A numerical study of rippling instability driven by the electron-phonon coupling in finite size graphene membranes

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Suspended graphene exhibits ripples of size ranging from 50 to 100 Å and height ~10 Å, however, their origin remains undetermined. Previous theoretical works have proposed that rippling in graphene might be generated by the coupling between the bending modes and the density of electrons. These studies theoretically proposed that in the thermodynamic limit a membrane of single layer graphene displays a lattice instability for large enough electron-phonon coupling, undergoing a phase transition from a flat phase to a rippled one. In this work we solve the elasticity equations for a finite membrane of graphene coupled to the charge distribution, modeled in the tight-binding approximation, we find that the electron-phonon coupling controls a transition from a stable flat configuration to a stable rippled phase.

Since its early discovery in 2004 [1–4] graphene attracts the attention of the scientific community due to its unconventional and remarkable features. From the electronic point of view, fermions in graphene behave as relativistic massless particles [2, 5], as confirmed by their peculiar Quantum-Hall effect [2, 4], allowing for an outstanding mobility of the charge carriers [6, 7] and hence enhancing its transport properties. On the other hand, graphene possesses exceptional mechanical properties. Monolayer graphene membranes display a huge resistance against strains, which prevents their fracture [8], and even their existence seemed to challenge the Mermin-Wagner theorem [9], according to which long-wavelength fluctuations are expected to make 2D crystals unstable. However, graphene is extracted after growing within a 3D structure using different methods [1, 3]. In addition, as a membrane embedded in 3D space it can bend, and the anharmonic coupling between the bending (or flexural) and stretching modes can suppress long range fluctuations and make wrinkled membranes stable [10, 12]. However, when suspended graphene membranes are studied using transmission electron microscopy [13], the membrane exhibits long-lived ripples, remarkably different from a stable flat configuration plus thermal fluctuations [10, 12]. The origin of rippling in suspended graphene is still undetermined [14], and motivates this work.

Flexural modes in free-standing graphene influence the electronic density distribution, changing the electrical conductivity [15–17] and generating spatially varying gauge potentials [5, 18, 19], which leads to charge inhomogeneity [20] and underlies the formation of electron-hole puddles [21]. Further theoretical studies [22, 24] showed that the coupling between elastic and electronic degrees of freedom might be at the origin of ripples in graphene, as it can strongly suppress the long-wavelength bending rigidity, leading to enhanced fluctuations in the direction orthogonal to the membrane. These works, supported by both perturbative (one-loop approximation) [22] and non perturbative techniques [23, 24], identify a possible phase transition between the flat and rippled phases for a critical value of the coupling between strain and electron density. Other approaches simplify the problem modeling the electronic degrees of freedom as Ising spins, and coupling them with an elastic membrane. This makes natural the introduction of an external temperature, what produces a rich phase diagram [26–28]. In 1D, the model can be studied analytically, displaying first and second order phase transitions when controlling the temperature and the interaction between the spins [29].

In this work we use a model for graphene elasticity coupled to the electronic degrees of freedom. The electrons are modeled in the tight-biding approximation and we solve the problem on the honeycomb lattice. We prove that the coupling of the Dirac fermions to the elastic degrees of freedom causes suspended graphene to develop stable ripples, and study the nature of the transition from the flat phase in [30]. We find that the spatial distributions of heights and electronic density are strongly correlated with each other in the corrugated phase.

I. THE MODEL

We describe the elastic deformations of a membrane of monolayer graphene by the vector field \( \mathbf{u} = (u_x, u_y, h) \), where \( u_x, u_y \) are the in-plane deformations of the membrane with respect to the equilibrium position and \( h \) the out-of-plane shift. In the long-wavelength limit, the elastic energy of the membrane can be defined in terms of the strain tensor \( u_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i + \partial_i h \partial_j h) \) as [31]:

\[
E_{el} = \frac{1}{2} \int d^2 \mathbf{r} \left[ \kappa (\nabla^2 h)^2 + \lambda u_{ii}^2 + 2\mu u_{ij}^2 \right],
\]  

\( \kappa, \lambda, \mu \) being the bending and stretching elastic constants.
where repeated indices $i,j = x,y$ are implicitly summed. Here $\kappa$ is the bending rigidity and $\lambda, \mu$ are the Lamé coefficients. Typical values for graphene are $\kappa = 0.82$ eVÅ, $\lambda = 19.67$ eVÅ$^2$ and $\mu = 57.13$ eVÅ$^2$, where $a_0 = 2.46$ Å is the lattice constant. Finally, we have: $\lambda_0 = 3.25$ eVÅ$^{-2}$ and $\mu_0 = 9.44$ eVÅ$^{-2}$ [14, 32].

The kinetic energy of the electronic degrees of freedom is modeled within the tight-binding approximation. For electrons that can hop to nearest neighbors this is given by the following Hamiltonian [5]:

$$\hat{H}^{(0)}_e = -t_0 \sum_{\langle i,j \rangle} (\hat{a}^\dagger_{i\sigma} \hat{b}_{j\sigma} + h.c.)$$

(2)

where $t_0 \approx 2.7$ eV is the hopping integral, $\hbar = 1$, $\hat{a}$ and $\hat{b}$ are the fermionic annihilation operators defined on the two sub-lattices of the honeycomb lattice of graphene, $i,j$ are lattice coordinates and $\sigma$ is the index of spin. The low energy physics of the Hamiltonian [2] is well described by the continuum model for massless Dirac fermions:

$$\hat{H}^{(0)}_e \approx -v_F \int d^2r \sum_\sigma \bar{\psi}^\dagger_\sigma(r) \tau \cdot (-i\nabla) \psi_\sigma(r),$$

(3)

where $v_F = \sqrt{3}t_0 a_0/2 \approx 1 \times 10^6$ m/s is the Fermi velocity and $\tau = (\tau_x, \tau_y)^T$ are the Pauli matrices. The field operator can be expressed as: $\hat{\psi}^\dagger_\sigma(R) = v_0^{-1/2} \hat{a}_{RS} \hat{b}_{RS} e^{-iK\cdot R}$, where $v_0 = a_0^2 \sqrt{3}/2$ is the volume of the unit cell and $K = (4\pi/3a_0,0)$ is the Dirac point.

We introduce now an interacting term coupling the elastic modes of the membrane to the electronic charge distribution. Previous works proposed different coupling terms, either a scalar potential inducing charge fluctuations, or a gauge field inducing current fluctuations, see e.g. [33]. Since the latter are suppressed in the long-wavelength limit [23, 24], we consider only the effects of the scalar potential, that are described by the following Hamiltonian:

$$\hat{H}_{e-ph} = -g \int d^2r \hat{\rho}(r) u_i(r),$$

(4)

$$\delta \hat{\rho}(r) = \sum_\sigma \bar{\psi}^\dagger_\sigma(r) \psi_\sigma(r) - \rho_0,$$

(5)

where $\rho_0$ is the carrier density at equilibrium counted from the neutrality point. There is no consensus about the magnitude of the electron-phonon coupling $g$, recent estimates give values in the range $g \sim 4 - 50$ eV [34, 56].

It’s worth noting that we do not include the Coulomb repulsion between the electrons. We expect this will not qualitatively change our main results: even though it would play against charge accumulation, and therefore against the formation of ripples, it has been shown that the small quantum capacitance of graphene preserves the rippled phase [22, 23]. The overall effect of the Coulomb interaction is to increase the critical value of the electron-phonon coupling as compared to its bare value [24]. In addition, this effect becomes completely negligible when the Coulomb forces are screened by the presence of a substrate.

Finally, in our approach, the Hamiltonian describing the behavior of the graphene membrane takes the form,

$$\hat{H} = H_{el} + \hat{H}^{(0)}_e + \hat{H}_{e-ph}.$$  

(6)

We study the Hamiltonian of Eq. [6] within the Born-Hoppeppeiner (adiabatic) approximation, in which the quantum problem for the electrons is solved by treating the phonon fields as classical fields. In this approach, the displacements $u$ enter in the quantum problem as external parameters, via the interaction term $\hat{H}_{e-ph}$. The total energy of the membrane is then a functional of the displacement fields:

$$E_{tot}[u] = \langle H \rangle,$$

(7)

where the brackets denote the quantum average as computed by means of $H$ itself:

$$\langle \hat{O} \rangle = \frac{\text{Tr} \{ e^{-\hat{H}/K_BT} \hat{O} \} }{\text{Tr} \{ e^{-\hat{H}/K_BT} \} },$$

(8)

where $K_B$ is the Boltzmann constant, $T$ the temperature and $\hat{O}$ any operator.

In this work we study the equilibrium configurations of the membrane at $T = 0$, what makes the quantum operators contained in $\langle H \rangle$ to reduce to the sum of their eigenvalues. Finally, at $T = 0$ the equilibrium state of the system minimizes the total energy $\langle H \rangle$ with respect to the displacements. The Euler-Lagrange equations for this minimization problem are:

$$\frac{\delta E_{tot}[u]}{\delta u(r)} = 0.$$

(9)

At $T = 0$ the functional derivatives of $E_{tot}$ can be performed by means of the Feynman-Hellmann theorem, which allows to switch the order in which the derivatives and the quantum average are computed: $\frac{\delta E_{tot}[u]}{\delta u(r)} = \langle \frac{\delta \hat{H}}{\delta u(r)} \rangle$. Then the equilibrium condition [9] can be written as:

$$\frac{\delta E_{el}[u]}{\delta u(r)} + \left( \frac{\delta \hat{H}_{e-ph}}{\delta u(r)} \right) = 0,$$

(10)

which, in turn, is equivalent to the following system:
\[
\lambda \partial_x \left( \partial_x u_x + \partial_y u_y + \frac{|h|^2}{2} \right) + \mu \partial_x \left[ 2 \partial_x u_x + (\partial_x h)^2 \right] + \mu \partial_y \left( \partial_y u_x + \partial_x u_y + \partial_x h \partial_y h \right) = g \partial_x \delta \rho(x), \quad (11a) \\
\lambda \partial_y \left( \partial_x u_x + \partial_y u_y + \frac{|h|^2}{2} \right) + \mu \partial_y \left[ 2 \partial_y u_y + (\partial_y h)^2 \right] + \mu \partial_x \left( \partial_x u_y + \partial_x u_y + \partial_y h \partial_x h \right) = g \partial_y \delta \rho(x), \quad (11b) \\
\lambda \nabla \cdot \left[ \left( \partial_x u_x + \partial_y u_y + \frac{|h|^2}{2} \right) \nabla h \right] + \mu \partial_x \left[ 2 \partial_x u_x + \partial_x u_x + \partial_x h \partial_y h + \nabla h^2 \partial_x h \right] + \\
\quad + \partial_y \left[ 2 \partial_y u_y \partial_y h + (\partial_y u_x + \partial_x u_y) \partial_x h + |\nabla h|^2 \partial_y h \right] - \kappa (\nabla^2)^2 h = g \nabla \cdot (\delta \rho \nabla h), \quad (11c)
\]

where \(\delta \rho = \langle \delta \hat{\rho} \rangle\) is the charge distribution corresponding to the ground state of the electronic Hamiltonian: \(\hat{H}_{e}^{(0)} + \hat{H}_{e-ph}\), which also depend on the displacements \(u\). Finally, to find the minimum of \(\langle \hat{H}_{e} \rangle\), one has to solve equation (11) and diagonalize the electronic Hamiltonian on equal footing, i.e., to minimize energy, we have to solve a nonlinear eigenvalue problem. In the following section we explain the procedure that we use to perform this minimization.

The physical role played by each term in Eqs. (11) can be made more clear if we rewrite the equations in terms of an Airy potential, \(\chi\), which is defined as: \(\partial_x^2 \chi = \lambda u_{ii} + 2\mu u_{yy} - g \delta \rho, \partial_y \partial_y \chi = \lambda u_{ii} + 2\mu u_{xx} - g \delta \rho, \partial_x \partial_y \chi = -2\mu u_{xy}\). As shown in appendix [A], Eqs. (11) are equivalent to the Föppl-von Kármán equations [27, 28]:

\[
\begin{align*}
\kappa \nabla^2 h - 2\chi, h &= 0 \quad (12a) \\
\frac{1}{Y} \nabla^2 \chi + [h, h] &= -\frac{g}{2B} \nabla^2 \delta \rho, \quad (12b)
\end{align*}
\]

where \(Y = \frac{4\mu(\lambda + \mu)}{\lambda + 2\mu}\) and \(B = \lambda + \mu\) are the Young and compression moduli, respectively. Also, \([\chi, h] = \frac{1}{2} [\partial_x^2 \chi \partial_y^2 h + \partial_y^2 \chi \partial_x^2 h - 2(\partial_x \partial_y \chi)(\partial_x \partial_y h)],\) so that \([h, h]\) is the curvature of the membrane, as defined in Ref. [31]. Thus, the spatially varying electronic density, which is a superposition of eigenfunctions oscillating in space, acts as the source of curvature according to Eq. (12b). In turn, the curved membrane modifies the potential term in the Hamiltonian that is being diagonalized.

## II. SELF-CONSISTENT NUMERICAL APPROACH TO SOLVE THE COUPLED PROBLEM

To solve the system of equations (11) coupled to the eigenvalue problem for the electrons we first discretize all the terms on the hexagonal lattice with coordinates \(R\).

The details of this procedure are shown in appendix [B]. The quantum contribution of the electrons to the total energy is given by the following Hamiltonian:

\[
\hat{H}_{e} = -t \sum_{\langle R, R' \rangle} \left( \hat{\alpha}^\dagger_{R, \sigma} \hat{\beta}_{R', \sigma} + h.c. \right) - g \sum_{R} (\hat{n} - 1)(R) u_{ii}(R), \quad (13)
\]

where the contribution \(g \sum_{R} u_{ii}(R)\) acts just as a constant term which can be included in the elastic energy. The first term of the Eq. (13) is the usual tight-binding Hamiltonian on the hexagonal lattice, with the sum running over nearest neighbors sites and spin index. The second term introduces the coupling between the electrons and the deformation degrees of freedom. Here the local occupation number, \(\hat{n}(R)\), is given by:

\[
\hat{n}(R) = \begin{cases} 
\sum_\sigma \hat{\alpha}^\dagger_{R, \sigma} \hat{\alpha}_{R, \sigma}, & \text{if } R \in A \\
\sum_\sigma \hat{\beta}^\dagger_{R, \sigma} \hat{\beta}_{R, \sigma}, & \text{if } R \in B 
\end{cases} \quad (14)
\]

where \(A\) and \(B\) represent the two sub-lattices forming the hexagonal lattice, as described in appendix [B].

To solve the discretized version of equations (11) (see the appendix [B]), we use an iterative procedure.
brane is computed as the sum of the elastic and electronic placement fields, $E_{el} = E_{el} \alpha + E_n$, where $E_{el}$ is given by the discretized version of Eq. (1), and $E_n = 2 \sum_{\alpha \leq N/2} E_{\alpha}$. Note that a completely flat configuration with an homogeneous distribution of charge is always a solution of the Eqs. (11), although it can be not stable.

It is not practical to use the Föppl-von Kármán equations (12) instead of the elasticity Eqs. (11): we need additional differentiations to recover the stress and strain tensors from the potential $\chi$; see Appendix A. Since we solve spatially discretized equations, the additional differentiations would involve extra approximations when we discretize them.

III. NUMERICAL SOLUTION AND PHASE TRANSITION FROM FLAT TO RIPPLED MEMBRANE

Figures 1 and 2 show two solutions of equations (11), obtained within the method described in section II. We use a hexagonal lattice with 1536 atoms and periodic boundary conditions. The coupling parameter for these cases takes the value $g = 12t_0$, 10.5$t_0$. We start the iterative procedure with a Gaussian profile for the height field, $h$, peaked in the center of the membrane. The stationary solutions shown in the figures display a non-homogeneous distribution of the height and electronic density. This shows that the coupling introduced in the equations is enough to bring the system out of the flat configuration and to stabilize rippled configurations. Panels (a) and (b) depict a 3D plot and a 2D density plot of the height distribution, respectively. Sizable ripples can be observed as red and blue zones. The electronic occupation number counted from half-filling is shown in panel (c). The Fourier amplitudes of height and electronic density are shown in the bottom panels of both figures. These plots also show that both fields are correlated and share similar symmetries.

In the related paper [30] we identify a phase transition from the flat to the rippled membrane occurring by increasing the coupling parameter $g$. Remarkably, this transition takes place at a critical value $g_c > 0$. Studying this transition lies out of the aim of the present work, however, in Fig. 3 we show the configuration obtained for the finite value $g = 8t$, which turn out to be completely flat, meaning that $g_c > 8t$ for this system size. The dependence of $g_c$ on the system size is addressed in the Ref. [30] via a scaling analysis.

IV. DISCUSSION

We study the stationary solutions of an elastic membrane of graphene coupled to Dirac fermions. We propose a numerical method to iteratively solve the elasticity equations, discretized on the honeycomb lattice, minimizing the electronic energy on equal footing. Our method converges in a wide range of initial conditions to either a flat –undeformed– configuration or to a rippled one. We find that when the coupling between deformations and electron charge density, $g$, is sufficiently large, a stable rippled phase appears. Our results provide numerical evidence that align with previous theoretical works [22–24], that proposed the coupling between the electronic charge and the elastic degrees of freedom as the driving mechanism at the origin of rippling in suspended graphene sheets. Although our results are suggestive and give foundation to previous theoretical work, our method is limited by our capability to simulate membranes of realistic sizes. We can deal with system sizes of up to $10^3 - 10^4$ atoms, but much larger membranes require a very expensive numerical effort. In [30] we propose a variation of our method that allows us to effectively reach much larger sizes. We use it to systematically study the transition from undeformed to rippled configurations as $g$ reaches a critical value ($g_c$), unveiling a critical behavior of $g_c$ with system size.

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Appendix A: Derivation of the Föppl-von Kármán equations

Here we show how to use the Airy potential to rewrite elasticity equations (11) of the main text in the form of Föppl-von Kármán equations.

First of all, it is useful to introduce the stress tensor $\sigma_{ij} = \lambda \delta_{kk} \delta_{ij} + 2\mu u_{ij}$, (A1) which allows us to write Eqs. (11) as:

$$\partial_i [\sigma_{ij} - g (\delta \rho) \delta_{ij}] = 0 \quad i, j = x, y \quad (A2a)$$

$$\partial_i \left[ (\sigma_{ij} - g (\delta \rho) \delta_{ij}) \partial_j h \right] - \kappa (\nabla^2)^2 h = 0. \quad (A2b)$$

Eq. (A2a) is identically satisfied if we define the Airy potential, $\chi$, as:

$$\sigma_{xx} - g \delta \rho = \partial_y^2 \chi, \quad (A3)$$

$$\sigma_{yy} = \partial_y^2 \chi, \quad (A4)$$

$$\sigma_{xy} = -\partial_y \partial_x \chi, \quad (A5)$$

whereas Eq. (A2b) becomes:

$$\kappa \nabla^2 h - 2[\chi, h] = 0, \quad (A6)$$
Then we use Eqs. (A1) and (A3) to rewrite the left hand side of Eq. (A8) in terms of the Airy potential,

$$\chi, h \equiv \frac{1}{2} \left[ \partial_x^2 \chi \partial_y^2 h + \partial_y^2 \chi \partial_x^2 h - 2 \left( \partial_x \partial_y \chi \right) \left( \partial_x \partial_y h \right) \right] \begin{equation}
\text{(A7)}
\end{equation}
$$

To get an equation for $\chi$, we first check that

$$2 \partial_x \partial_y u_{xy} - \partial_x^2 u_{yy} - \partial_y^2 u_{xx} = [h, h]. \begin{equation}
\text{(A8)}
\end{equation}$$

Then we use Eqs. [A1] and [A3] to rewrite the left hand side of Eq. [A8] in terms of the Airy potential,

$$\frac{1}{Y} \nabla^2 \chi + [h, h] = - \frac{g}{2B} \nabla^2 \delta \rho, \begin{equation}
\text{(A9)}
\end{equation}$$

where $Y = \frac{4(\lambda + \mu)}{\lambda + 2\mu}$ and $B = \lambda + \mu$ are the Young and compression moduli, respectively. This equation, along with Eq. [A6], represent the Föppl-von Kármán equations for the membrane.

Appendix B: Discretizing the elasticity equations and the coupling to the electrons on the honeycomb lattice

In the following we describe the procedure used to discretize the continuum elasticity equations (10) of the main text on the honeycomb lattice, which basically recalls the approach of the Refs. [39] [40]. We also explain the general method that we used to solve the problem of the elastic membrane coupled to the electrons.

As usual, we describe the honeycomb lattice as consisting of two sub-lattices, that here we call of type $A$ and $B$. This is depicted in the Fig. 4 where the atoms of type $A$ are represented in red and those of type $B$ in cyan, although in the case of graphene the two species correspond to identical carbon atoms. Each atom of type $A$ has three first nearest neighbors of type $B$, that we labeled with the indices 1, 2, 3, and six second nearest neighbors of type $A$, labeled by the indices 4, ... 9. If the atom $A$ has coordinates $(x, y)$ then, according to the scheme of the Fig. 4, the coordinates of its nine nearest neighbors are:

$$n_1 = \left( x - \frac{a}{2}, y - \frac{a}{2\sqrt{3}} \right), \quad n_2 = \left( x + \frac{a}{2}, y - \frac{a}{2\sqrt{3}} \right),$$

$$n_3 = \left( x, y + \frac{a}{\sqrt{3}} \right), \begin{equation}
\text{(B1)}
\end{equation}$$

$$n_4 = \left( x - \frac{a}{2}, y - \frac{a\sqrt{3}}{2} \right), \quad n_5 = \left( x + \frac{a}{2}, y - \frac{a\sqrt{3}}{2} \right),$$

$$n_6 = \left( x - a, y \right), \quad n_7 = \left( x + a, y \right),$$

$$n_8 = \left( x - \frac{a}{2}, y + \frac{a\sqrt{3}}{2} \right), \quad n_9 = \left( x + \frac{a}{2}, y + \frac{a\sqrt{3}}{2} \right),$$

where $a$ stands for the lattice constant.

An analogous scheme, of course, holds for each atom of type $B$, with a similar definition of the nearest neighbors.

The first and second order partial derivatives that appear in the continuum equations (10) of the main text can be replaced by their corresponding finite differences on the lattice by introducing the following operators [39] [40]:

$$T f(A) = f(n_1) - f(A) + f(n_2) - f(A) \begin{equation}
\text{(B2a)}
\end{equation}$$

$$+ f(n_3) - f(A) \sim \frac{a^2}{4} \nabla^2 f$$

$$H f(A) = f(n_6) - f(A) + f(n_7) - f(A) \begin{equation}
\text{(B2b)}
\end{equation}$$

$$\sim a^2 \partial_x^2 f$$

$$D f(A) = f(n_4) - f(n_5) + f(n_9) - f(n_8) \begin{equation}
\text{(B2c)}
\end{equation}$$

$$\sim a^2 \sqrt{3} \partial_x \partial_y f,$$

$$\Delta_x f(A) = f(n_2) - f(n_1) \sim a \partial_x f \begin{equation}
\text{(B2d)}
\end{equation}$$

$$\Delta_y f(A) = \frac{f(n_3) - f(A) - [f(n_1) - f(A) + f(n_2) - f(A)]}{2} \begin{equation}
\text{(B2e)}
\end{equation}$$

$$\sim \frac{a}{\sqrt{3}} \partial_y f,$$

$$B f(A) = T f(n_1) - T f(A) + T f(n_2) - T f(A) \begin{equation}
\text{(B2f)}
\end{equation}$$

+ $T f(n_3) - T f(A)$, where $f$ is a generic function of the lattice positions.

The continuum electronic density $\rho$ and its deviation $\delta \rho$ appearing in the rhs of the Eq.s (10) of the main text can be replaced by the occupation number per site $n(R)$ and by $\delta n(R) = n(R) - n_0$, $n_0$ being the filling (we use $n_0 = 1$). Thus, the elasticity equations on the honeycomb lattice can be written as:
\[ 4\mu T u_x + (\lambda + \mu) H u_x + \frac{\lambda + \mu}{\sqrt{3}} \frac{D u_y}{a} + \frac{\lambda + \mu}{a} [\Delta_x h H h + \Delta_y h D h] + \frac{4\mu}{a} \Delta_x h Th = g \frac{\Delta_x \delta n}{a}, \quad (B3a) \]

\[ 4 (\lambda + 2\mu) T u_y - (\lambda + \mu) H u_y + \frac{\lambda + \mu}{\sqrt{3}} \frac{D u_x}{a} + \frac{4\lambda H}{a} (\lambda + 2\mu) \Delta_y h Th + \frac{\lambda + \mu}{a} \sqrt{3} [\Delta_x h Dh - 3\Delta_y h H h] = \]

\[ = g \frac{\sqrt{3} \Delta_y \delta n}{a}, \quad (B3b) \]

\[ \left( \frac{\lambda + 2\mu}{a} \right) \left\{ \Delta_x h (H u_x + 2\Delta_x h Dh / a + \Delta_x h H h / a) + \Delta_y h \left[ \sqrt{3} (4T - H) u_y + 3\Delta_y h (4T - H) h / a \right] \right\} + \]

\[ + \frac{\lambda + \mu}{a} \left[ D u_x \Delta_y h + \Delta_x h D u_y / \sqrt{3} \right] + \frac{4\lambda H}{a} \left[ \Delta_x u_x + \sqrt{3} \Delta_y u_y \right] + \frac{2(\lambda + 2\mu)}{a^2} Th \left[ (\Delta_x h)^2 + 3(\Delta_y h)^2 \right] + \]

\[ + \frac{\mu}{a} \left[ \sqrt{3} H u_y \Delta_y h + (4T - H) u_x \Delta_x h + 2\Delta_x u_x H h + 2\sqrt{3} \Delta_y u_y (4T - H) h + 2D h \left( \Delta_y u_x + \Delta_x u_y / \sqrt{3} \right) \right] - \]

\[ - \frac{16\kappa}{a^2} Bh = \frac{g}{a^2} \left[ 4T \delta n + \Delta_x h \Delta_x \delta n + 3\Delta_y h \Delta_y \delta n \right]. \quad (B3c) \]

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Figure 1. Displacements and charge distribution corresponding to a solution of the Eqs. (11), found following the iterative method described in section II. We simulate a hexagonal lattice with periodic boundary conditions, 1536 atoms and $g = 12t_0$. The simulation uses as initial condition a Gaussian profile for the height field $h$. (a) Position of each atom in real space. (b): Contour plot displaying the out-of-plane deformation of the membrane. (c) Contour plot displaying the electronic distribution throughout the system counted from the neutrality point $n = 1$. Red (blue) regions present a higher (lower) charge density compared to the homogeneous case where the charge density is the same at every site. (d)-(e) Amplitude of the Fourier components of the height and charge fields, in the Brillouin zone of monolayer graphene. Arbitrary units are used. Note that the height and charge distribution are spatially correlated.
Figure 2. As in Fig. 1 but obtained by using a smaller value of the electron-strain coupling: $g = 10.5t$. 
Figure 3. Height (a)-(b) and charge (c) corresponding to the completely flat solution obtained for $g = 8t$.

Figure 4. Neighbors of a given site of type $A$ (red). There are three first nearest neighbors 1, 2, 3 of type $B$ (cyan) and six second nearest neighbors 4, . . . 9 of type $A$. 