.573$ Å\textsuperscript{35}, $\epsilon_{Ar-Ar}=0.0123$ eV, $\sigma_{Ar-Ar}=3.573$ Å\textsuperscript{36}. The Au-Au (gas-substrate) interactions were neglected, and the substrate layer remained static during the simulation. Most of the graphene layer was unconstrained, except for a 0.5 nm region around the outer edges of the simulation box where it remained pinned. The third and final scenario considers a different substrate to assess any consequence of varying degrees of interaction with the substrate, we chose the surface (111) for the closeness of its lattice parameter to graphene’s, which promotes the interaction between the two surfaces. Our goal is to assess whether any features in the conductance of the system when deformed under realistic conditions of contact with a substrate are robust, or dependent on the degree of substrate-graphene interaction. The fact that these two are metals is secondary for our purposes since we consider the electronic transport within the graphene layer only, without any possibility of conduction through the substrate. Our approach is directly transferable to any other substrate for which an accurate interaction potential with two-dimensional carbon is known.

### B. Tight-binding calculations

The scattering region used in the electronic transport calculations contains the entire MD simulation cell (including the flat portions between the bubble’s perimeter and the edge of the cell). The cell accommodates 15088 lattice sites, an example of which is shown in Fig. 1. For convenience, we assume the ZZ chains are parallel to the $x$ direction. Most low energy electronic properties of graphene are captured by the $\pi$ band nearest-neighbor TB Hamiltonian

$$H = \sum_{<i,j>} t_{ij}(c_i^\dagger c_j^\dagger + c_j c_i),$$  \hfill (1)

where $c_i$ represents the annihilation operator on site $i$ and $t_{ij}$ is the hopping amplitude between nearest neighbor $\pi$ orbitals (in the unstrained lattice $t_{ij} = t_0 \approx -2.7$ eV). The link between the MD simulation and the TB Hamiltonian is performed when the positions of the carbon atoms in the deformed configuration, obtained by MD, are incorporated into the TB Hamiltonian through the modification of the hopping parameter $t_{ij}$ between all nearest-neighbors. The modification that accounts simultaneously for the distance $d$ between neighbors and the local rotation of the $p_z$ orbitals is given by:

$$t_{ij}(d) = V_{pp\sigma}(d_{ij}) \hat{n}_i \cdot \hat{n}_j + V_{pp\pi}(d_{ij}) \frac{(\hat{n}_i \cdot \vec{d}_{ij})(\hat{n}_j \cdot \vec{d}_{ij})}{d_{ij}^2},$$  \hfill (2)

where $\hat{n}_i$ is the unit normal to the surface at site $i$, $\vec{d}_{ij}$ is the distance vector connecting two sites $i$ and $j$, and $V_{pp\sigma}(d)$ and $V_{pp\pi}(d)$ are the Slater-Koster bond integrals for $\sigma$ and $\pi$ bonds. Their dependence on the inter-atom distance is taken as\textsuperscript{31,39}

$$V_{pp\sigma}(d_{ij}) = t e^{-\beta(d_{ij}/a-1)},$$  \hfill (3)
$$V_{pp\pi}(d_{ij}) = 1.7 V_{pp\sigma}(d_{ij}),$$  \hfill (4)

where $t = 2.7$ eV, $a \approx 1.42$ Å represents the equilibrium bond length in graphene, and $\beta = 3.37$ captures the exponential decrease in the hopping with interatomic distance. Once the values of $t_{ij}$ are obtained, we use the TB Hamiltonian of the strained system as the scattering central region, to which two ideal contacts are attached. Since the edges of the system are of ZZ or AC type, the
central region is seamlessly stitched to the contacts resulting in a perfect ZZ or AC ribbon. We then study the quantum transport characteristics of such a GNR containing a central region deformed by the presence of the nano-bubble. The zigzag graphene nanoribbon (ZGNR) is created attaching two pristine semi-infinite ZZ nanoribbons to the left and right edges of the strained graphene square. The metallic armchair graphene nanoribbon (AGNR) is constructed by connecting two perfect metallic semi-infinite AGNR to the upper and lower edges of the central region. The conductance of these nanoribbons is calculated within the Landauer-Büttiker formalism using Caroli’s formula\(^{40–42}\): \(G = \frac{2e^2}{h} \text{Tr}[G_\varphi G_\varphi^T G_\varphi^\dagger]\), where \(G_\varphi = [G_\varphi^0]^{\dagger} = [E + i\eta - H - \Sigma_p - \Sigma_q]^{-1}\) is the retarded [advanced] Green’s function, the coupling between the contacts and the central region is represented by \(\Gamma_\varphi = i[\Sigma_q - \Sigma_q^\dagger]\), and \(\Sigma_q\) is the self-energy of contact \(q\) which is calculated recursively for ZZ and AC contacts\(^{43}\).

Having calculated the retarded and advanced Green’s functions, other electronic properties such as the density of states (LDOS), \(\rho_{ii} = -\text{Im}[G_\varphi^{ij}(\vec{r}_i, \vec{r}_j, E)]/\pi\), and the total density of states (DOS), \(p = \text{Tr}(\rho_{ii})\) are readily calculated. For a local mapping of the current distribution in the central region we consider the current density between nearest neighbors\(^{40}\), \(I_{ij} = \frac{e}{\hbar} \int dE [t_{ij} G_\varphi^{ji} - t_{ji} G_\varphi^{ij}]\), that is calculated from the lesser Green’s function, and which can be obtained exactly in the absence of electronic interactions as\(^{42}\) \(G^\text{<} = G_\varphi^{<}(E)[\Gamma_L(E) f_L(E) + \Gamma_R(E) f_R(E)]G_\varphi^{\dagger}(E)\). We stress again that the interaction graphene-substrate is included in the MD simulation part to realistically describe the interaction and sliding of graphene in contact with the substrate by the combined action of gas pressure and substrate aperture\(^{44}\). From the electronic point of view, the substrate plays no direct role in electronic tunneling or other electronic processes.

In order to compare the local current distribution to the spatial pattern of the PMF the latter is calculated directly from \(t_{ij}\) introduced in eq. (2) via

\[
A_x(r) - iA_y(r) = \frac{2\hbar}{3t_{\text{ae}}} \sum_n \delta_{r,r+n} e^{i\mathbf{k} \cdot \mathbf{n}}.
\]

This defines the two-dimensional pseudomagnetic vector potential, \(\mathbf{A} = (A_x, A_y)\)\(^{12,13}\), from where the PMF is calculated using \(B = \partial_x A_y - \partial_y A_x\).

**II. PSEUDOMAGNETIC FIELDS, MODE MIXING AND CONFINEMENT**

In order to recognize the incremental contributions of the different factors determining the conductance characteristics of the system (geometry, substrate interaction, and edge type of the GNR), we start with the simplest scenario described above: a ZGNR where all carbon atoms outside the aperture are rigidly attached to their original position; any deformation occurs only within the aperture region. Under this scheme the only scattering center is the nanobubble in the middle of the ZGNR, which allows us to isolate the effect of the bubble geometry and the corresponding PMF on the conductance. For a meaningful comparison among different geometries, all bubbles are chosen with approximately the same area \(\approx 50\, \text{nm}^2\), and centered within the square simulation cell. Polygonal apertures were used with side lengths of 7.1 nm (square), 5 nm (rectangle), 4 nm (circle radius), 4.4 nm (hexagon), 5.7 nm (pentagon), and 10.6 nm (triangle). In a second stage, we analyze graphene lying flat on a substrate, with no hole nor gas pressure, to determine whether the epitaxial strain that sets in at equilibrium perturbs the ideal conductance traces of free-standing graphene. Finally, we obtain the conductance traces arising from the nanobubbles inflated against the Au and Cu substrates.
A. Clamped bubbles

There is one key feature in the quantum transport of these systems stemming from the presence of the central bubble in an otherwise perfect GNR, and which is independent of the bubble geometry. Irrespective of the shape, the conductance of a ZGNR with \( W \approx 20 \text{ nm} \) of transverse dimension with an embedded bubble exhibits reproducible dips just at the onset of a new conductance plateau. The conductance traces for clamped nanobubbles are shown in Fig. 2(a)-(e) for a gas pressure of 19 Kbar, equivalent to a deflection of \( \approx 0.9 \text{ nm} \). The difference in sharpness and depth of these dips, as well as the roundness of the conductance steps, can be attributed to the geometry of the bubbles which, together with the spatial extent and magnitude of the local PMF, contributes to defining the strength of the scatterer. The weaker the scatterer, the narrower the line-shape of the conductance dips will be\(^{45,46}\). The red dashed traces in Fig. 2 represent the conductance of the ideal ZGNR. By direct inspection, we see that rectangular and square bubbles do not significantly affect the electron transport, since their impact translates only into a slight rounding of the conductance steps and a few shallow dips before each step, which is characteristic of a weak scatterer. For an intermediate scatterer, the conductance is generally lowered relative to perfect quantization, and dips remain sharp. This behavior can be observed for circular, pentagonal, and hexagonal bubbles. The triangular bubble is seen to be the strongest scatterer of the six considered in Fig. 2, as its conductance exhibits the largest reduction from the quantized value within each plateau, together with broader dips (notwithstanding, the original plateau structure is still identifiable). Despite the noticeable differences in the degree of perturbation that different bubble shapes bring to the conductance, and our usage of the terms weak and strong to conveniently distinguish those differences, it should be clear that, in a broad sense, all six nanobubbles should be classified as weak scatterers: the stepwise structure of the conductance versus Fermi energy, \( E_F \), is approximately preserved, and the conductance values do not differ significantly from the pristine case\(^{45,46}\).

The spectral counterpart of the conductance dips is the appearance of strong and narrow peaks in the DOS of the ribbons, just below the van Hove singularities (VHS) of the unpressurised system. The DOS for each bubble shape are shown in Fig. 3. The energy position of these shallow peaks is nearly the same for all bubbles, as can be seen in the figure. The weakest scatterers (rectangle and square) lead to the sharpest (and shallowest with respect to the nearest VHS) peaks in the DOS. Many of them are not associated with noticeable features in the conductance, such as the peaks observed at \( E = 0.048 t_0 \) for the rectangular bubble or at \( E = 0.216 t_0 \) for the square one. The DOS peaks of stronger scatterers (hexagon, pentagon, circle, triangle) are broader, and the VHS in the DOS are also broadened; in these cases, each DOS peak corresponds to a dip in the conductance.

Before proceeding further with our analysis we want to discuss the origin and physics behind the shallow and sharp features observed right before the onset of the plateaus (in the conductance) or the VHS (in the DOS). This resonant behavior is a multimode effect previously observed in quasi-one dimensional systems with impurities\(^{47,48}\), finite-range local potential scattering\(^{49,50}\), and short-range impurity potentials\(^{45,46,51–53}\). It can be understood by recalling that in quantum wires electric current is carried by independent transverse modes. When an impurity is present an electron incident upon the defect in a given mode will be scattered into a number of available modes with the same energy, including evanescent states\(^{45}\). The transition probability for this process depends on the density of final modes and, therefore, by virtue of the high density of evanescent states at the edge of each sub-band (mode), the electron has a high probability of scattering to an evanescent state, which is a state predominantly confined within the defect region, with an energy close to the bottom of the sub-band\(^{45}\). Of course, the transition rate depends also on the scattering potential itself, in addition to the density of evanescent states. As we

![FIG. 3: (Color online) Density of states of the same ZZ GNRs with nanobubbles described in Fig. 2. The red dashed lines correspond to the DOS of a pristine graphene ribbon with ZZ edges.](image-url)
outlined in the introduction, electrons in graphene perceive non-uniform local changes in the electronic hopping parameter as a PMF, and it is this non-uniform PMF pattern created by the inflation of graphene that determines the strength of the scattering at each nanobubble. The detailed analysis of the PMF created by each of the nanobubbles considered here can be found in reference 21. We briefly recall that one of the conclusions from this previous work was that the leading characteristic of the PMF distribution arising from an inflated nanobubble is an intense magnetic barrier that is narrowly localized within a few atomic distances from its perimeter. This results from the large bending and high bond stretching that occurs at the edge of the apertures. Different geometries have an impact in the local polarity of the PMF and its magnitude and space dependence in the central regions of the bubble. Two representative case are shown in Fig. 4.

In ascending order of the scattering barrier strength inferred from the conductance and DOS results of Fig. 2 and Fig. 3, square and rectangular bubbles display a sharp PMF barrier along the horizontal (zigzag) edges of the bubble $\sim 2000$ T (on the vertical edge (armchair) the PMF is much smaller). These configurations offer low resistance to electron flow since the barriers are parallel to the direction of propagation of electrons in a ZGNR. Circular, hexagonal, and pentagonal bubbles exhibit high PMF barriers ($\sim 2000$ T) at the corners and edges, followed by a fast decay towards the center of the bubble. Triangular bubbles, the strongest scatterer from the transport point of view, create PMFs of magnitude equally large around the edges and a roughly constant field of $\sim 100$ T in the inner area. In triangular nanobubbles the intensity and polarity of the peripheral barrier remains constant at all the three edges.

Based on the above we can attribute the conductance dips observed in Fig. 2 to scattering of propagating modes into a confined state around the bubble. However, it remains unclear how such different strengths and patterns of PMF created by the bubbles produce nearly the same effect on the conductance. To clarify this point let us inspect a map of the LDOS for a square bubble (weak scatterer), circular and hexagonal (intermediate scatterers), and a triangular bubble (strong scatterer). The LDOS maps at selected energies are shown in Fig. 5. The square bubble was seen earlier to display a sharp DOS peak at $E = 0.216 t_0$ that has no signature on the conductance. Circular, hexagonal and triangular bubbles, on the other hand, have a DOS peak at $E = 0.215 t_0$ with a corresponding conductance dip. Inspection of the LDOS maps in Fig. 5 at those energies immediately shows that there is no fingerprint of a strictly confined state: the shape of the bubble is faintly recognizable in each panel and, although the highest LDOS is seen within the bubble, the values there are not markedly different from those outside. To interpret these maps it is important to note that the unpressurized conductance of these systems at these energies is $G(0.215 t_0) = G(0.216 t_0) = (2e^2/h) \times 11$. From the conductance quantization sequence of an ideal GNR, $G = (2e^2/h)(2n + 1)^{54,55}$, we conclude that there are 5 conducting modes in an ideal GNR at the energies represented in Fig. 5. The inclusion of the square bubble brings essentially no change to this tally, as Fig. 2 shows that the conductance in its presence is scarcely changed: $G(0.216 t_0) = (2e^2/h)(10.9)$. On the other hand, at $E = 0.215 t_0$ for stronger scatterers one or more channels are backscattered because $G = (2e^2/h)(10.1)$ for the circle, $G = (2e^2/h)(9.6)$ for the hexagon, and
$G = (2e^2/h)(9.4)$ for the triangle. Hence, despite the nominal suppression of 1 to 2 conducting modes, the conductance is never zero at these energies and, consequently, the LDOS maps include contributions from conducting, backscattered, and confined states in the same picture.

A better insight into the extent to which the local PMF arising from different geometries disrupts the electron flow can be obtained from the local current density that we have calculated at each C-C bond, and whose results are presented in Fig. 6. The current map shown in Fig. 6(a) for the circular bubble reveals current bands where the current is directed forwards and backwards in an alternating pattern, signaling electron trapping within and its bouncing back and forth by the action of the strong PMF barriers at the perimeter of the bubble (cf. Fig. 4). Over the central region of the bubble the current remains predominantly horizontal by virtue of the negligible PMF inside. These strong bands decay outside bubble, confirming that this current pattern is associated with an evanescent mode created by the bubble through mode mixing. Qualitatively similar features are seen with hexagonal and pentagonal perimeters, which we omit for brevity.

Contrarily to the other shapes, a triangular bubble sustains a high and constant PMF $\sim 100$ T in the inner region (cf. Fig. 4). Inspection of the current’s spatial distribution in Fig. 6(b) reveals that the PMF within is seemingly enough to permanently trap a fraction of the electronic density in closed orbits, as suggested by the presence of a local vortex of counterclockwise current at the center of the bubble. We note that an electron in graphene with energy $E = 0.215 t_0$ in a constant magnetic field of 100 T has a magnetic length $\ell_B \approx 2.6$ nm and a cyclotron radius of $r_c = e^2/\hbar B \approx 6.8$ nm. Since such $r_c$ is larger than the bubble, and since other geometries still display conductance dips despite the absence of such localized current features, we conclude that those effects are not just dominated by the PMF, but bubble geometry and mode mixing are important ingredients. Finally, note that an electron should have an energy higher than $E \approx h v_F \pi / L$ to be sensitive to a scatterer of typical size $L$. The average radius of the polygonal apertures that we considered is $L \approx 4$ nm, which means that only above energies of $E \approx 0.16 t_0$ should the electrons begin to be noticeably affected by the presence of the nanobubble. This estimate is quantitatively consistent with the fact that in panels (c-f) of Fig. 2 the conductance dips only develop above this energy, and are not present at lower energies.

B. Flat graphene interacting with different substrates

Whereas the previous section discusses transport in the presence of a nanobubble, but having graphene rigidly clamped everywhere except the aperture region, in a realistic scenario the graphene-substrate interaction must be accounted for. The pressure-induced bulging of the graphene sheet through the aperture will be accompanied by its sliding and stretching in the regions outside the hole. The final strain distribution will thus be different which, in turn, will lead to modifications of the PMF barriers. Since the modification of electronic conductance discussed above stems from these barriers, one should naturally assess how robust they are in a realistic substrate scenario.

As introduced in Sec. I, we carried out MD simulations for two substrates fully interacting with the graphene
quantization is destroyed for $E \gtrsim 0.15 t_0$. Each dip is accompanied by a sharp peak in the DOS (not shown), analogously to the behavior previously seen in Fig. 3.

It is surprising that the Cu substrate alone has such a strong impact in the conductance. The underlying cause is the large epitaxial strain arising from the strong coupling between Cu and graphene\cite{8} that leads to strong PMFs even in the flat situation. As reported elsewhere\cite{21}, on Cu these fields can reach values of $\sim 200$ T (four times stronger than on Au). The typical scenario for graphene on Cu is shown in Fig. 7(c). Moreover, the epitaxial PMF pattern is not uniform through the system, but has a superlattice structure. This superlattice of PMF barriers derived from the underlying Moiré-type mismatch of the two lattice parameters is an effective source of electron scattering, and its extended and periodic nature leads to strong perturbations to the conductance of the system. Confirmation of this can be seen in Fig. 7b, where we show the LDOS at the energy of a representative conductance dip ($E = 0.215 t_0$). Most of the density appears around points distributed with an hexagonal periodicity that exactly matches the periodicity of the PMF superlattice in graphene. States in the vicinity of these energies are thus strongly scattered by the PMF field pattern.

The study of how a (Moiré) superlattice potential arising from the interaction of graphene and a substrate of different lattice constant has been a subject of considerable theoretical and experimental interest lately\cite{56–59}. One of the reasons is the experimental observation that, for certain substrates such as boron nitride, the superlattice potential can be strong enough to induce an energy gap $\sim 20$ meV at the Dirac point\cite{56–59}, to introduce satellite Dirac points\cite{60,61}, and to allow the observation of a Hofstadter spectrum\cite{62} in the presence of a magnetic field\cite{63}. In the case of a wide ZGNR on Cu analyzed here in more detail, the conductance does not develop a gap. However, a glimpse of conductance suppression in the vicinity of the Dirac point is seen in the inset of Fig. 7a. There, we amplify the low energy portion of the main panel to highlight the dip near the Dirac point.

C. Nanobubbles on Au and Cu substrates

When graphene is allowed to slide and bulge into the aperture under the combined effect of gas pressure and substrate interaction, electrons see a completely different PMF landscape. It is neither the characteristic PMF profile characteristic of the clamped, isolated bubble, nor the uniform superlattice structure of flat graphene + substrate discussed in the previous section. The main effect of creating the nanobubble in the PMF distribution is rather simple\cite{21}: (i) in the flat regions in contact with the substrate the superlattice structure gets perturbed but the underlying periodicity and polarity of the field is still observed, with field extrema reaching 300–400 T; (ii) within the bubble region the PMF has considerably smaller magnitudes, fluctuating about zero

![Image of a ZGNR on Cu](image-url)
in a random manner, so that the typical PMF patterns of an isolated bubble are lost. These modifications are, of course, gradual and strongly dependent on the type of substrate: graphene on Cu exhibits this contrast with the clamped case quite clearly, whereas on Au the field polarity, the marked barriers at the edges and corners of the bulge, and the field variation inside still resemble much of the clamped bubble behavior, except that now the PMF is seen to “leak” considerably beyond the aperture region.

The implications of the modified PMF pattern to the conductance can be analyzed in two different energy ranges, according to whether the electron’s Fermi wavelength, $\lambda_F = k/2\pi$, is larger ($E < 0.150 t_0$) or smaller ($E > 0.150 t_0$) than the characteristic size of the central nanobubble. In Fig. 8 we show the conductance of a ZGNR with embedded bubbles of different shapes for graphene on Au and Cu. We can see that the conductance traces are now richer than in Fig. 2 or Fig. 7. First, in the low energy region, the conductance is strongly perturbed with respect to the behavior of a free-standing ribbon. This is different from what we saw for either the substrate or the bubble alone, and results from how these two elements interplay to determine the final PMF distribution through the entire system. Interestingly, at low energies there is no marked difference between the conductance on a weakly interacting substrate like Au, or on a strong one like Cu. The conductance dip observed around the Dirac point in Fig. 7a also disappears which, according to our previous discussion, we interpret as a consequence of losing translation invariance in the PMF superlattice. At higher energies, the conductance on Au and Cu are visibly different and bear some resemblance with the conductance of the unpressurized ZGNR on the same substrate. The presence of the bubble translates only into deeper and wider conductance dips. Note also that the association that we made in the context of Fig. 2 between the bubble geometry and the corresponding scattering strength (based on the amplitude of the conductance dips) cannot be made with respect to the data shown in Fig. 7. It thus follows that, on a realistic substrate simulation, the aperture/bubble geometry plays a minor role in determining the deviation of the conductance traces from the ideal ribbon behavior and, consequently, all shapes share the same qualitative and quantitative features from the point of view of transport, as we see in this figure.

One new feature detected in Fig. 8 (common to all but
the triangular bubble) is the presence of a resonant peak right at the start of the second plateau at $E \simeq 0.05t_0$. The dips and resonances in the conductance are just two particular manifestations of a Fano resonance in the electron’s scattering cross-section\textsuperscript{24-26} that get imprinted in the conductance. In simple terms, a Fano resonance is characterized by a transmission probability of the form

$$T(E) \propto \frac{(\epsilon + q)^2}{\epsilon^2 + 1}, \quad \epsilon = E - E_{\text{res}} \quad (6)$$

in the neighborhood of $E = E_{\text{res}}$, where $\epsilon$ is the reduced energy and $q$ the phenomenological Fano asymmetry parameter measuring the degree of coupling between a localized (evanescent) state and propagating states\textsuperscript{25,64}. Whereas in general the lineshape described by eq. (6) has a characteristic asymmetric profile, if the coupling is strong ($|q| \to \infty$) it reduces to a resonant symmetric peak (Breit-Wigner), while weak coupling ($|q| \to 0$) is characterized by a a dip, or anti-resonance. To elucidate the origin of the low-energy resonance prevalent in nearly all panels of Fig. 8, it is instructive to inspect the LDOS at that energy, which is shown in Fig. 9 for two bubble shapes, and on both Cu and Au substrates. The LDOS in the presence of the square bubble on Au is strongly peaked in the regions between the horizontal edges of the aperture (top and bottom) and the outer edges of the ribbon. A fingerprint of the high coupling between the states can be seen as high LDOS on the edges\textsuperscript{65}. For this energy $E \simeq 0.05t_0$ at the threshold of the 1st to 2nd conductance plateau, the current is carried by a single mode (one can notice that $G = G_0$ throughout the 1st plateau) which is strongly localized around the edges of the nanoribbons because it is one of the characteristic edge states of a ZGNR. The LDOS profile in Fig. 9a shows the tendency to localize electrons between the horizontal PMF barriers and the ribbon edges, which means that the entire current path coming from the ZZ edge state overlaps spatially with the localized state, leading to a strong-coupling scenario between the confined and propagating modes. This, of course, is a consequence of the underlying PMF for this case: the fact that there is a considerable “leakage” of the PMF between the aperture and the outer edge drives electron confinement in that region of strong field and promotes the localization of electrons in a region through which all the current would be passing, thus promoting a strong coupling that leads to a well defined resonance. Comparison of panels a and b reveals that the LDOS obtained on Cu for the same bubble shape is not as sharply localized as on Au. And, as a result, the coupling to the propagating mode will not be as strong, which explains the fact that the resonance at $E \simeq 0.05t_0$ in Fig. 8a is not as sharp on Cu as it is on Au. While the conductance of the triangular bubble does not show resonant peaks, the effect of the corners is pronounced in Fig. 9c-d, where the high PMF at the corners favor the coupling of the confined state to its closer edge, and where in this case the upper zigzag edge presents high LDOS. This asymmetric coupling is reflected in the asymmetric conductance lineshape at $E \simeq 0.08t_0$.

Following the procedure employed in the analysis of the clamped bubbles, we analyze the local current density profile in order to understand the nature of the confinement hinted by the LDOS distribution seen in Fig. 9. Fig. 10 shows the current density for the triangular bubble at $E = 0.08t_0$. On Au, the current develops a local wide counterclockwise loop, dominated by a straight right-to-left current band near the top vertex of the substrate aperture and a straight left-to-right current band near the bottom side of the triangle. In this bubble, the PMF inside is negligible, and the current is only deflected outside the triangle, closing the loop. The corresponding current pattern on the Cu substrate shows two current loops within the triangle. Starting from the left edge of the panel where the ideal contacts are attached, the current flow is split by the strong PMF outside the sub-

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig10.png}
\caption{(Color online) Current density in the vicinity of the triangular bulges when graphene lies on (a) Au(111) and (b) Cu(111) substrates, both at $E = 0.08t_0$. The red outline marks the portion of the system corresponding to the bubble region.}
\end{figure}
substrate aperture into an upward and downward stream, which backflow towards the inside of the triangle upon reaching its leftmost side. Hence, in both Au and Cu, the current distribution in Fig. 10 is consistent with a strong tendency for electron confinement in the vicinity of the bubbles at energies near the conductance steps (or the VHS of the clean system). This confirms that the fine resonant features (peaks or dips) imprinted in the global conductance of the system are a reflection of this tendency for electron confinement that arises from the peculiar PMF pattern around the nanobubbles.

D. Armchair nanoribbons

So far we analyzed the quantum transport response of one square cell containing a nanobubble by attaching horizontal leads made of ideal graphene. This has resulted in an infinite ZGNR. In the same way, by connecting metallic leads to the vertical sides of the square cell the full system becomes an infinite AGNR of the same width (W \simeq 20 \text{nm}). The resulting conductance profiles for the various bubble shapes and the Au and Cu substrates are qualitatively and quantitatively similar to the behavior seen in the ZZ transmission configuration. For that reason, we omit a detailed analysis of the same physics in the interest of brevity. Nevertheless, for completeness, we show in Fig. 11 the conductance of an AGNR with a central square bubble in the three substrate scenarios (note that the fact that Fig. 11a seems to indicate a stronger detriment of the ideal conductance than in the ZGNR orientation stems from the fact that a square bubble in this orientation offers a strong PMF barrier perpendicular to the current flow).

III. FINAL REMARKS

Using a combined molecular dynamics–tight-binding simulation scheme we have investigated the electronic transport properties of graphene nanostructures containing nanobubbles of different geometries, and on top of different substrates. The local strain that develops within and nearby the bubble regions leads the rich patterns of strong PMF with alternating polarity on length scales of a few nm. The combination of both strong field and spatially sharp reversal of its polarity intuitively suggest a tendency for electron localization at certain energies. In this report, we have determined how this localization manifests itself (and impacts) the perspective of electronic transport. The analysis of the LDOS and local current distribution reveals the microscopic details of this localization process, and establishes that low-energy electrons can be confined in the vicinity or within the nanobubbles by the interplay of the specific PMF barrier created by the geometry of the bubble, mode mixing, and substrate interaction. Interestingly, graphene substrate interaction – unavoidable in real samples – facilitates the appearance of confined states at the same time that it determines their coupling to the propagating ones. At low energies, the coupling of the evanescent electron states in the vicinity of the nanobubbles leads to two distinct signatures in the conductance as a function of \( E_F \): (i) the appearance of peaks and asymmetric Fano resonances when the evanescent states spread considerably to the outside of the nanobubble; (ii) dips, or anti-resonances, when these states are confined mostly inside the nanobubble by the back and forth scattering of electrons between the PMF and, consequently, couple less effectively to the continuum.

We conclude that, even though under realistic conditions the interaction between graphene and the substrate is seen to strongly modify the spatial profile of the PMF distribution in relation to an ideal (clamped) scenario, the electrons can still be significantly confined under the rearranged local strain. If one follows the evolution of the PMF distribution, the progression from clamped bubbles to weakly interacting substrate (e.g. Au) to strongly interacting substrate (e.g. Cu) is characterized by, first, the “leakage” and broadening of the strong and sharp PMF barriers in the vicinity of the bubble edges, accompanied by the reduction of the overall field strength inside. Subsequently, the PMF pattern is dominated by the interfacial strain outside the bubble region, where the presence of the bubble becomes less important as compared to the graphene-substrate interaction. The spatial profile of the PMF is, hence, initially bubble-dominated evolving to substrate-dominated with the increase in substrate coupling. In any of these cases our calculations show that the tendency for electron confinement persists, despite the rearrangement of the pseudomagnetic barriers.
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