Spontaneous Strains and Gap in Graphene on Boron Nitride

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The interaction between a graphene layer and a hexagonal Boron Nitride (hBN) substrate induces lateral displacements and strains in the graphene layer. The displacements lead to the appearance of commensurate regions and the existence of an average gap in the electronic spectrum of graphene. We present a simple, but realistic model, by which the displacements, strains and spectral gap can be derived analytically from the adhesion forces between hBN and graphene. When the lattice axes of graphene and the substrate are aligned, strains reach a value of order 2%, leading to effective magnetic fields above 100T. The combination of strains and induced scalar potential gives a sizeable contribution to the electronic gap. Commensuration effects are negligible, due to the large stiffness of graphene.

I. INTRODUCTION

Hexagonal Boron Nitride (hBN) has been demonstrated as a promising insulating substrate for graphene. Both systems share the same lattice structure, with a lattice mismatch of $\delta = 1.8\%$. hBN is an insulator with a $\sim 5.2$ eV gap. The electronic carriers in graphene on hBN exhibit very large mobilities. $^{1-5}$

The electronic band structure of graphene placed over hBN is being intensively studied, both theoretically $^{6-15}$ and experimentally. $^{16-20}$ The earliest experiments on different samples showed conflicting results on the existence of an insulating state at the neutrality point. Some different samples showed conflicting results on the existence of a correlation between the electronic gap and the presence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)).

A recent experiment Re. $^{20}$ strongly suggests the existence of a correlation between the electronic gap and the formation of a peculiar strain pattern on graphene, measured both through conductive atomic force microscopy (AFM) and scanning tunnel microscopy (STM). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)). In the absence of strains (i. e. at large enough rotation angles (AFM) and scanning tunnel microscopy (STM)).

The paper is organized as follows. In Sec. [II] we set our notation and characterize the geometric moiré pattern as a function of lattice mismatch and twist angle. In Sec. [III] we describe our model for the energetics of adhesion and strain, and write the equilibrium solution for the displacements. We also obtain expressions for the associated pseudomagnetic fields. In Sec. [IV] we plot and discuss the results, including the spectral gap caused by the deformations in Sec. [V]. Finally, we draw our conclusions in Sec. [VI].

II. MOIRÉ SUPERLATTICE

Graphene and hBN exhibit a $\delta \approx 1.8\%$ lattice mismatch, $a_0' = (1 + \delta)a_0$, where $a_0 = 0.246$ nm and $a_0' = 0.251$ nm are the lattice parameters of graphene and...
hBN, respectively. Thus, a graphene monolayer placed on an hBN crystal will not be in perfect registry, even if their crystallographic axes are perfectly aligned. If both crystals remain strain-free when brought into contact, this results in the formation of a smooth hexagonal moiré pattern of period \( A_0 \approx 14 \) nm. If the two crystals are rotated by a relative angle \( \theta \), the moiré period is reduced.

The general form of \( A_0 \) is

\[
A_0 = |\vec{A}_1| = |\vec{A}_2| = \frac{1 + \delta}{\sqrt{1 + (1 + \delta)^2 - 2(1 + \delta)\cos \theta}} a_0
\]

where \( \vec{A}_i \) are the superlattice vectors and \( |\theta| \leq 30^\circ \). This result, and also general expressions for \( \vec{A}_1 \), is derived as follows. We write \( \vec{A}_i \), and the corresponding graphene (hBN) lattice vectors \( \vec{a}_i \), as the columns of the \( 2 \times 2 \) matrices \( \vec{A} = (\vec{A}_1, \vec{A}_2) = \vec{G}^{-1}/2\pi \), \( \vec{a} = (\vec{a}_1, \vec{a}_2) = \vec{g}^{-1}/2\pi \) and \( \vec{a}' = (\vec{a}_1', \vec{a}_2') = \vec{g}'^{-1}/2\pi \). By defining the mismatch-plus-rotation transformation \( \vec{a}' = \vec{R} \vec{a} \) between the two lattices,

\[
R = (1 + \delta) \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix},
\]

and noting that the conjugate momenta of the moiré pattern (rows of matrix \( \vec{G} \)) are defined as the mismatch between lattice momenta \( \vec{G} = \vec{g} - \vec{g}' \) we find \( \vec{A} = \vec{a} \vec{N} = \vec{a}' \vec{N}' \), where \( \vec{N} = \vec{a}^{-1}(1 - \vec{R})^{-1} \vec{a} \) and \( \vec{N}' = \vec{a}'^{-1}(1 - \vec{R}^{-1})^{-1} \vec{a}' \). Eq. (1) follows.

Note that an atomically periodic (commensurate) minimal superlattice is achieved for those values of \( \delta \) and \( \theta \) that result in fully integer matrices \( \vec{N} = 1 + \vec{N}' \). The analysis of the elastic properties that follows, however, are continuum theories that do not rely on precise commensuration, and are generally valid as long as \( A_0 \gg a_0 \).

For later convenience we define here \( \vec{G}_0' = 0 \), and the momentum “first star”, which extends the basis \( \vec{G}_{1,2,3} \) to the six integer combinations thereof that have equal modulus

\[
\begin{align*}
\vec{G}_0' &= 0 \\
\vec{G}_1' &= -\vec{G}_{-1} = (1,0) \vec{G} \\
\vec{G}_2' &= -\vec{G}_{-2} = (0,1) \vec{G} \\
\vec{G}_3' &= -\vec{G}_{-3} = (-1,-1) \vec{G},
\end{align*}
\]

We make similar definitions for \( \vec{g}_j' \) and \( \vec{g}_j'' \), where \( j = 0, \pm 1, \pm 2, \pm 3 \). A sketch of the reciprocal lattice vectors considered is shown in Fig. 1.

III. EQUILIBRIUM GRAPHENE DEFORMATION

The moiré superlattice defined in the absence of displacements consists in a smooth spatial variation of the local stacking pattern, which shifts continuously between AA-type (local alignment of both carbons in a unit cell to Boron and Nitrogen), AB-type (Carbon-on-Boron) and BA-type (Carbon-on-Nitrogen). Each of these configurations has a different associated adhesion energy density. Ab-initio calculations yield a lower energy for AB-stacking, while BA and AA are roughly similar. The difference between \( \epsilon_{AB}, \epsilon_{BA} \) and \( \epsilon_{AA} \) adhesion energies in different regions is denoted by

\[
\Delta \epsilon_{AB} = \epsilon_{AB} - \epsilon_{AA} \\
\Delta \epsilon_{BA} = \epsilon_{BA} - \epsilon_{AA}
\]

These differences in adhesion create in-plane forces in the two crystals. These forces induce distortions which maximize the area of the favorable AB-stacked regions, at the expense of the elastic energy. For a graphene monolayer placed on a thick hBN crystal, it is reasonable to neglect the distortions of hBN. We derive here expressions for the equilibrium graphene displacement field \( \vec{u}(\vec{r}) \), defined as a minimum of the total energy \( U = U_E + U_S \), where \( U_E \) is the elastic energy and \( U_S \) is the stacking energy (we neglect thermal effects).

A. Elastic energy

The elastic energy \( U_E \) per unit cell of a graphene deformation \( \vec{u}(\vec{r}) \) that is smooth on the atomic spacing is given by continuum elasticity theory,

\[
U_E = \frac{1}{N} \int_A \frac{1}{2} \left[ 2\mu \text{Tr}(\vec{u})^2 + \lambda (\text{Tr} \vec{u})^2 \right] d^2 r,
\]

where the integral covers a deformation supercell, assumed equal to the moiré supercell \( A \), which contains \( N \) graphene unit cells. Here \( \vec{u} = u_{ij} \) is the strain, and \( \lambda \approx 3.5 \) eV/Å² and \( \mu \approx 7.8 \) eV/Å² are the Lamé factors for graphene. Next, we expand the
deformation in harmonics $\tilde{u}_q = \tilde{u}_{-q}$

$$\tilde{u}(\vec{r}) = \sum_q \tilde{u}_q e^{i\vec{q} \cdot \vec{r}}$$

(4)

Note that, if we assume $C_3$-symmetric deformations, its harmonics are related by $2\pi/3$-rotations. Taking this into account, we may write all possible distortions as a combination of four pure classes, see Fig. 2. These are either even or odd respect to a given origin $\vec{r}_0$, depending on whether $\tilde{u}(\vec{r} - \vec{r}_0) = \mp \tilde{u}(-\vec{r} - \vec{r}_0)$ (imaginary or real harmonics if $\vec{r}_0 = 0$). They may also be purely longitudinal or purely transverse, depending on whether $\tilde{u}_q$ is parallel or perpendicular to $\vec{q}$.

In terms of the $\tilde{u}_q$ harmonics, we may diagonalize $U_E$,

$$U_E = \frac{1}{2} \sum q \tilde{u}_{-q} W_q \tilde{u}_q$$

The dynamic matrices $W_q$ read

$$W_q = (B \det a) W_q^\parallel + (\mu \det a) W_q^\perp,$$

where $\det a$ is the area of the graphene unit cell, $B = \lambda + 2\mu \approx 21.6 \text{ eV/Å}^2$ is graphene’s bulk modulus, and

$$W_q^\parallel = \left( \begin{array}{cc} q_x^2 & q_x q_y \\ q_x q_y & q_y^2 \end{array} \right), \quad W_q^\perp = \left( \begin{array}{cc} -q_x q_y & -q_x q_y \\ -q_x q_y & -q_x q_y \end{array} \right)$$

(5)

They satisfy $W_q = W_{-q} = W_q^T$. Note that purely transverse (longitudinal) distortions have only elastic energy contributions from $\mu W_q^\perp$ ($BW_q^\parallel$).

**B. Adhesion potential**

We next consider the periodic adhesion potential created by the hBN crystal on the graphene lattice. The simplest model for this potential $V_S(\vec{r})$ (“first star” model), is parameterized by $\Delta_{AB}$ and $\Delta_{BA}$ defined above, and is written, using the definition Eq. (3) of the first star hBN basis $\vec{g}_j$, as

$$V_S(\vec{r}) = 2 \Re \left[ v_S \left( e^{i\vec{g}_1 \cdot \vec{r}} + e^{i\vec{g}_2 \cdot \vec{r}} + e^{i(-\vec{g}_1 - \vec{g}_2) \cdot \vec{r}} \right) \right] + v_0$$

$$= \sum_{j = \pm 1}^3 v_j e^{i\vec{g}_j \cdot \vec{r}} + v_0$$

(6)

**FIG. 2.** Different types of $C_3$-symmetric distortions, depending on their longitudinal/transverse character, and their parity respect to the origin.

**FIG. 3.** Displacement field $\vec{u}$ in real space for rotation angle $\theta = 0$ (left), $\theta = 1.5^\circ$ (center) and $\theta = 4^\circ$ (right). Spatial positions are normalized to the moiré period $A_0$.

**FIG. 4.** Relative local expansion $\frac{1}{2}\Tr \epsilon$ in real space for rotation angle $\theta = 0$ (left), $\theta = 1.5^\circ$ (center) and $\theta = 4^\circ$ (right). Large values of the strain are obtained for $\theta = 0$.

**FIG. 5.** Adhesion energy density $\tilde{V}_S(\vec{r}, \tilde{u}(\vec{r})$) in real space, relative to the average adhesion $v_0$, for rotation angle $\theta = 0$ (left), $\theta = 1.5^\circ$ (center) and $\theta = 4^\circ$ (right).

**FIG. 6.** Normalized full width at half maximum (FWHM) of the hexagonal boundaries in the adhesion energy density, see Fig. 3 (left), as a function of rotation angle $\theta$, or moiré period $A_0$. 

$\theta^\circ$
Vector \( \vec{r} \) in Eq. (6) is the position, in the crystal plane, of the center of any given graphene unit cell, so that \( \vec{r} = 0 \) corresponds to AA stacking, and \( \vec{r} = \pm \vec{r}_0 = \pm (\vec{a}_1 + \vec{a}_2) / 3 \) corresponds to AB/BA stacking. The complex numbers \( v_j \) are defined as

\[
v_{j>0} = v_{j<0} = v_S = -\frac{\Delta \epsilon_{AB} + \Delta \epsilon_{BA}}{18} - \frac{\Delta \epsilon_{AB} - \Delta \epsilon_{BA}}{6\sqrt{3}}
\]

so that the adhesion potential is a local extremum at these points, and their difference is indeed \( \Delta \epsilon_{AB/BA} \). Note that the constant energy offset in Eq. (6), \( v_0 = (\epsilon_{AB} + \epsilon_{BA} + \epsilon_{AA}) / 3 \), is irrelevant for the purpose of computing the equilibrium deformations.

The total adhesion energy per graphene unit cell is the sum, over all \( N \) graphene unit cells positions \( \vec{R}_n \) contained in a moiré supercell, of the adhesion potential

\[
U_S = \frac{1}{N} \sum_n \tilde{V}_S(\vec{R}_n)
\]

The positions \( \vec{R}_n \) above are

\[
\vec{R}_n = \vec{r}_n + \vec{u}(\vec{r}_n)
\]

where \( \vec{r}_n = n \vec{a} \) are the unstrained unit cells positions, and \( n = (n_1, n_2) \) is a vector of integers. Using the fact that \( g_{\vec{a}} = 2\pi \), we have \( e^{i \vec{g}_j \vec{r}_n} = e^{i \vec{G}_j \vec{r}_n} = e^{-i \vec{G}_j \vec{r}_n} \), so that \( U_S \) reads

\[
U_S = \frac{1}{\det A} \int_A d^2 r \tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] \quad (7)
\]

\[
\tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] = \sum_{j=\pm 1}^{\pm 3} v_j e^{-i \vec{G}_j \bullet \vec{r}} e^{i \vec{G}_j \bullet \vec{u}(\vec{r})} \quad (8)
\]

where we have transformed the sum into an integral over the moiré supercell, of area \( \det A \), since the form of the integrand \( \tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] \) is now smooth on the atomic scale. This last step transforms our description into a continuum theory on the moiré supercell. Note however, that the large hBN momenta \( \vec{g}_j \) are retained, associated to the displacements \( \vec{u}(\vec{r}) \).

To minimize the total energy analytically we need to assume that displacements \( \vec{u} \) are small as compared to the hBN lattice constant. This is the linear distortion regime, and allows us to expand \( \tilde{V}_S \) to first order in \( \vec{u}(\vec{r}) \)

\[
\tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] \approx \tilde{V}_S [\vec{r}, 0] + \vec{u}(\vec{r}) \partial_\vec{r} \tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] \big|_{\vec{u}=0}
\]

Using, once again, a harmonic decomposition for \( \vec{u}(\vec{r}) \), Eq. (6), we arrive at an adhesion energy that depends only on the harmonics \( \vec{u}_j \) for momenta \( \vec{q} = \vec{G}_j \) in the first star of the moiré superlattice,

\[
U_S = i \sum_{j=\pm 1}^{\pm 3} v_j \vec{G}_j \vec{u}(\vec{G}_j)
\]

This is a generic feature of the linear distortion theory: if the microscopic adhesion profile \( \tilde{V}_S(\vec{r}) \) is composed of a set of harmonics with momentum \( \vec{q}_i = m_i \vec{g}_j \) (integer \( m_i \)), the linearised adhesion energy will depend only on distortion harmonics with momentum \( m_i \vec{G}_j \).

The equilibrium value of distortion harmonics \( \vec{u}_j \) are obtained by minimising \( U = U_S + U_E \). Since \( U_E \) is quadratic on \( \vec{u}_j \), all harmonics different from the \( \vec{u}_j \) in the adhesion energy will be zero in equilibrium. For the remaining six harmonics, we obtain, by differentiating \( U \),

\[
\vec{u}(\vec{G}_j) = \frac{i v_j \vec{G}_j}{\partial_\vec{G}_j \tilde{V}_S(\vec{G}_j)}
\]

This is the main analytical result of this section. At \( \theta = 0 \), the \( \vec{u}(\vec{G}_j) \) become \( \vec{u}(\vec{G}_j) = i(1 + \delta) v_j / (25\pi \vec{G}_j^2) \), since the form of the integrand \( \tilde{V}_S \) is now smooth on the atomic scale. This last step transforms our description into a continuum theory on the moiré supercell. Note however, that the large hBN momenta \( \vec{g}_j \) are retained, associated to the displacements \( \vec{u}(\vec{r}) \).

To minimize the total energy analytically we need to assume that displacements \( \vec{u} \) are small as compared to the hBN lattice constant. This is the linear distortion regime, and allows us to expand \( \tilde{V}_S \) to first order in \( \vec{u}(\vec{r}) \)

\[
\tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] \approx \tilde{V}_S [\vec{r}, 0] + \vec{u}(\vec{r}) \partial_\vec{r} \tilde{V}_S [\vec{r}, \vec{u}(\vec{r})] \big|_{\vec{u}=0}
\]

Using, once again, a harmonic decomposition for \( \vec{u}(\vec{r}) \), Eq. (6), we arrive at an adhesion energy that depends only on the harmonics \( \vec{u}_j \) for momenta \( \vec{q} = \vec{G}_j \) in the first star of the moiré superlattice,

\[
U_S = i \sum_{j=\pm 1}^{\pm 3} v_j \vec{G}_j \vec{u}(\vec{G}_j)
\]

This quantity has been measured to be greater than 2% (2043).

\section{C. Pseudogauge fields}

A strain field in graphene is known to produce an effective pseudogauge field, due to the modulation of nearest neighbor hopping amplitude \( t \approx 2.78 \) eV with the

\[
\mathbf{B}(\vec{r}) \text{ in real space for rotation angle } \theta = 0 \text{ (left), } \theta = 1.5^\circ \text{ (center) and } \theta = 4^\circ \text{ (right). Large fields above 200 T are produced by the strains.}
\]
displacements.\cite{25} In terms of the dimensionless parameter $\beta = d \log t/d \log a_0 \approx 2$, the pseudogauge potential is given by

$$\vec{A}(\vec{r}) = \pm \frac{\beta t}{e v_F} \left( \begin{array}{c} u_{xx} - u_{yy} \\ -2u_{xy} \end{array} \right) , $$

(12)

where the strain tensor $\vec{u}(\vec{r}) = u_{ij}(\vec{r})$ is written in a coordinate frame with AB bond aligned along the $y$ direction, and the $\pm$ sign correspond to each of the two valleys (we will specialize on the $+$ sector in the follows, the opposite one trivially related by time reversal symmetry). In the next section we will analyse the effect of this field on the low energy electronic structure.

If we consider, conf. the solution Eq. (10) that only the first star harmonics of $\vec{u}(\vec{r})$ are non-zero, we obtain a pseudogauge potential that is likewise within the first star, $\vec{A}(\vec{r}) = \sum_{j=\pm 1}^{3} \vec{A}_j e^{i\vec{G}_j \cdot \vec{r}}$, where the $\vec{A}_j = \vec{A}^\pm_j$ harmonics can be written, conf. Eq. (12), as

$$\vec{A}_j = \frac{\beta t}{e v_F} \left( \begin{array}{c} i \vec{G}_j \sigma_x \vec{u}_j \\ -i \vec{G}_j \sigma_y \vec{u}_j \end{array} \right) , $$

(13)

where $\vec{G}_j$ are Pauli matrices. The associated pseudomagnetic field $\vec{B}(\vec{r}) = \partial_x \vec{A}_y - \partial_y \vec{A}_x = \sum_{j=\pm 1}^{3} \vec{B}_j e^{i\vec{G}_j \cdot \vec{r}}$ has harmonics $\vec{B}_j = \vec{B}^\pm_j = -\vec{G}_j \sigma_y \vec{A}_j$.

It is interesting to note that while the typical equilibrium distortions of Eq. (10) scale as $A_0^2$ (since $W_{\vec{G}_j} \sim A_0^{-2}$), the pseudomagnetic field $\vec{B}$ contains two spatial derivatives that cancel this scaling, so, unlike $\vec{u}$, it is not expected to vanish as the angle $\theta$ increases. Its effect on the electronic structure, however, will be diminished, since the physically relevant ratio of magnetic length to moiré period will increase.

For the case when the hBN and graphene axes are aligned, we can use the estimate for the strain in Eq. (11), and obtain a typical value for the effective magnetic length $\ell_B = \sqrt{h/|\vec{B}|}$ in terms of the elastic properties of graphene and the adhesion to the substrate

$$\ell_B = \frac{3}{4 \sqrt{\pi}} \frac{h(1+\delta)A_0^2}{|\beta| \epsilon_{AA} - \epsilon_{AB}|} a_0 $$

(14)

FIG. 8. Range of variation of magnetic field $B$ throughout the sample as a function of rotation angle $\theta$, or moiré period $A_0$. Note the large $\sim 200$ T maximum fields, even for large angles, and the zero at $\theta_B \approx 1.5^\circ$.

FIG. 9. Pseudogauge potential $\vec{A}(\vec{r})$ in real space for rotation angle $\theta = 0$ (left), $\theta = 1.5^\circ$ (center) and $\theta = 4^\circ$ (right). Note the vorticity inversion at $\theta = \theta_B = 1.5^\circ$.

IV. DISCUSSION

The different quantities computed in the preceding section depend critically on the adhesion energy differences $\Delta \epsilon_{AB}/\epsilon_{BA}$, as compared to the typical elastic energy of graphene $\sim a_0^2 B \approx 97$ eV, multiplied by some power of $\delta \approx 1.8%$ (recall that $\lambda \approx 3.5$ eV/Å$^2$ and $\mu \approx 7.8$ eV/Å$^2$). The adhesion energies have been computed using different ab-initio and semi-empirical approaches\cite{19,20,21,22,23,24,25}. These calculations give values in the range of some tens of meV per unit cell for $\Delta \epsilon_{AB}$, and much lower for $\Delta \epsilon_{BA}$.

On the other hand, the experiment of Ref. 20 has observed a difference of at least 2% in the local lattice parameter between AB and AA regions. Using Eq. (11), we see that, if the elastic moduli of graphene are not significantly modified by the presence of hBN, the adhesion energy differences should be at least -60 meV/unit cell to account for the observed deformation, with Refs. 23 and 26 suggesting values even greater than -100 meV/unit cell when taking into account London dispersion forces. We use this latter value for $\Delta \epsilon_{AB}$, with $\Delta \epsilon_{BA}$ a tenth of that, which yields results in good agreement with the experiment.

The solution for the strain field of Eq. (10) is plotted in Fig. 3 for rotation angles $\theta = 0^\circ$, $\theta = 1.5^\circ$ and $\theta = 4^\circ$. We see that the magnitude of the displacements is indeed much smaller than the lattice constant $a_0$, but much larger than the lattice constant $a_0/2$, which justifies our linear expansion in $\vec{G} \vec{u}(\vec{r})$. We also see that at $\theta = 0$, the solution approaches a pure longitudinal mode, that is even respect to the AB point, see Fig. 2. This solution is thus dominated by local expansion. As the angle is increased, we see how the solution crosses over to an even-transverse mode respect to the AB point, which is dominated by local twists and increased shear. The local expansion $1/4 \text{Tr} \vec{u}$ associated to these distortions is shown in Fig. 4. The equilibrium strain for the adhesion and elasticity parameters used reaches very large values for $\theta = 0$. In the AB region the lattice expands by $da_0$, so that $a_0 + da_0 \approx a_0'$. The relative expansion $da_0/a_0 = 1/4 \text{Tr} \vec{u}$ reaches its maximum value $\delta = 1.8\%$, as corresponds to adhesion dominating the total energy. In the other regions the lattice compresses by a comparable, though somewhat smaller amount, so that the difference
surpasses 2%, as found experimentally\textsuperscript{20}.

The adhesion energy $V_\text{S}[^\mathbf{r}, \bar{u}(\mathbf{r})]$ is shown in Fig. \ref{fig:adhesion_energy}. The flat blue regions around $\theta = 0$ (left panel) correspond to AB regions in near-perfect registry, where the lattice locally expands by the effect of the adhesion. Surrounding these flat regions are sharp hexagonal boundaries, with (different) local maxima at the AA and BA points. It is clear that as the rotation angle $\theta$ increases and the moiré period decreases, the adhesion energy loses to the elastic energy, and the strain field is quickly suppressed. One way to quantify this effect is to analyse the $\theta$-dependence of the full width at half maximum (FWHM) of the adhesion potential as one moves between an AB region to the next. This is plotted in Fig. \ref{fig:adhesion_fwhm} A purely unstrained bilayer has a FWHM = $A_0/2$. We can see how this value decreases as $A_0$ is increased.

The spatial patterns of vertical Young modulus recently measured with atomic force microscopy (AFM) by Woods et al\textsuperscript{20} are strongly reminiscent of the adhesion potential profiles shown in Fig. \ref{fig:adhesion_energy}, including the small difference between AA and BA vertices along the hexagonal boundary (which are due to the finite $\Delta t_{BA} < 0$). It can be argued that the measured elastic modulus should indeed reflect, to certain extent, the spatial modulation of the adhesion potential, since a stronger adhesion should correlate to a stiffer elastic modulus with respect to vertical deformations. The FWHM of the experimental elastic modulus also shows a strong decrease as the angle approaches zero. However, the way this decrease happens is far more abrupt in the experiment than in our model, apparently dropping discontinuously at around $A_0 \approx 10$ nm ($\theta = 1^\circ$). This suggests effects beyond our present model, such as the possibility of additional contribution to the total energy, the formation of ripples whereby the interlayer distance acquires a spatial texture, or even a global commensurate-incommensurate transition, associated to a sudden jump in the area of the graphene sample as the angle is decreased\textsuperscript{27}. These considerations remain beyond the scope of this work, and require numerical computation of a rather different kind. We have evaluated within our analytical framework the effect of including additional harmonics to the adhesion potential in Eq. (9), as those described in Ref. \textsuperscript{12} but the results of Fig. \ref{fig:adhesion_fwhm} do not change qualitatively. We have likewise excluded the possibility of a first- and second-order phase transitions as a result of non-linear terms in Eq. (9). This is clear from the profile of the total energy $U$ around $\theta = 0$, shown in Fig. \ref{fig:total_energy} as a function of longitudinal/transverse and even/odd distortion amplitudes, $u_{\text{even/odd}} - L/T$. Note that the potential minimum in Eq. (10) (white dot in the figure) remains stable and is the true absolute minimum of the potential. This remains valid even in the unrealistic extreme of vanishing shear modulus (not shown).

Finally, the pseudomagnetic field associated to the strain is shown in Fig. \ref{fig:pseudomagnetic_field}. The large strains involved in the equilibrium configuration produce very large pseudomagnetic fields up to 200 T. Surprisingly, however, the spatial pattern experiences an inversion at a finite but small angle $\theta_B$, around which the pseudomagnetic field is suppressed and changes sign. The range of spatial variation of $B$ as a function of $\theta$ is shown in Fig. \ref{fig:pseudomagnetic_field} which reveals the inversion at $\theta_B \approx 1.5^\circ$. Analysing the vector potential $\vec{A}(\mathbf{r})$ at this particular rotation angle, we find a similar pattern as that in Fig. 3(left): while $\vec{A}(\mathbf{r})$ is non-zero, it has a vanishing curl, so it is a pure gauge (purely longitudinal field, odd respect AB, see Fig. 2). It’s vorticity, in fact, becomes inverted at this $\theta_B$. This is shown in Fig. \ref{fig:pseudomagnetic_field}. Apart from the field inversion, the typical magnitude of the pseudomagnetic field is roughly in the 100-200 T throughout all angles, although its physical effects on the electronic structure should be stronger at small angles, where the magnetic length greatly exceeds the moiré period.

\section{V. Spectral Gap}

The problem of assessing the spectral gap of graphene coupled to the gapped hBN crystal can be analysed assuming that the hBN gap ($\Delta_{\text{hBN}} \approx 5.2$ eV) is much larger than the energy scales under consideration. In this limit, its effect on graphene’s low energy effective Dirac Hamiltonian is the addition of a position dependent SU(2) self-energy $\Sigma^{(0)}(\mathbf{r})$. Its absolute magnitude is $m_0 = t_\perp^2/(\Delta_{\text{hBN}}/2) \approx 35$ meV, where $t_\perp \sim 0.3$ eV is the graphene-hBN hopping amplitude. The gap at the Dirac point can be approximated to first order in $m_0$ as
the spatial average average in a supercell $A$ of area $\det A$

$$\Delta_{\text{eff}} = \frac{1}{\det A} \int_A d^2 \mathbf{r} \left[ \mathbf{r} \cdot \nabla \mathbf{r} \cdot \nabla \mathbf{r} \right] + O(m_0^2)$$  \hspace{1cm} (15)

In the absence of strains, it can be shown that the local gap $\Delta_{\text{eff}} = \Delta_{\text{eff}}(\mathbf{r})$ has a zero average, so that the average gap is zero. The AB and BA regions will have a positive local gap $\Delta_{\text{eff}}(\mathbf{r}) = \Delta_{\text{eff}}(\mathbf{r}) = m_0$, while the AA region will have a negative local gap that exactly cancels the former, $\Delta_{\text{eff}}(\mathbf{r}) = -2m_0$.

The effect of spontaneous strains, as we saw, is to expand the AB regions at the expense of BA and AA. This breaks the cancelation of the average $\Delta_{\text{eff}}(\mathbf{r})$, and hence, strains will create a gap $\Delta_{\text{eff}} \neq 0$ at the Dirac point. In the extreme case that the effective AB-stacked area grows from $A/3$ to cover most of the supercell area $A$, the average gap will become $m_0 \approx 35$ meV. In the more realistic case described here, the linear size of the AB region at $\theta = 0$ is around 70% – 75% of the supercell diameter, which yields an estimate for the gap around 15 meV. A figure closer to the maximum $m_0$ would be obtained for stronger adhesion parameters, which would result in a larger AB region (smaller FWHM in Fig. 6).

Interestingly, it has been noted\textsuperscript{23} that in the presence of strains, there is another contribution to Eq. (15) that further increases the effective gap by around 40% [actually $\beta/(\sqrt{3}\pi)$, to be precise]. This comes about in second order of perturbation theory in the pseudogauge field $A(\mathbf{r})$ and the scalar potential $\Delta_{\text{eff}}(\mathbf{r})$. Crucially, both the $\sim m_0$ term in the preceding paragraph and this second order contribution are parametrically equal in a systematic expansion in the deformations $u$ and the inverse hBN gap $\Delta_{\text{hBN}}^{-1}$. A careful evaluation of the two contributions yields at $\theta = 0$,

$$\Delta_{\text{eff}} = \frac{2}{\sqrt{3}} \frac{1 + \delta}{\delta^2} \left( 1 + \frac{\beta}{\sqrt{3}\pi} \right) \times \frac{|m_{-}(\Delta_{\text{BA}}) - m_{+}(\Delta_{\text{AB}})|}{9a_0^2 B}$$

Here, $m_{\pm} = (\epsilon^{-1} \pm \epsilon^{-1}_v) / 2$ is given in terms of the conduction and valence band edges $\epsilon_{c,v}$ in hBN respect to graphene's neutrality point (if the gap is centered, $m_{-} = m_0$, and $m_{+} = 0$). Recall also that $\delta \approx 1.8\%$, $\beta \approx 2$, and $B \approx 19.1$ meV/$\AA^2$ is the bulk modulus of graphene. With our assumption for the adhesion energies, the gap at $\theta = 0$ is approximately $\Delta_{\text{eff}} \approx 20$ meV. This value for $\Delta_{\text{eff}}$ is in qualitative agreement with experimental observations\textsuperscript{21}.

VI. CONCLUSIONS

We have presented a model for the in-plane deformations of a graphene layer on a hBN substrate. The deformations, effective magnetic field, and average gap can be expressed in terms of the elastic properties of graphene, the lattice mismatch, and the adhesion energy between graphene and hBN, see Eqs. (11), (14), and (16). The estimates presented here give an electronic gap of a few tens of meV, in line with experiments. The average strains near perfect alignment are a few percent $\sim \delta$, and give rise to effective pseudomagnetic fields of order 50-100T. The pseudomagnetic length is a few nanometers, about one order of magnitude smaller than the dimensions of the superlattice unit cell, which should therefore lead to strong effects in the electronic structure.

The different components of the potential induced by the moiré superlattice include even and odd terms under spatial inversion of similar magnitude, as expected from an hBN substrate. The combination of a modulated scalar and gauge potential gives a contribution to the average gap which has the same parametric dependence and order of magnitude as the gap arising from the enlargement of the energetically favorable AB regions.

The main results arise from a competition between the rigidity of the graphene layer and the adhesion potential provided by the substrate. For realistic parameters, the graphene deformations are small, and pinning and commensuration effects are not important. In terms of an effective Frenkel-Kontorova model, the results presented here are consistent with a floating phase, with gapless acoustic modes.

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