



Cite this: *Nanoscale*, 2015, 7, 15300

Conductance signatures of electron confinement induced by strained nanobubbles in graphene

Dario A. Bahamon,^{*a} Zenan Qi,^b Harold S. Park,^b Vitor M. Pereira^{c,d} and David K. Campbell^e

We investigate the impact of strained nanobubbles on the conductance characteristics of graphene nanoribbons using a combined molecular dynamics – tight-binding simulation scheme. We describe in detail how 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 of or within the nanobubbles by the delicate interplay among the pseudo-magnetic field pattern created by the shape of the bubble, mode mixing, and substrate interaction. The coupling between confined evanescent states and propagating modes can be enhanced under different clamping conditions, which translates into Fano resonances in the conductance traces.

Received 22nd May 2015,
Accepted 13th August 2015

DOI: 10.1039/c5nr03393d

www.rsc.org/nanoscale

The fine control over nanofabrication techniques has not only increased the performance of existing electronic devices,¹ 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 regime.^{2–5} 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 transmission.^{4,5} In addition, strong and sharp barriers generally beget richer transmission characteristics, including the stabilization of confined states within the barrier.⁶ 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 flow.^{7–11} The need for robust and tunable

confinement strategies is more fundamental in graphene electronic devices than in conventional semiconductors because the massless Dirac character of the charge carriers in graphene renders them more vulnerable to the phenomenon of Klein tunneling, and they cannot be adequately confined by standard electrostatic means, particularly in the ballistic regime. However, although 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 graphene electrons in largely the same way they would react to an external magnetic field in the bulk by purely mechanical means (*i.e.*, strain).^{12,13} 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) profiles.^{14–16} The development of Landau quantization in the absence of magnetic fields is one such prediction¹⁷ that was recently confirmed in local tunneling spectroscopy experiments.^{18,19} This shows that, even though strain doesn't break time-reversal

^aMackGraphe – Graphene and Nano-Materials Research Center, Mackenzie Presbyterian University, Rua da Consolação 896, 01302-907 São Paulo, SP, Brazil. E-mail: darioabahamon@gmail.com

^bDepartment of Mechanical Engineering, Boston University, Boston, MA 02215, USA

^cCentre for Advanced 2D Materials & Graphene Research Centre National University of Singapore, 6 Science Drive 2, Singapore 117546, Singapore

^dDepartment of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542, Singapore

^eDepartment of Physics, Boston University, 590 Commonwealth Ave, Boston, MA 02215, USA

symmetry, and consequently cannot generate a quantum Hall effect or chiral edge modes as a real field would, the spectral analogy is robust and supported by experimental evidence. Time-reversal symmetry can be explicitly broken by combining strain and magnetic fields, which breaks the valley degeneracy and can be explored for pseudomagnetic quantum dots whose sharp resonant tunneling characteristics might provide a very sensitive strain detector.^{20,21} The experiments of Levy¹⁸ and Lu¹⁹ with graphene nanobubbles confirm 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 Tesla; (ii) the possibility of having these fields localized in regions of only a few nm, if strain can be locally concentrated; (iii) the prospect of continuously varying the strength of the local PMF, in particular being able to establish and remove it on demand; and (iv) not requiring drastic extrinsic modifications of the graphene layer, thus preserving most of its intrinsic superlatives, namely the high mobility and the Dirac nature of its carriers. Recently, in order to gain more insight into details of the PMF magnitude and spatial profile associated with graphene nanobubbles, as well as to understand the role played by typical substrates, we (with several colleagues) conducted a study of the effects of nano-sized bubbles in graphene under different geometries and substrate conditions.²² In order to have a continuous and tunable range of deflection, the nanobubbles were generated by inflation under gas pressure against selected apertures on the substrate.²² In the present article, we revisit this problem from the point of view of electronic transport to elucidate the main signatures that circular and triangular nanobubbles, and their strong PMFs, imprint on the conductance characteristics. We are particularly interested in whether the large and local PMF leads to scattering and/or confinement that is significant enough to translate into modified transmission characteristics. This is directly relevant to scenarios such as the one explored in a recent experiment that shows selective 3-point electronic transmission across pressurized triangular graphene nano-blisters.²³ Existing theoretical work approaches this problem by straining graphene according to deformation fields that are either prescribed analytically or obtained numerically, but always following from the equations of continuum elasticity thus treating the graphene sheet as a continuum medium.^{24,25} Hence, even when performing tight-binding calculations on the honeycomb lattice, the widespread practice has been to obtain the deformations from continuum elasticity theory. If this is justifiable for deformation profiles that vary over characteristic distances that are large compared to the lattice parameter, it isn't so in the cases we are interested to describe here. One notable exception is the approach based on discrete differential geometry recently pioneered by Barraza-Lopez *et al.*^{26,27} which retains all the quantities parameterized on the lattice.

We tackle this in the same framework developed in ref. 22, 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, without assumptions, since they play an important role at these scales of less than 50 nm. Similar to what is observed for real magnetic barriers⁶ or Gaussian bump deformations,^{28,29} 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^{30–32} 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 circular and triangular graphene nanobubbles on hexagonal boron nitride.

1. 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 nanobubble 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).

It is beneficial to underline from the outset the role we attribute to the substrate in our modeling with regards to the electronic structure and transport: all the electronic action is taken to happen within the graphene sheet, which we assume not to be chemically perturbed in a significant way by the presence of the substrate underneath. This amounts to assuming that the electronic properties of graphene are completely decoupled from those of the substrate, the latter playing a rather passive role from this perspective, in that it simply stabilizes the static lattice configuration of graphene on which all the electronic action unfolds. This is a reasonable assumption for most current experimental scenarios, where graphene is physically transferred and deposited on a target substrate with a random orientation of the respective lattice directions. It also implicitly assumes substrates without reactive/dangling bonds that could strongly interact with those p_z orbitals that happen to be in registry and become a significant source of disorder. The most important aspect of this scenario of weak electronic coupling between graphene and the substrate is that we consider

electronic conduction taking place *only* through the graphene system, and its characteristics are determined solely by the electronic states derived from the p_z orbitals in the deformed and curved graphene. This is done so that the computations can be easily extended to tens of thousands of atoms, and relies on a tight-binding parameterization of the electronic dynamics that has been repeatedly shown to be reliable to describe low energy processes such as those involved in the electronic conduction. Moreover, a full *ab initio* consideration of the relaxation, electronic structure and quantum transport is unattainable in this context because (i) the deformation fields are highly non-uniform, (ii) graphene, substrate and gas atoms have to be all taken into account, and (iii) we wish to tackle the characteristic deformation scales seen in the experiments quoted above, all of which entail a large number of atoms in the minimal supercell. This justifies and motivates the multi-scale approach to this problem that we now describe in more detail.

1.1 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.^{34,35} 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 Tersoff potential was used to describe the C–B–N interactions. The parameters were adopted from ref. 36–38, the dimension of the simulation box was $20 \times 20 \times 8 \text{ nm}^3$, and circular and triangular apertures 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 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 1 nm. All simulations in the presence of the gas were carried out at room temperature (300 K) using the Nose–Hoover thermostat.³⁹

Since a previous study established that the magnitudes and spatial dependence of the strain-induced PMFs can be very sensitive to the clamping conditions and substrate type,²² we considered two 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.^{14,20,40} In the second scenario, we included a 1 nm thick substrate of h-BN and its interaction with the graphene sheet is explicitly taken into account. The Ar–BN (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 choice of the substrate is motivated by is the experimental observation that, for certain substrates such as boron nitride, graphene develops a nonuniform strain strong enough to induce an energy gap $\approx 20 \text{ meV}$ at the Dirac point,^{41–44} to introduce satellite Dirac points,^{45,46} and to allow the observation of a Hofstadter spectrum⁴⁷ in the presence of a magnetic field.⁴⁸ 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.

1.2. 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 15 088 lattice sites, an example of which is shown in Fig. 1. For convenience, we take the x axis parallel to the ZZ direction. Most low energy electronic properties of graphene are captured by the π band nearest-neighbor TB Hamiltonian

$$H = \sum_{\langle i,j \rangle} t_{ij} (c_i^\dagger c_j + c_j^\dagger c_i), \quad (1)$$

where c_i represents the annihilation operator on site i and t_{ij} is the hopping amplitude between nearest neighbor π orbitals (in the unstrained lattice $t_{ij} = t_0 \approx -2.7 \text{ eV}$). The link between the MD simulation and the TB Hamiltonian is made 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

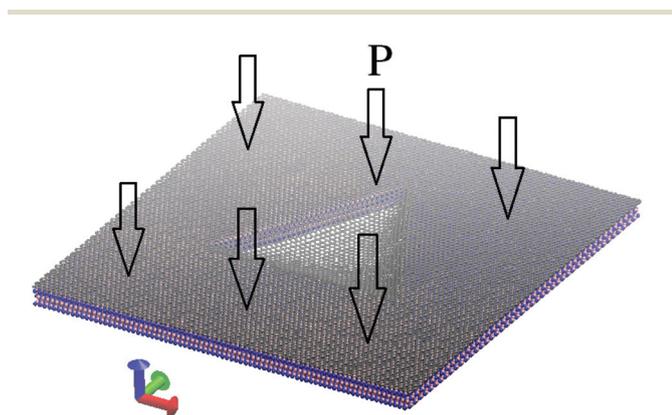


Fig. 1 Illustration of a MD simulation cell conveying the strategy used to generate the graphene nanobubbles. An aperture (a triangle in this case) is perforated on hexagonal boron nitride on which rests a monolayer of graphene (gray). Argon gas is then pressurized against graphene which bulges through 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.³³

all nearest-neighbors. The modification that accounts simultaneously for the changing distance d between neighbors and the local rotation of the p_z orbitals is given by:

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

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 σ and π bonds. Their dependence on the inter-atom distance is taken as^{22,49}

$$V_{pp\pi}(d_{ij}) = te^{-\beta(d_{ij}/a-1)}, \quad (3)$$

$$V_{pp\sigma}(d_{ij}) = 1.7 V_{pp\pi}(d_{ij}), \quad (4)$$

where $t = 2.7$ eV, $a \simeq 1.42$ 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. This approach captures all the possible modifications of the π -derived bands at the level of the Slater–Koster approximation. In particular, since nothing is assumed with regards to the position of the carbon atoms, it naturally includes effects such as the so-called pseudomagnetic field induced by non-uniform deformations, the scalar local deformation potential, and sublattice symmetry breaking terms if the atomistic configurations so allow.^{12,13,26,28,50} Since the edges of the central 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:^{51–53} $G = \frac{2e^2}{h} \text{Tr}[\Gamma_q G^r \Gamma_p G^a]$, where $G^r = [G^{a\dagger}]^\dagger = [E + i\eta - H - \Sigma_p - \Sigma_q]^{-1}$ is the retarded [advanced] Green's function, the coupling between the contacts and the central region is represented by $\Gamma_q = i[\Sigma_q - \Sigma_q^\dagger]$, and Σ_q is the self-energy of contact q which is calculated recursively for ZZ and AC contacts.⁵⁴ Having calculated the retarded and advanced Green's functions, other electronic properties such as the density of states (LDOS), $\rho_{ii} = -\text{Im}[G^r(\vec{r}_i, \vec{r}_i, E)]/\pi$, and the total density of states (DOS), $\rho = \text{Tr}(\rho_{ii})$ are readily calculated. For a local mapping of the current distribution in the central region we consider the current density between nearest neighbors,⁵¹ $I_{ij} = \frac{2e}{h} \int dE [t_{ij} G_{ij}^< - t_{ij} G_{ji}^<]$, that is calculated with the lesser Green's function, and which can be obtained exactly in

the absence of electronic interactions as⁵³ $G^< = G^r(E)[\Gamma_L(E)f_L(E) + \Gamma_R(E)f_R(E)]G^a(E)$. 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.⁵⁵ 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 eqn (2) via

$$A_x(\mathbf{r}) - iA_y(\mathbf{r}) = \frac{2\hbar}{3tae} \sum_n \delta t_{r,r+n} e^{i\mathbf{k}\cdot\mathbf{n}}. \quad (5)$$

This defines the two-dimensional pseudomagnetic vector potential, $A = (A_x, A_y)$,^{12,13} from where the PMF is calculated using $B = \partial_x A_y - \partial_y A_x$. Note that eqn (5) is used here only as a practical and direct means of quantifying the effect of the non-uniform strain in the electronic properties of graphene. It *does not* imply that we use this as an approximation for the PMF in graphene for, as stressed above, the general and realistic hopping model eqn (2) that we use in the transport calculations naturally includes effects that are not captured by such an approximation.

2. 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 (thus artificially) attached to their original position; any deformation occurs only within the aperture region under the gas pressure. Under this scheme the nanobubble in the middle of the ZGNR is the only extended scattering center, which allows us to isolate the effect of the bubble geometry and the corresponding PMF on the conductance. We chose two representative cases of aperture geometry for discussion: triangular and circular. The triangular aperture is particular because it begets a PMF that is appreciably uniform within most of the bubble area, and which does not alternate in sign within. The circular hole, on the other hand, is used because it captures most of the qualitative features of the PMF that sets in for a class of different shapes.²² For a meaningful comparison, circular and triangular bubbles are chosen with approximately the same area $\simeq 50$ nm², and centered within the square simulation cell; specifically, the radius of the circular aperture is 4 nm and the side length of the triangle is 10.6 nm. In a second stage, we analyze the conductance traces arising from the nanobubbles inflated against a h-BN substrate to determine whether the graphene–substrate interaction perturbs the conductance traces of the ideal clamped situation.

2.1. 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 $W \simeq 20$ nm of transverse dimension with an embedded bubble exhibits reproducible dips just at the onset of a every new conductance plateau. The conductance traces for circular and triangular nanobubbles are shown in Fig. 2(a) and (b) for a gas pressure of 19 Kbar, equivalent to a deflection of 1 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.^{56,57} The red dashed traces in Fig. 2(a) and (b) represent the conductance of the ideal ZGNR. By direct inspection, we see that the conductance is generally lowered relative to perfect quantization, and dips remain sharp for the circular bubble. The triangular bubble exhibits larger reduction from the quantized value within each plateau, together with broader dips (notwithstanding, the original plateau structure is still identifiable). The spectral fingerprint 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, as observed in Fig. 2(c) and (d).

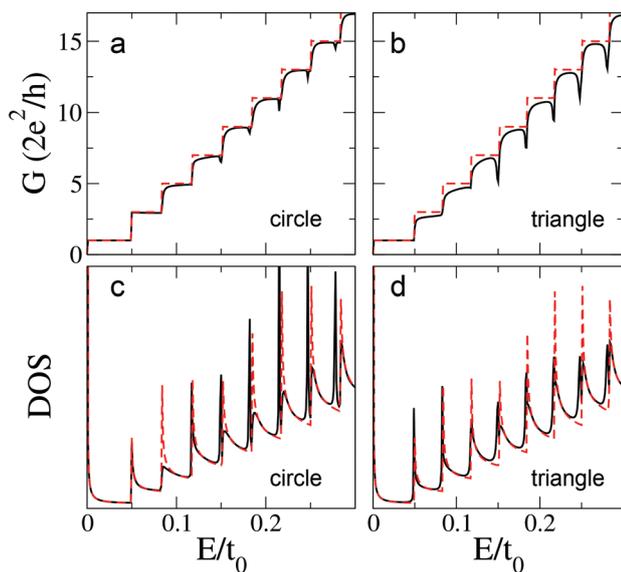


Fig. 2 Top rows present the conductance as function of the Fermi energy, E_F , for a ZZ GNR 20 nm wide with an embedded (a) circular and (b) triangular nanobubble. Bottom rows correspond to the Density of States (DOS) of the same ZGNR with (c) circular and (d) triangular bubbles. In all panels the carbon atoms outside the bubble region are rigidly clamped to the substrate and remain (artificially) undisplaced. The red dashed lines correspond to the conductance and DOS of a pristine graphene ribbon with ZZ edges state.

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,^{58,59} finite-range local potential scattering,^{60,61} and short-range impurity potentials.^{56,57,62–64} 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.⁵⁶ 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.⁵⁶ Of course, the transition rate depends also on the scattering potential itself, in addition to the density of evanescent states. As we 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 the clamped circular and triangular nanobubbles, and other geometries not considered here, can be found in ref. 22. For our current purposes, Fig. 3(a) and (b) shows the spatial profile of the PMF in the two geometries considered. We recall briefly that one of the leading characteristics 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.

The PMF graphs in Fig. 3(a) and (b) show that the circular bubble has high PMF barriers (~ 2000 T) at the perimeter, followed by a rapid decay towards the center of the bubble. Triangular bubbles, on the other hand, create PMFs of magnitude equally large around the perimeter and a roughly constant field of ~ 100 T in the inner central area. Unlike the behavior in circular bubbles, in triangular nanobubbles the intensity and polarity of the peripheral barrier remain constant at all the three edges. Based on this, 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 the wave function of the confined electron is distributed under such different strengths and patterns of PMF created by the bubbles. To clarify this point, let us inspect the LDOS maps shown in Fig. 3(c) and (d), each taken at the energy of the conductance dips observed at $E = 0.215t_0$. We see no fingerprint of a strictly confined state: the shape of the bubble itself is not even identifiable in either panel and,

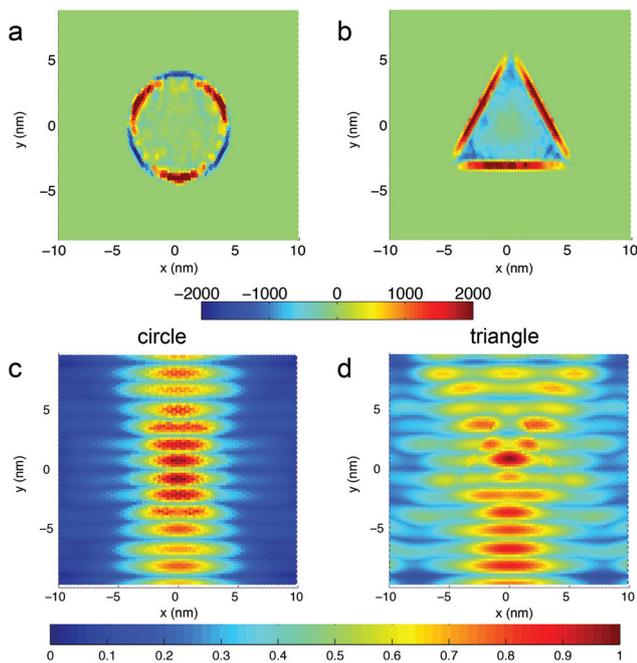


Fig. 3 Spatial maps of the PMF in the central scattering cell used in the transport calculations for the representative cases of a circular (a) and a triangular (b) nanobubble. The PMF calculated according to eqn (5) includes the hopping perturbations brought in by bond stretching and bending, as per eqn (2). Normalized local DOS for (c) circular and (d) triangular bubbles at $E = 0.215t_0$.

although the highest values of the LDOS are found within the bubble region, they are not significantly different from those outside.

To interpret these maps it is important to note that the unpressurized conductance of these systems at $E = 0.215t_0$ is $G(0.216t_0) = (2e^2/h) \times 11$. From the conductance quantization sequence of an ideal GNR, $G = (2e^2/h)(2n + 1)$,^{65,66} we conclude that there are 5 conducting modes in an ideal GNR at the energy represented in Fig. 3(c) and (d). The inclusion of the bubbles brings only a small change to this tally, as Fig. 2 shows that the conductance in their presence is, for the most part, scarcely modified: at $E = 0.215t_0$ one or more channels are backscattered because $G = (2e^2/h) \times (10.1)$ for the circle, and $G = (2e^2/h) \times (9.4)$ for the triangle. Despite this nominal suppression by 1 to 2 of the conducting modes, the conductance is never zero.

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 as described earlier, and whose results are presented in Fig. 4. The current map shown in Fig. 4(a) for the circular bubble reveals current streams 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. 3). Over the central region of the bubble the current remains predominantly horizontal

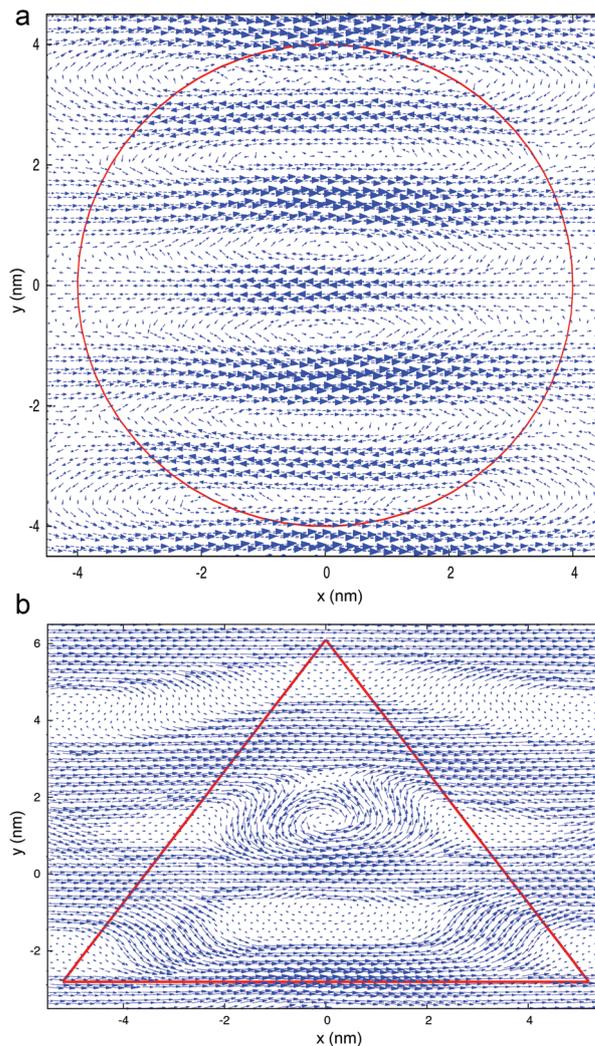


Fig. 4 (Color online) Current density at $E = 0.215t_0$ around the clamped circular bubble (a) and triangular bubble (b). The red outline marks the portion of the system corresponding to the bubble region. Each blue arrow indicates the local current flow, and has a magnitude proportional to the current at each lattice site.

by virtue of the negligible PMF inside a circular bubble. These strong bands decay outside bubble, confirming that this current pattern is associated with an evanescent mode created by the bubble through mode mixing. In contrast to the circle, a triangular bubble sustains a high and constant PMF ~ 100 T in the inner central region (*cf.* Fig. 3). Inspection of the current's spatial distribution in Fig. 4(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 eddy of current of at the center of the bubble. We note that an electron in graphene with energy $E = 0.215t_0$ in a constant magnetic field of 100 T has a magnetic length $\ell_B \approx 2.6$ nm and a cyclotron radius of $r_c = \ell_B^2 k_F \approx 6.8$ 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 dominated solely by the PMF but that bubble geometry and mode mixing are important ingredients. Finally, note that an electron should have an energy higher than $E \approx \hbar v_F \pi / L$ to be sensitive to a scatterer of typical size L . The average radius of the substrate apertures that we considered is $L \approx 4$ nm, which means that only above energies of $E \approx 0.16t_0$ should the electrons begin to be noticeably affected by the presence of the nanobubble. This estimate is quantitatively consistent with the fact that the conductance dips and DOS peaks, observed in Fig. 2, develop only above this energy and are not present at lower energies.

2.2. Nanobubbles on hexagonal boron nitride substrate

Whereas the previous section discusses transport in the presence of a nanobubble, but with the graphene layer rigidly clamped everywhere except the aperture region, in a realistic scenario, we must account for the graphene–substrate interaction. 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. To answer this question, we explicitly incorporate the graphene–substrate interaction at the atomistic level by carrying out MD simulations of triangular and circular graphene nanobubbles on a h-BN substrate, letting all the atoms in graphene to relax under the constraint imposed by the gas pressure. The PMF that obtains in this case is very similar to that shown previously in Fig. 3(a) and (b). This is, of course, not surprising given that outside the aperture region graphene is still being pressed against the rigid BN substrate; the magnitudes of the fields are, however, smaller, which is a direct consequence of the in-plane relaxation of the carbon atoms and the smaller in-plane strain that, consequently, sets in for the same deflection imposed on the bubble.

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 ($E < 0.150t_0$) or smaller ($E > 0.150t_0$) than the characteristic size of the central nanobubble. In Fig. 5(c) and (d) we show the conductance of a ZGNR with embedded circular and triangular bubbles on h-BN; we can see that the conductance traces – specially at low energies – are now richer than before. Interestingly, there is no marked difference between the two geometries; at higher energies, the presence of the bubble translates only into shallower and wider conductance dips.

One new feature detected in Fig. 5(c) and (d) is the presence of a resonant peak right at the start of the second plateau at $E \approx 0.05t_0$, and which replaces the conductance plateau of the unstrained system. The dips and resonances in the conductance are just two particular manifestations of a Fano resonance in the electron's scattering cross-section^{30–32} that are

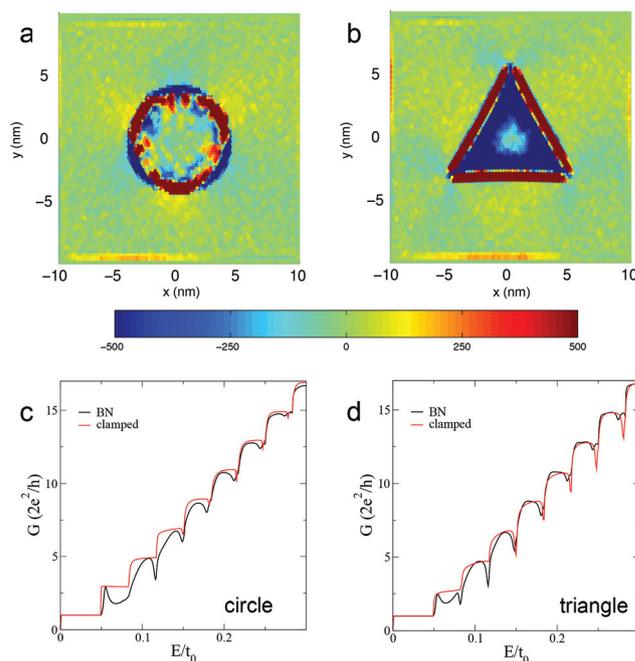


Fig. 5 (Color online) The top row shows the PMF spatial distribution for (a) circular and (b) triangular bubbles on h-BN substrate. Bottom rows show the conductance as a function of E_F for ZZ nanoribbons 20 nm wide placed on h-BN substrate, and containing a: (a) circular nanobubble and (b) triangular nanobubble. The red lines represent the conductance of the same geometry bubble in the clamped configuration.

imprinted in the conductance. In simple terms, a Fano resonance is characterized by a transmission probability of the form

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

in the neighborhood of $E = E_{\text{res}}$, where ε is the reduced energy and q the phenomenological Fano asymmetry parameter measuring the degree of coupling between a localized (evanescent) state and propagating states.^{31,67} Whereas in general the line shape described by eqn (6) has a characteristic asymmetric profile, if the coupling is strong ($|q| \rightarrow \infty$) the shape reduces to a resonant symmetric peak (Breit–Wigner), while in weak coupling ($|q| \rightarrow 0$) it becomes a dip, or anti-resonance.

To elucidate the origin of the low-energy resonance it is instructive to inspect the LDOS at that energy, which is shown in left panels of Fig. 6. The LDOS in the presence of the circular bubble on h-BN is strongly peaked in the regions between the top and bottom edges of the aperture and the outer edges of the ribbon. Such an enhancement of the LDOS at the edges constitutes a fingerprint of coupling between states.⁶⁸ For this energy $E \approx 0.05t_0$ 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. 6(a) shows the tendency to localize

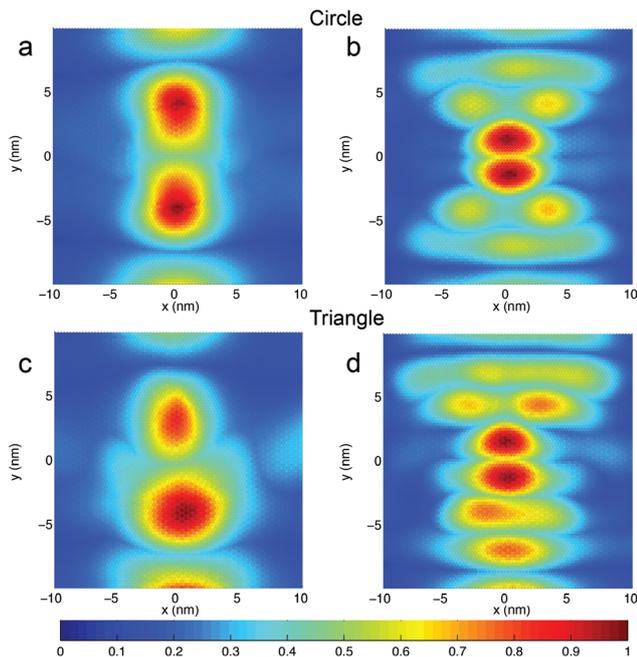


Fig. 6 (Color online) The top row shows the normalized local DOS for a circular bubble in graphene lying on a h-BN substrate for (a) conductance peak at $E = 0.05t_0$ and (b) conductance dip at $E = 0.116t_0$. The bottom row refers to a triangular bubble on h-BN substrate, at (c) the conductance peak for $E = 0.05t_0$ and (d) the conductance dip seen at $E = 0.116t_0$.

electrons between the perimeter of the circular bubble and the ribbon edges, which means that the entire current path coming from the ZZ edge mode 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 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. A comparison between panels a and c at the same energy for the triangular bubble shows, for the latter, an asymmetric enhancement of the LDOS in the vicinity of the upper and lower edges of the ribbon. As a result, the coupling to the propagating mode will not be as strong, which explains the fact that the resonance at $E \approx 0.05t_0$ in Fig. 5(d) is not as sharp as it is for the circular bubble. In contrast to the conductance resonances, the LDOS snapshots associated with dips are characterized by a strong enhancement in the central area, as can be seen in panels b and d of Fig. 6 for the conductance dip at $E = 0.116t_0$. For completeness, we show in Fig. 7 the respective current densities at the $E = 0.116t_0$ dip, which support the previous interpretation but show that the tendency for current localization is diminished in comparison with the rigidly clamped scenario, a consequence of the reduced strain in the present case.

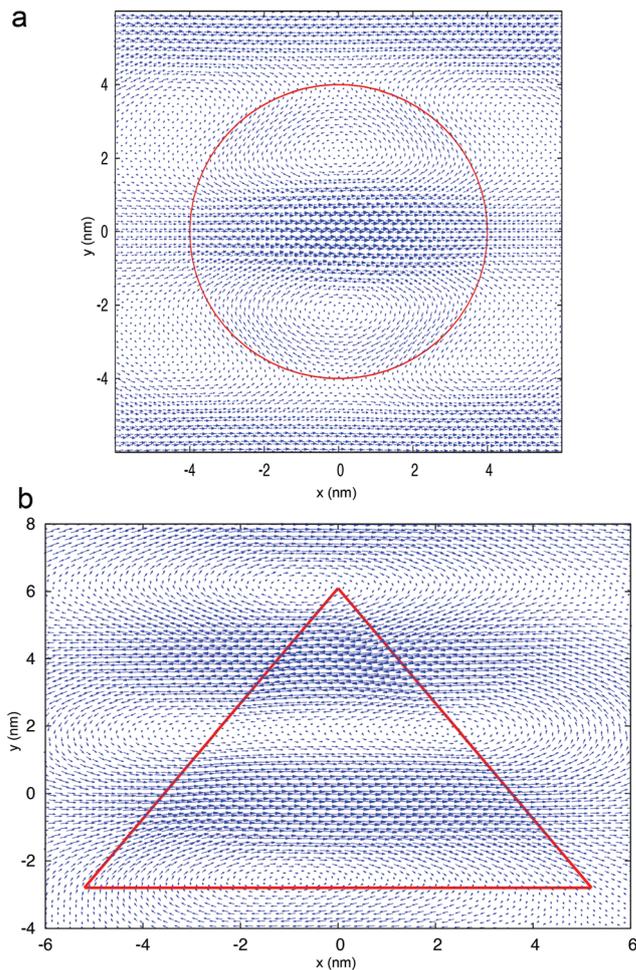


Fig. 7 (Color online) Current density in the vicinity of the (a) circular and (b) triangular bulges when graphene lies on h-BN substrate, both at $E = 0.116t_0$. The red outline marks the portion of the system corresponding to the bubble region.

Finally, we note that the type of graphene lead considered in computing the conductance has no bearing on the validity of the discussion and conclusions above. To illustrate this, we show in Fig. 8 the conductance of the same nanobubbles obtained with AC graphene nanoribbons as leads. This was done by connecting metallic AC leads to the vertical sides of the square system cell. The resulting conductance profiles are entirely similar to those seen in the ZZ transmission configuration, and the differences observed in the triangular case are due to the different orientation of the triangle (a 90° rotation) with respect to the incoming current.

3. Conclusions

Using a combined molecular dynamics – tight-binding simulation scheme we have investigated the electronic transport properties of graphene nanostructures containing circular and triangular nanobubbles and under two graphene–substrate

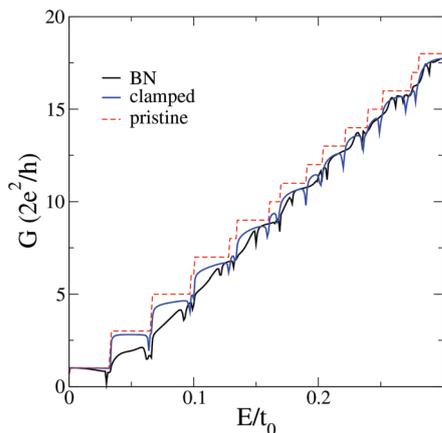


Fig. 8 (Color online) Conductance of a 20 nm AC nanoribbon with a triangular bubble in the central region. The different curves correspond to the conductance of a pristine ribbon (red), a bubble under clamped conditions (blue), and a bubble on the h-BN (black) substrate.

adhesion conditions. The local strain that develops within and near the bubble leads to rich patterns of strong PMF with alternating polarity on length scales of a few nm. The combination of both a strong field and spatially sharp reversal of its polarity intuitively suggests a tendency for electron localization at certain energies. We have determined how this localization manifests itself in (and impacts) the electronic transport. Analyses of the LDOS and local current distribution reveal the microscopic details of this localization process and establish that low-energy electrons can be confined in the vicinity of 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, or Breit–Wigner resonances, when the evanescent states spread considerably to the outside of the nanobubble; and (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 modify the magnitude and spatial profile of the PMF in relation to an ideal (clamped) scenario,²² there remains a significant tendency for electron confinement under the rearranged local strain.

Acknowledgements

VMP acknowledges support through Singapore NRF CRP grant “Novel 2D materials with tailored properties: beyond gra-

phene” (R-144-000-295-281). ZQ acknowledges the support of the Mechanical Engineering and Physics Departments at Boston University.

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