

Straintronics and twistrionics in bilayer graphene

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(Received 26 November 2025; accepted 6 April 2026; published 29 May 2026)

The interplay of twist and strain in bilayer graphene enables the formation of moiré patterns and narrow bands that host correlated and topological phases. While magic-angle twisted bilayer graphene has been widely studied, strain provides an additional and realistic control knob for band engineering. In this work, we first generate a global method to construct commensurate supercells for arbitrary twist and heterostrain. Then, using atomistic tight-binding and strain-extended continuum models to study the commensurate structures, we identify configurations that minimize the bandwidth beyond the magic angle. The results reveal a strong dependence of band narrowing and topology on strain type, magnitude, direction, and lattice relaxation. Particularly, shear strain produces a stronger distortion than uniaxial strain. Including electron-electron interactions through a self-consistent Hartree potential shows that strain broadens the bare bands while reducing electrostatic renormalization. Strain also drives topological transitions as the narrow and remote bands hybridize, establishing twisted and strained bilayer graphene as a tunable platform for flat-band and topological phenomena.

DOI: [10.1103/r8sv-6xmp](https://doi.org/10.1103/r8sv-6xmp)

I. INTRODUCTION

The discovery of correlated phases and unconventional superconductivity in twisted bilayer graphene (TBG) has attracted significant attention over the last few years [1–11]. These phenomena are intrinsically connected to the emergence of very flat bands due to the moiré potential [12–15], induced by the lattice mismatch created by the twist or strain [16–21]. The quenching of the kinetic energy in the flat bands promotes the appearance of the observed electronic correlations. Any approach to understand the nature of the correlated phases in TBG must then start from a solid understanding of the nature and origin of the flat bands, supported by accurate modeling methods.

With only a relative twist, the flat bands are well known to arise at an infinite set of *magic angles*, the largest one being around 1° [12,15,22]. However, in practice the samples usually have at least some residual strain [23,24], defects [25–27], or even twist angle disorders [28–30], typically arising during their fabrication [31]. The presence of strains,

in particular, can significantly modify the geometrical and electronic properties of the system since the moiré acts as a magnifying glass [20,21,32–37]. Although this may be seen as undesirable, one can conversely use strains as an additional tune parameter in the system [23,33,38–40]. Compared to the twist, which only rotates the layers, strains distort the layers and thus can lead to a plethora of moiré patterns with potentially rich properties [21,41]. This has motivated recent experimental advances in developing techniques to induce and manipulate the strain in moiré heterostructures [40,42–44], opening a path to straintronics and twistrionics, whereby the electronic properties can be tuned by the combined interplay between twist and strain. Among different types of strain, uniaxial heterostrain is the most common type and has been observed in many experimental samples [4,32,34,37,45]. Consequently, most theoretical works focus on the effects of the uniaxial heterostrain. Recently, under some well-developed techniques, shear heterostrain is introduced to manipulate the moiré patterns [46–48].

A natural question, then, is how the presence of arbitrary strain and twist modifies the narrow bands in twisted bilayer graphene. An initial step involves computing the electronic spectra of the system and study its evolution under different kinds of relevant strain. Since narrow bands generally arise only under small lattice mismatches [12,15], at which the supercells can contain tens of thousands of atoms, previous studies have mostly employed extensions of effective continuum models under strain [19–21], or topological heavy fermion models [49,50]. Yet, despite its importance, there is

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no comprehensive study of the electronic properties under strain by means of more realistic approaches, such as atomistic models. The challenge for that relies not only on the huge size of the supercell, but also on the fact that under twist and strain the system is in general incommensurate, and it is not clear at which configurations there can actually be a commensurate solution [51]. The commensurate and incommensurate structures may in fact have distinct ground-state properties [52].

In this work, we present a comprehensive analysis of the tight-binding (TB) properties of twisted and strained bilayer graphene (TSBG), focusing on the optimal conditions for the emergence of narrow bands. Two relevant types of heterostrain are considered: uniaxial and shear (in the following, without specifying, strain refers to heterostrain). We first tackle the problem of obtaining commensurate structures under both twist and strain. We find that by generally adding a small biaxial strain, one can always find particular twist and strain values at which the system is commensurate. Using these commensurate structures, we then obtain the band structure and the density of states (DOS) by using a full atomistic TB model. We find that (1) albeit the strain tends to increase the bandwidth at the (nonstrain) magic angle [20,21], there are yet other twist angles at which the bandwidth can be minimum, resulting in a shift of magic angle with strain; (2) the emergence of narrow bands depends critically on the strain direction; (3) the shear strain produces a stronger distortion of the geometry and electronic properties of TSBG; and (4) the gap between the narrow and remote bands (induced by the lattice relaxation) is mainly determined by the strain-dependent bandwidth of the narrow bands.

Our atomistic results are then compared with those of the strain-extended continuum model [53–56], which introduces two main modifications: (1) the change in the moiré vectors by which electrons in the different layers are coupled through the moiré potential [21,41]; and (2) the introduction of strain-induced fields [57,58]. We show that with just a few suitable parameter choices, the continuum model yields results in excellent agreement with the TB ones. In particular, we find that the strain-induced gauge potential, accounting for the change in the hopping energies within the Dirac approximation [57], plays a key role in capturing the electronic behavior in TSBG. Using the strain-extended continuum model, we extend our analysis of the bandwidth evolution under twist and strain. We find that the twist angle at which the bandwidth is minimum sensitively depends on the strain direction. Yet, we remarkably see that the minimum bandwidth of the narrow bands (at the optimal twist angle) increases practically linearly with the strain magnitude.

We further consider the effect of electrostatic interactions, as accounted by the Hartree potential [59–61]. Due to the increase in bandwidth under strain, the Hartree effect is weaker than that in the only twisted configurations. Consequently, as the strain increases, there is a competition between the increase of bandwidth of the bare bands and the decrease of the Hartree potential. We show that the synergy between these effects can lead to bandwidths under twist and strain that are actually comparable, if not smaller, than those with only twist angles. As any comprehensive account of correlated phases must consider such strong renormalization of the spectra by

electrostatic interactions [62–66], we conclude that TSBG has the potential to be a platform for rich correlated phenomena.

Finally, we analyze the influence of strain on the topology of the narrow bands around the magic angle. By introducing a small mass term that breaks the inversion symmetry, we compute the valley Chern number C of the narrow bands for different strain magnitudes and directions. Due to the strain effect in both increasing the narrow bandwidth and reducing the remote bandgap, there are topological ($C = \pm 1$) to trivial ($C = 0$) transitions as the strain increases, with a nontrivial dependence on the strain direction. We show that these topological transitions take place when the narrow bands close their gap with the remote bands. In the noninteracting case, we find that the sum of Chern numbers in top and bottom narrow bands is always zero, i.e., they are both topological or both trivial. However, upon taking into account the electrostatic interactions we find asymmetrical topological transitions, whereby one narrow band can be topological while the other is trivial. We associate this behavior with the asymmetrical renormalization of the narrow bands due to the Hartree potential, which implies that they close their gap with the remote bands at different strain magnitudes.

The paper is organized as follows: In Sec. II, we introduce a general formalism for moiré commensurability with any twist and strain, and discuss the Dirac point shifts due to the moiré deformation. In Sec. III, we calculate the electronic structures by using the TB and continuum methods, including the uniaxial strain, shear strain, and lattice relaxations. These two models yield results in excellent agreement. Then, we investigate the narrow-band modulation by both twist and strain. In Sec. IV, we study the effect of the electronic interactions. The band topology with strain is investigated in Sec. V. Our conclusions follow in Sec. VI.

II. MOIRÉ COMMENSURABILITY WITH TWIST AND STRAIN

In order to employ the TB method to obtain the band structure, we first require a commensurate structure. Although for only twist configurations the set of commensurate twist angles is well known, there is no close expression for the set of twist and strain that give commensurate structures. In what follows, we will explicitly describe a global method to construct a commensurate structure of TSBG for a given twist angle and strain, taking into account different types of strain observed in experiments.

A. Structural analysis of the moiré patterns

1. Commensurate structures with twist

We consider two graphene layers rotated in the plane by an angle θ , with the rotation origin at the AA site, and assume the constructed supercell is commensurate with only one moiré pattern [67]. Each moiré pattern contains three different high-symmetry stackings, namely, AA, AB, and domain wall (DW) stackings, similar to the strained configuration shown in Fig. 1(a). For the nonstrain case, the rotation angle for the commensurate condition is [12,68]

$$\cos \theta = \frac{3i^2 + 3i + 1/2}{3i^2 + 3i + 1}, \quad i = 0, 1, 2, \dots, \quad (1)$$

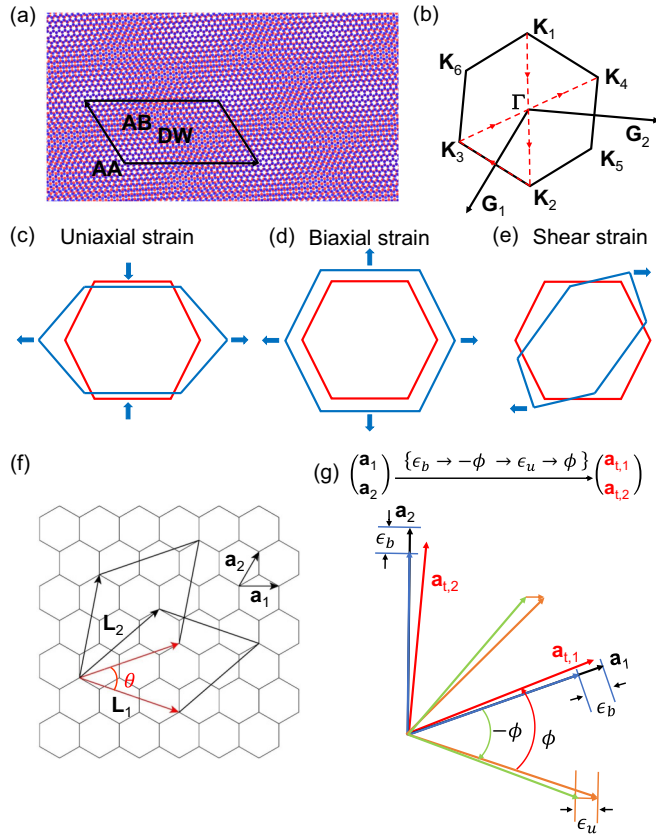


FIG. 1. (a) Moiré pattern of bilayer graphene with a twist angle $\theta = 3.89^\circ$ and uniaxial strain $\epsilon_u = 3.7\%$. The atoms in the top and bottom layers are plotted with blue and red dots, respectively. The AA, AB, and DW stacking regions are labeled. Due to the strain, the AA regions are elliptical. (b) Illustration of the moiré Brillouin zone, with the reciprocal lattice vectors labeled by $\mathbf{G}_1$ and $\mathbf{G}_2$. We label six corner K points. The red dashed line is the momentum path for the band structure plots. (c)–(e) Schematically show the uniaxial, biaxial, and shear strains, respectively. Only the top layer (blue line) is deformed. The undeformed bottom layer is plotted with red lines. (f) Schematic construction of the moiré cell with the lattice vectors of the two graphene layers. (g) Schematic construction of the moiré cell in three steps by following Eq. (9) with $\mathcal{E} \rightarrow \mathcal{E}_b + \mathcal{E}_{u/s}$: (1) an isotropic rescaling corresponding to ϵ_b ; (2) an anisotropic rescaling corresponding to ϵ_u in a direction given by ϕ ; and (3) a rotation by an angle θ . We only plot the first two steps in panel (g).

where i is an integer. The commensurate supercell vectors are

$$\begin{aligned} \mathbf{L}_1 &= i\mathbf{a}_1 + (i+1)\mathbf{a}_2, \\ \mathbf{L}_2 &= -(i+1)\mathbf{a}_1 + (2i+1)\mathbf{a}_2, \end{aligned} \quad (2)$$

where $\mathbf{a}_1 = a(1, 0)$ and $\mathbf{a}_2 = a(1/2, \sqrt{3}/2)$ are the lattice vectors of monolayer graphene, with $a \simeq 2.46 \text{ \AA}$ being the lattice constant. Therefore, a commensurate supercell with twist angle θ and vectors $\mathbf{L}_{1,2}$ is exclusively identified by the integer i .

When strain is introduced into the system, Eqs. (1) and (2) become invalid, and a general formalism is needed to determine the twist, strain, and moiré vectors of the commensurate structure.

2. Uniaxial, shear, and biaxial strains

We introduce three important strains that are reported by experiments. Assuming that the two-dimensional (2D) system has a homogeneous (position-independent) strain, an arbitrary two-dimensional strain tensor is given by

$$\mathcal{E} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} \\ \epsilon_{xy} & \epsilon_{yy} \end{pmatrix}, \quad (3)$$

where $\epsilon_{ij} = (\partial u_i / \partial x_j + \partial u_j / \partial x_i) / 2$, with $\mathbf{u}$ the displacement vector that accounts for the deformation induced by stress [69,70]. The three relevant types of strain that we shall consider are uniaxial, shear, and biaxial [Figs. 1(c)–1(e)]. Their corresponding strain tensors read [20,21,41,53]

$$\mathcal{E}_u = R_\phi \begin{pmatrix} \epsilon & 0 \\ 0 & -\nu\epsilon \end{pmatrix} R_{-\phi} \quad (\text{uniaxial}), \quad (4)$$

$$\mathcal{E}_s = R_\phi \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix} R_{-\phi} \quad (\text{shear}), \quad (5)$$

$$\mathcal{E}_b = \begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix} \quad (\text{biaxial}). \quad (6)$$

Here, $R_\phi \equiv R(\phi)$ is the rotation matrix, ϵ is the strain magnitude, ϕ is the strain direction relative to the x axis, and ν is the Poisson's ratio ($\nu \simeq 0.16$ in graphene). The shear strain can be written as

$$\mathcal{E}_s = R_{\phi+\pi/4} \begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix} R_{-\phi-\pi/4}. \quad (7)$$

Comparing with the uniaxial strain tensor, we then have the relation

$$\mathcal{E}_s(\epsilon, \phi) = \mathcal{E}_u(\epsilon, \phi + \pi/4, \nu \rightarrow 1). \quad (8)$$

This means that a shear strain with magnitude ϵ and direction ϕ_s can be thought of as uniaxial strain with magnitude ϵ and direction $\phi_u = \phi_s + \pi/4$, but with Poisson's ratio $\nu \rightarrow 1$ (i.e., the limit case in which the lateral contraction is equal to the applied longitudinal tension).

In this paper, we restrict ourselves to TBG with a heterostrain, which refers to relative strains between two layers. In general, the heterostrain can be unintentional or intentional. The unintentional heterostrain is commonly generated without control during the sample growth or fabrication [32]. The intentional heterostrain can be induced externally and designed carefully by well-established strain techniques, for instance, the substrate out-of-plane bending [43], process-induced strain [40], and sliding-based strain [23,44,48] (see, e.g., Ref. [71] for more details about these strain techniques). In our model, we will specifically assume that the top layer is strained and the bottom layer is rotated. Note that our definition of heterostrain differs from that in Refs. [20,21], where the two layers are strained in opposite directions with equal magnitude, i.e., a symmetric configuration. Instead, our definition is closer to the experimental cases in Refs. [4,32], where the concept of heterostrain was first introduced. These two types of heterostrain show slightly different modifications of the geometrical and electronic properties of the moiré systems. However, these two definitions induce practically the same perturbation effects to the TBG around the first magic angle and are indistinguishable in both theory [72] and experiments [46,48].

3. Moiré geometry with twist and strain

An application of strain in the top layer and a rotation in the bottom layer transform their lattice vectors as

$$\begin{aligned}\mathbf{a}_{t,i} &= (\mathbb{I} + \mathcal{E})\mathbf{a}_i, \\ \mathbf{a}_{b,i} &= R_\theta \mathbf{a}_i,\end{aligned}\quad (9)$$

where $\mathbb{I}$ is the 2×2 identity matrix. The reciprocal vectors follow as

$$\begin{aligned}\mathbf{b}_{t,i} &= (\mathbb{I} + \mathcal{E})^{-1}\mathbf{b}_i, \\ \mathbf{b}_{b,i} &= R_\theta \mathbf{b}_i,\end{aligned}\quad (10)$$

where $\mathbf{b}_i$ are the reciprocal lattice vectors of the honeycomb lattice. The reciprocal moiré vectors $\mathbf{G}_i$ [see Fig. 1(b)] can then be calculated by taking the difference between the deformed lattice vectors in each layer [18,21,41,73]

$$\mathbf{G}_i = \mathbf{b}_{t,i} - \mathbf{b}_{b,i}. \quad (11)$$

The real space moiré vectors $\mathbf{L}_i$ are determined by the relation $\mathbf{L}_i \cdot \mathbf{G}_j = 2\pi\delta_{ij}$. In principle, the moiré vectors $\mathbf{G}_i$ and $\mathbf{L}_i$ define the moiré structure [20,41]. However, in practice, the definition of $\mathbf{L}_i$ does not guarantee commensurability in the supercell.

4. Commensurate structures with twist and strain

In this part, we develop a general geometrical formalism for commensurate structures in TSBG. The analysis of the commensurate supercell can be performed by expressing the moiré lattice vectors as a function of those of the two graphene layers, as shown in Fig. 1(f):

$$\begin{pmatrix} \mathbf{L}_1 \\ \mathbf{L}_2 \end{pmatrix} = \begin{pmatrix} i & j \\ k & l \end{pmatrix} \begin{pmatrix} \mathbf{a}_{t,1} \\ \mathbf{a}_{t,2} \end{pmatrix} = \begin{pmatrix} m & n \\ q & r \end{pmatrix} \begin{pmatrix} \mathbf{a}_{b,1} \\ \mathbf{a}_{b,2} \end{pmatrix}. \quad (12)$$

Then, the top and bottom graphene lattices can be related by a Park-Madden transformation matrix

$$\begin{aligned}\begin{pmatrix} \mathbf{a}_{t,1} \\ \mathbf{a}_{t,2} \end{pmatrix} &= \frac{1}{il - jq} \begin{pmatrix} lm - jq & ln - jr \\ -km + iq & -kn + ir \end{pmatrix} \begin{pmatrix} \mathbf{a}_{b,1} \\ \mathbf{a}_{b,2} \end{pmatrix} \\ &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \mathbf{a}_{b,1} \\ \mathbf{a}_{b,2} \end{pmatrix}.\end{aligned}\quad (13)$$

For an arbitrary transformation matrix composed of contributions of twist and strain, there are four variables (a, b, c, d) corresponding to a pair of eight integers (i, j, k, l, m, n, q, r) that define the Park-Madden matrix. The set of eight integers can be determined experimentally through atomically resolved microscopy [32,73].

The analysis of the commensurate supercell also can be expressed as a function of the elementary geometrical deformations in Eq. (9), which in general depends on four parameters: the twist angle and the three components of the strain tensor. These four parameters completely determine, in principle, the (2×2) matrix in Eq. (13). If, for simplicity, one assumes that the system contains only uniaxial or shear strain, then one is left with only three parameters, namely, the twist and the strain magnitude and direction. Therefore, we introduce an additional—extremely small—biaxial strain in the top layer, so that Eq. (9) becomes $\mathbf{a}_{t,i} \rightarrow (\mathbb{I} + \mathcal{E}_{u/s} + \mathcal{E}_b)\mathbf{a}_i$ [see Fig. 1(g)]. Then, the system has four parameters

$(\theta, \epsilon_{u/s}, \phi, \epsilon_b)$ that can *fully* determine the set of eight integers in Eq. (13). To obtain the commensurate solutions, it is convenient to rewrite $\mathbf{a}_{t,i} \simeq (\mathbb{I} + \mathcal{E}_b)(\mathbb{I} + \mathcal{E}_{u/s})\mathbf{a}_i$ by taking $\mathcal{E}_b \mathcal{E}_{u/s} \rightarrow 0$ under the limit of small deformations. The transformation matrix that links $(\mathbf{a}_{t,1}, \mathbf{a}_{t,2})$ with $(\mathbf{a}_{b,1}, \mathbf{a}_{b,2})$ can then be written as

$$\begin{pmatrix} \mathbf{a}_{t,1} \\ \mathbf{a}_{t,2} \end{pmatrix} = P(1 + \epsilon_b)(\mathbb{I} + \mathcal{E}_{u/s})R_\theta P^{-1} \begin{pmatrix} \mathbf{a}_{b,1} \\ \mathbf{a}_{b,2} \end{pmatrix}, \quad (14)$$

where $P = \begin{pmatrix} 1 & 0 \\ 1/2 & \sqrt{3}/2 \end{pmatrix}$ is the basis of the triangular lattice vectors. By combining Eqs. (13) and (14), we can relate the physical parameters $(\theta, \epsilon_{u/s}, \phi, \epsilon_b)$ to the eight integers (i, j, k, l, m, n, q, r) [73].

The described procedure to obtain commensurate structures can be generalized to any arbitrary strain tensor, with the inclusion of lattice relaxation effects [74]. A detailed, step-by-step algorithm of how to obtain commensurate structures with any twist and strain, with some example solutions, can be found in Secs. S1 and S2 of the Supplemental Material [75].

B. Dirac point shifts from moiré geometry deformation

When the strain is small, we can consider that the length of the two moiré vectors remains, to a first approximation, practically equal. In that case, the borders of the moiré Brillouin zone (mBZ) are given by the three points [see Fig. 1(b)] [21]:

$$\begin{aligned}\mathbf{K}_1 &= -\frac{(1 + 2\chi)\mathbf{G}_1 - \lambda\mathbf{G}_2}{2(1 + \chi)}, \\ \mathbf{K}_3 &= \mathbf{K}_1 + \mathbf{G}_1, \\ \mathbf{K}_5 &= \mathbf{K}_1 + \mathbf{G}_1 - \lambda\mathbf{G}_2,\end{aligned}\quad (15)$$

and their negatives. Here, $\chi = |\mathbf{G}_1 \cdot \mathbf{G}_2|/|\mathbf{G}_1| |\mathbf{G}_2|$ and $\lambda = \text{sign}(\mathbf{G}_1 \cdot \mathbf{G}_2) + \delta_{0, \mathbf{G}_1 \cdot \mathbf{G}_2}$. When the angle between $\mathbf{G}_1$ and $\mathbf{G}_2$ is 120° , the moiré pattern is triangular and the points above collapse to yield a hexagonal mBZ.

Next, we check how the undeformed Dirac points, at the corners of the graphene BZ, are mapped into the mBZ. First, we translate Eq. (12) to the reciprocal space as

$$\begin{aligned}\begin{pmatrix} \mathbf{b}_{t,1} \\ \mathbf{b}_{t,2} \end{pmatrix} &= \begin{pmatrix} i & k \\ j & l \end{pmatrix} \begin{pmatrix} \mathbf{G}_1 \\ \mathbf{G}_2 \end{pmatrix}, \\ \begin{pmatrix} \mathbf{b}_{b,1} \\ \mathbf{b}_{b,2} \end{pmatrix} &= \begin{pmatrix} m & q \\ n & r \end{pmatrix} \begin{pmatrix} \mathbf{G}_1 \\ \mathbf{G}_2 \end{pmatrix}.\end{aligned}\quad (16)$$

The projection of a Dirac point at $\mathbf{K}_0 = \mathbf{b}_1/3 + 2\mathbf{b}_2/3$ is then given by

$$\begin{aligned}\mathbf{K}_0 &= (\mathbf{G}_1, \mathbf{G}_2) \begin{pmatrix} \frac{1}{3}i + \frac{2}{3}j \\ \frac{1}{3}k + \frac{2}{3}l \end{pmatrix} \\ &= (\mathbf{G}_1, \mathbf{G}_2) \begin{pmatrix} \frac{1}{3}m + \frac{2}{3}n \\ \frac{1}{3}q + \frac{2}{3}r \end{pmatrix}.\end{aligned}\quad (17)$$

For different pairs of (i, j, k, l, m, n, q, r) , there are five different types of projections: $(0, 0)$, $(0, \frac{1}{3})$, $(\frac{1}{3}, 0)$, $(\frac{1}{3}, \frac{1}{3})$, $(\frac{1}{3}, \frac{2}{3})$. These projections will always fall into the five high-symmetry points.

The situation under strain changes because the borders of the mBZ are no longer located at $\mathbf{G}_1/3 + 2\mathbf{G}_2/3$ (and

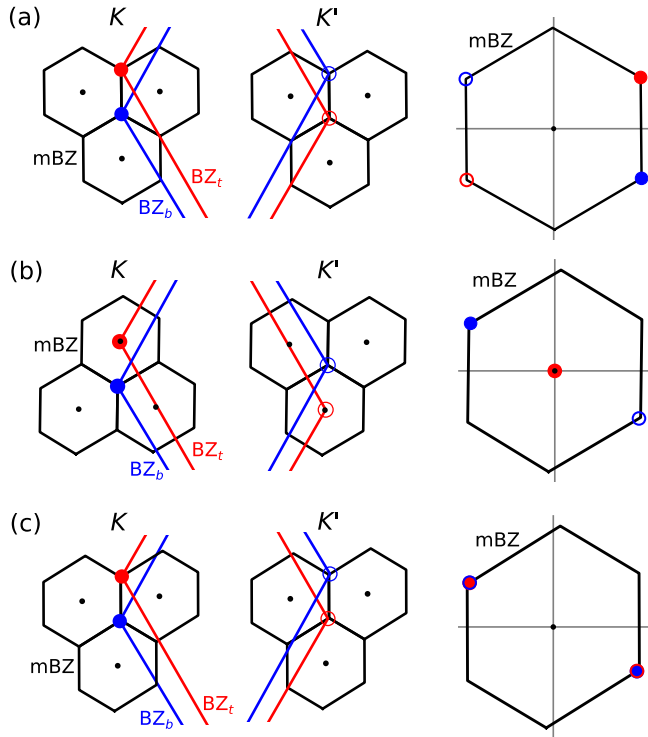


FIG. 2. (a) Position of the Dirac points projected within the mBZ, for the commensurate solutions of magic angle $\theta \sim 1.05^\circ$ without strain. (b) The same case as panel (a) for uniaxial strain $\epsilon_u \sim 0.1\%$. (c) The same case as panel (a) for shear strain $\epsilon_s \sim 0.1\%$. In each case, plots on the left and middle sides show the Dirac points in the top (red) and bottom (blue) layers, and the mBZ periodically translated from the origin for the K and K' valleys, respectively. Plots on the right side show the position of the Dirac points within the mBZ, when translated by the moiré vectors. In panels (b) and (c), the positions of Dirac points from the top strained layer are slightly shifted from the five possible positions in the mBZ [see Eq. (17)].

translations by reciprocal moiré vectors), as in the nonstrain case. Consequently, the Dirac points in the mBZ are rather located at arbitrary, strain-dependent positions. Some examples of the geometrical positions of the Dirac points in TSBG are plotted in Figs. 2(b) and 2(c). The Dirac points are effectively away from the corners of the mBZ and are no longer degenerate. It should be noted that our analysis here only accounts for the geometrical position of the Dirac points in each layer, i.e., the projection of the borders of their respective BZ. As we will discuss in the following sections, under strain and relaxation the Dirac points are also slightly shifted by strain-induced fields. Moreover, due to the broken symmetries under strain, the actual position of the moiré Dirac points is further influenced by the moiré potential that couples the two layers [21,36,72].

In the particular nonstrain case, the commensurate condition is given by Eq. (1), and Eq. (17) becomes

$$\mathbf{K}_0 = (\mathbf{G}_1, \mathbf{G}_2) \begin{pmatrix} 2/3 \\ 1/3 \end{pmatrix}, \quad (18)$$

which means that if there is no strain, the Dirac cones are always projected to the corners of the mBZ [Fig. 2(a)]. As discussed in the following section, the shift of the Dirac cones

and the deformation of the mBZ under strain explain why, in the TB calculations, the K_1 , K_2 , K_3 , K_4 , and Γ points appear displaced compared to the unstrained case.

C. Numerical models

We first compute the electronic structure of commensurate TSBG by using a full atomistic TB Hamiltonian. Then, we construct a general effective continuum model to describe the TB results. A key step for comparing the TB and continuum results is identifying the Dirac points in the strained mBZ, discussed in Sec. II B (see also Fig. 2).

1. Tight-binding model

The TB Hamiltonian of the TSBG is generated by only considering the p_z orbital of the carbon atom as [68]

$$H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j, \quad (19)$$

where c_i is an annihilation operator for the i state, ε_i is the on-site potential, $\langle i, j \rangle$ is the sum over index with $i \neq j$, t_{ij} is the hopping integral between i and j orbitals, which follows the Slater-Koster formalism [76,77]. As detailed above, including a very small biaxial strain guarantees commensurate solutions for arbitrary twist and uniaxial/shear strain, from which we calculate the bands. For conciseness, in the main text we quote the approximate twist and strain values of the commensurate solutions. The exact strain and twist parameters are listed in Sec. S2 of the Supplemental Material [75]. We identify the valley character with a valley operator [78,79], and relax the moiré supercell with LAMMPS [80]. All the TB calculations are performed in the TBPLaS simulator [81]. Details of the TB calculations are given in Sec. S3 of the Supplemental Material [75,82,83].

2. Strain-extended continuous model

In the continuum model, the electronic properties of the system are accounted for by the coupling of the Dirac points in each layer with an effective moiré-induced interlayer potential. Neglecting couplings between different valleys in each layer, the continuum model Hamiltonian for the K valley takes the form [20,32,84]

$$H = \begin{pmatrix} h_b(\mathbf{k}) + S_b & U^\dagger(\mathbf{r}) \\ U(\mathbf{r}) & h_t(\mathbf{k}) + S_t \end{pmatrix}, \quad (20)$$

where the index $\ell = b, t$ refers to the bottom and top layers, respectively. $h_\ell(\mathbf{k})$ is the Dirac Hamiltonian relative to the twisted and strained Dirac points:

$$h_\ell(\mathbf{k}) = -\hbar v \boldsymbol{\sigma} \cdot \mathbf{R}_{\theta_\ell}^T (1 + \mathcal{E}_\ell)(\mathbf{k} - \mathbf{K}_\ell), \quad (21)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the Dirac matrices and $\mathbf{K}_\ell = (1 - \mathcal{E}_\ell) \mathbf{R}_\ell(\theta_\ell) \mathbf{K}_0$, where $\mathbf{K}_0 = -(2\mathbf{b}_1 + \mathbf{b}_2)/3$ is the Dirac point of a honeycomb layer. The strain introduces an additional term S_ℓ that includes a deformation and gauge potential [54,57,58,85,86]

$$S_\ell = \mathbb{I} V_\ell - \hbar v \boldsymbol{\sigma} \cdot \mathbf{R}_{\theta_\ell}^T (1 + \mathcal{E}_\ell) \mathbf{A}_\ell, \quad (22)$$

where

$$V_\ell = g(\epsilon_{xx}^\ell + \epsilon_{yy}^\ell), \quad (23)$$

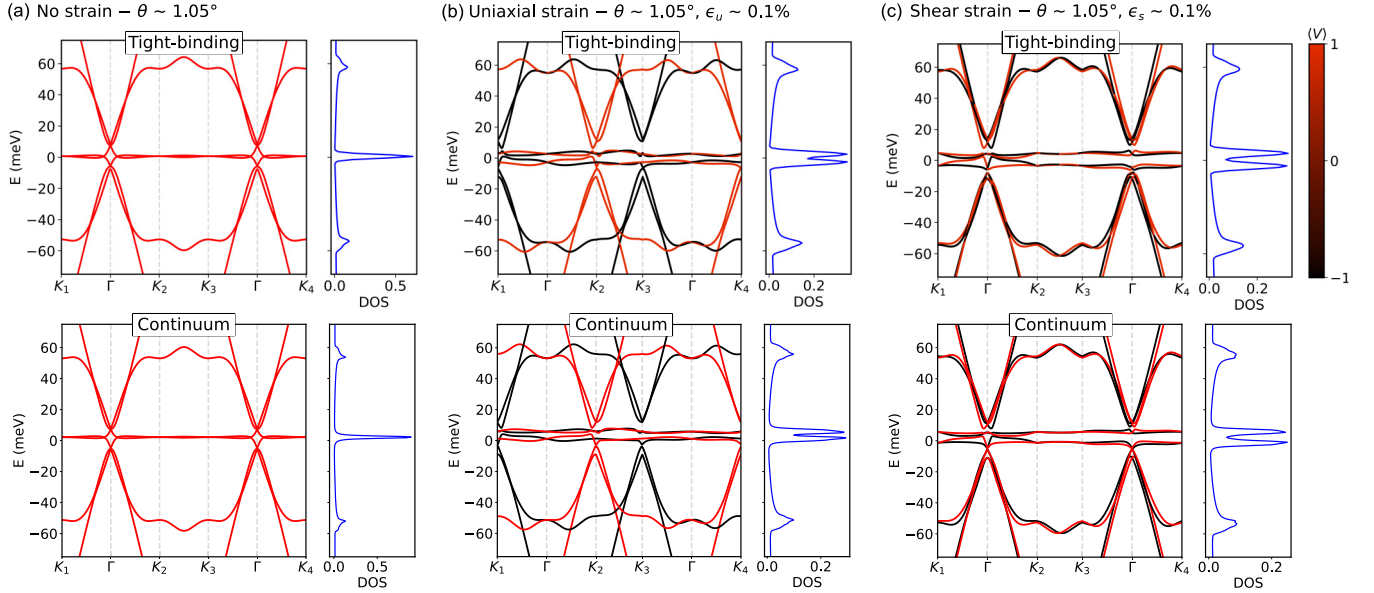


FIG. 3. Band structure and DOS for the commensurate structures of TBG with $\theta = 1.05^\circ$, $\phi = 0^\circ$ and (a) no strain, (b) uniaxial strain $\epsilon_u = 0.1\%$, and (c) shear strain $\epsilon_s = 0.1\%$, calculated by the TB (top panel) and continuum (bottom panel) models. In the TB band structures of panels (b) and (c), the color represents the expectation of the valley operator, with $\langle \hat{V}_z \rangle \approx 1$ if a state belongs to valley K (red line) and $\langle \hat{V}_z \rangle \approx -1$ if a state belongs to valley K' (black line). The momentum path is illustrated in Fig. 1(b).

$$\mathbf{A}_\ell = \frac{\sqrt{3}}{2a} \beta (\epsilon_{xx}^\ell - \epsilon_{yy}^\ell, -2\epsilon_{xy}^\ell), \quad (24)$$

with $g = 4 \text{ eV}$ and $\beta = 3.14$ for graphene [20,54]. The scalar potential V_ℓ shifts the Dirac points in energy, resembling the effect of a perpendicular electric field. The vector potential $\mathbf{A}_\ell$ shifts the Dirac points in momentum and accounts for the strain-induced change in the hopping energies within the Dirac approximation [57,58].

The moiré-induced coupling potential $U(\mathbf{r})$ depends on the interplay between twist and strain through its Fourier expansion in terms of the moiré vectors [17,18,21]. At small deformations (i.e., low twist and strain), the Fourier expansion can be truncated to the first three leading order terms [21]

$$U(\mathbf{r}) = U_1 + U_2 e^{i\mathbf{G}_1 \cdot \mathbf{r}} + U_3 e^{i(\mathbf{G}_1 + \mathbf{G}_2) \cdot \mathbf{r}}, \quad (25)$$

where

$$U_j = \begin{pmatrix} u_0 & u_1 e^{-i\omega_j} \\ u_1 e^{i\omega_j} & u_0 \end{pmatrix}, \quad (26)$$

with $\omega_j = (j-1)2\pi/3$. Here, u_0 and u_1 are the effective AA and AB/BA hopping amplitudes. The values of these hopping energies are expected to depend on the local lattice deformations. In general, a rigid configuration implies equal hopping energies $u_0 = u_1$. This results in the remote bands always touching the flat middle bands, i.e., there is no gap between them [15,17]. However, relaxation effects tend to shrink and increase the interlayer distance of the energetic AA regions, compared to the most favorable AB/BA, thus leading to an effective smaller hopping $u_0 < u_1$ [87–92]. The main effect of this is to open a gap between the flat middle bands and the remote bands.

III. ELECTRONIC STRUCTURES

A. Strain effect

Figure 3 shows both the TB and continuum model results for the band structure and DOS at the first magic angle $\theta \sim 1.05^\circ$, for different cases: without strain, and with uniaxial and shear strains, both with directions $\phi = 0$ (see also Sec. S4 of the Supplemental Material [75] for the cases with $\theta = 1.6^\circ$ and $\theta = 0.93^\circ$, and with different strain strengths). The fitted continuum model parameters $u_0 = u_1 = 0.1 \text{ eV}$ and $\hbar v/a = 2.15 \text{ eV}$ provide excellent agreement with the TB calculations. As described below, strain introduces four generic features in the electronic structures.

First, the middle narrow bands are extremely sensitive to strain. In the absence of strain, the band structure at the first magic angle exhibits characteristic flat bands near the charge neutrality point (CNP), leading to a pronounced peak in the DOS. Upon introducing strain into the system, we see that the narrow peak splits into two peaks in the DOS, with reduced magnitude [93]. The strain broadens the width (the difference between the extreme values within one band) of the narrow bands. Moreover, the energy separation [indicated by the separation of the van Hove singularities (vHs)] between the conduction and valence bands increases with increasing strain strength [75]. In TSBG with $\theta = 1.6^\circ$, strain induces multiple DOS peaks from both the valence and conduction bands, showing that strain can effectively generate higher-order vHs [20,32,34]. We emphasize that for each twist angle, the minimum bandwidth always appears around the small strain region (see narrow band dome in Sec. S5 of the Supplemental Material [75]).

Second, the strain breaks the C_3 symmetry and lifts the valley degeneracy along the high-symmetry points of the mBZ [20,32,94]. In the unstrained case, the Dirac points are located at the corners of the mBZ. The conduction and valence narrow

bands are connected by two Dirac crossings in each valley, protected by the $C_{2z}T$ symmetry. When strain is introduced, the breaking of C_3 symmetry lifts the valley degeneracy, as confirmed by the expectation value of the valley operator at each band state (details in Sec. S3 of the Supplemental Material [75]). In the band structure, this manifests as a separation between the red and black curves corresponding to different valleys. A similar valley splitting occurs in TBG/hexagonal boron nitride (hBN) heterostructures, where the aligned hBN substrate breaks valley degeneracy [94,95]. This lifting of valley degeneracy may account for the experimentally observed fourfold, rather than eightfold, Landau level degeneracy near the CNP [3,5]. Nevertheless, the band structures of the K and K' valleys remain related by time-reversal symmetry, and the conduction and valence narrow bands stay connected, indicating that strain alone cannot open a gap in TBG due to the preserved $C_{2z}T$ symmetry.

Third, the Dirac points are no longer located at the corner of the mBZ, but rather around the five possible projections without strain [see Eq. (17)]. This further reflects the lack of C_3 symmetries in the presence of strain. The geometric position of the Dirac points with 0.1% strain (uniaxial and shear) is plotted in Figs. 2(b) and 2(c). However, the exact positions of the Dirac points, identified from the energy maps (Fig. 6), are found to be slightly different. As noted before and discussed in detail in the continuum model results, there are two additional sources of corrections of the Dirac point position: (1) the gauge potential induced by strain (external strain and lattice relaxation) and (2) the deformed moiré potential that couples the two graphene layers [72]. Moreover, there is an energy shifting of the two Dirac points within a valley, resulting in a finite (lower) density of states at the CNP.

Finally, we observe that the remote bands always give two additional peaks flanking the middle narrow bands, which do not change under low strain. In particular, the DOS peaks around ± 60 meV from the remote bands are unchanged in the presence of strain [75]. This behavior is consistent with recent experimental results that suggest that the remote bands are insensitive to strain [46] and their optical interband transitions can be used as a fingerprint of the twist angle [96].

B. Comparison between uniaxial and shear strain

When comparing the effects of uniaxial and shear strain, we observe clear differences. Under shear strain, the energy separation between the vHs is larger, and the middle bands become narrower across most regions of the mBZ (see also Fig. 6). This can be attributed to geometric modulation: For the same strain magnitude, shear strain produces a stronger distortion of the moiré pattern than uniaxial strain [see Eq. (8)]. Similar trends are found for twist angles beyond the first magic angle [75].

In many experimental TSBG samples, the distorted moiré pattern is commonly interpreted under the assumption of uniaxial heterostrain. This assumption is frequently used when extracting twist and strain from scanning tunneling microscope (STM) topography. However, recent STM measurements have shown that shear strain can also appear as the dominant contribution [46,48]. Particularly, the large energy separation of the narrow bands can only be explained by the

effect of the shear strain [46]. Therefore, in order to properly interpret the experimental observations, it is necessary to identify the strain type.

Within the continuum model, the difference between the uniaxial and shear strain effects can be related to their corresponding scalar and gauge potentials. For uniaxial strain, the scalar potential is independent of the strain direction

$$V_u = g\epsilon(1 - \nu) \sim 3.35\epsilon \text{ eV}, \quad (27)$$

while for shear strain it vanishes, $V_s = 0$. On the other hand, the magnitude of the vector potential for uniaxial reads

$$|\mathbf{A}_u| = \frac{\sqrt{3}}{2a}\beta\epsilon(1 + \nu) \sim 12.8\epsilon \text{ nm}^{-1}, \quad (28)$$

which is independent of the strain direction. For shear strain, one has the same expression, but with $\nu \rightarrow 1$ [or, equivalently, with a strain magnitude $\epsilon_s \rightarrow \epsilon(1 + \nu)$; see Eq. (8)]. Since $|\mathbf{K}| \sim 17 \text{ nm}^{-1}$ in graphene, the momentum space shift induced by $\mathbf{A}$ is very small at low strain magnitudes, even on the scale of the moiré BZ. However, such a small shift can still significantly alter the electronic properties. It is worth noting that the net shift of the decoupled Dirac points in each monolayer, namely, $\mathbf{K} \rightarrow (1 - \mathcal{E})R_\theta\mathbf{K}^0 - \mathbf{A}$, does not generally match the actual position of the moiré Dirac points within the mBZ. This is due to the effect of the moiré potential and the role of the strain in breaking the symmetries of the system [21,72].

C. Strain direction effect

In unstrained TBG, the system possesses sixfold rotational symmetry, allowing the strain direction to be restricted to the range $\phi \in [0, 60^\circ)$. Since uniaxial and shear strains are related by a 45° rotation [cf. Eq. (8)], we focus on the uniaxial strain case. The evolution of the DOS as a function of strain direction is shown in Fig. 4 (see also the Secs. S6 and S9 of the Supplemental Material [75] for extended results). The results agree well with previous continuum model studies [20]. We again observe an excellent agreement between the TB and continuum results. Interestingly, we see that the main features of the DOS, namely, the highly sensitive splitting of the vHs as a function of the strain direction, are well captured only when the strain fields V and $\mathbf{A}$ are included. Thus, although the strain effect in the continuum model Hamiltonian generally comes from both the change in the moiré potential $U(\mathbf{r})$ (due to the geometric variation of the strained moiré vectors) and the inclusion of the strain-induced potential $\mathcal{S}_\ell$, the latter seems to have a greater effect on the middle narrow bands.

As the strain direction changes, the DOS peaks exhibit strong variations in both intensity and energy, particularly for $\theta = 1.05^\circ$. At the magic angle, when $\phi = 30^\circ$ only one prominent peak appears in each band, while for $\theta = 1.6^\circ$ a sharp peak emerges at the CNP when $\phi = 20^\circ$ [75]. The strain direction also shifts the position of the Dirac points within the mBZ (see Fig. S6 of the Supplemental Material [75]). Our results reveal an important aspect often overlooked in previous studies: The strain direction plays a decisive role in determining both the bandwidth and the energy separation of the narrow bands.

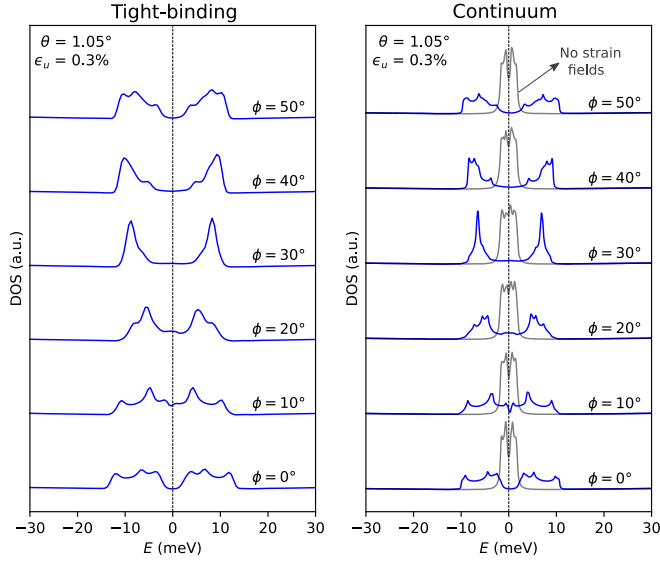


FIG. 4. Evolution of DOS with uniaxial strain direction ϕ in TSBG with $\theta = 1.05^\circ$ and $\epsilon_u = 0.3\%$, calculated by the TB (left side) and continuum (right side) models. We label $E = 0$ meV with black vertical dashed lines. The curves are relatively shifted to make the plot clear.

Specifically, we observe that at low twist angles the main effect of the strain on the electronic properties—in particular, the strain direction—comes from the gauge potential $\mathbf{A}$. For any rotation ϕ of the strain tensor $\mathcal{E} \rightarrow R_\phi \mathcal{E} R_{-\phi}$, as considered in Fig. 4, the gauge potential $\mathbf{A}$ transforms as

$$\mathbf{A}(\mathcal{E}) \rightarrow \mathbf{A}(R_\phi \mathcal{E} R_{-\phi}) = R_{-2\phi} \mathbf{A}(\mathcal{E}), \quad (29)$$

that is, it simply rotates by -2ϕ . Thus, the magnitude of the gauge potential is invariant, and only the direction of $\mathbf{A}$ changes when the strain direction is modified. The high sensitivity of the DOS to the strain direction around the magic angle, as seen in Fig. 4, then reflects that it is the actual direction of the vector potential that plays the most significant role in modifying the electronic spectra. This is in line with previous studies indicating that the moiré coupling and the emergence of flat bands depend critically on the relative orientation between the Dirac points and the momentum transfer vectors [20,21,97].

In fact, in linear Dirac band systems, the gauge potential is the relevant term that significantly modifies the electronic properties [20], and the scale potential only shifts the Dirac points in energy [20,21]. However, in parabolic band systems, the scale potential has a prominent contribution to the band structure, for example, by controlling the energy gap and flattening the band edges [98]. In particular, in rhombohedral multilayer graphene with a quasi-one-dimensional geometry, the scalar term [99] induces enriched correlated behaviors.

D. Lattice relaxation effect

The relaxed geometry exhibits two main global features. First, the lattice relaxation patterns of graphene moiré structures, with and without strain, are qualitatively similar: The AA regions shrink, while the AB regions expand into triangular domains [100]. Particularly, at low strain, the in-plane

and out-of-plane displacements of TBG without and with strain show a high degree of consistency (see Sec. S7 of the Supplemental Material [75]). Second, strain drives a structural transition in the DW network [47]. In nonstrain TBG, the DWs are of the shear type, characterized by a Burgers vector parallel to the DW. When strain is applied, the angle between the Burgers vector and the DW boundary changes, leading to a mixed configuration containing both shear and tensile DWs [101,102]. The atomic displacements within the DW region differ significantly between the strained and unstrained cases. This structural discrepancy may alter the electronic states localized at the DWs, which typically lie at higher energies [103,104].

As noted above, the simplest way to account for relaxation effects in the continuum model is to consider an unequal ratio $u_0 < u_1$ between the hopping energies of AA and Bernal stacking. However, although this captures the opening of a gap between the narrow and remote bands, it still misses to capture a relaxation-induced particle-hole asymmetry [88,105]. This effect can be captured by including next-order nonlocal (momentum-dependent) corrections to the moiré potential [88,106,107]. To leading order, the matrix elements of the nonlocal moiré potential U_{NL} read [106,107]

$$\langle \mathbf{k}, t | U_{\text{NL}} | \mathbf{k}', b \rangle = \sum_{j=1}^3 U_{\text{NL},j}(\mathbf{k}, \mathbf{k}') \delta_{\mathbf{k}' - \mathbf{k}, \mathbf{G}'_j}, \quad (30)$$

where $\mathbf{G}'_1 = \mathbf{0}$, $\mathbf{G}'_2 = \mathbf{G}_2$, $\mathbf{G}'_3 = \mathbf{G}_1 + \mathbf{G}_2$, while $U_{\text{NL},j}(\mathbf{k}, \mathbf{k}') = -(T_j p_- + T_j^\dagger p_+)/2$ with

$$T_j = \begin{pmatrix} \lambda_1 e^{-i\omega_j} & \lambda_2 e^{i\omega_j} \\ \lambda_3 & \lambda_1 e^{-i\omega_j} \end{pmatrix}. \quad (31)$$

Here, as before, $\omega_j = (j-1)2\pi/3$, while $p_\pm = p_x \pm ip_y$, where $\mathbf{p} = (p_x, p_y)$ is the vector sum of the momenta in the top and bottom layers, relative to the positions of their Dirac points, i.e., $\mathbf{p} = (\mathbf{k} - \mathbf{K}_t) + (\mathbf{k}' - \mathbf{K}_b)$.

Figure 5 presents a comparative analysis of the relaxed and rigid band structures and DOS under strain in both TB and continuum cases. To fit the TB results, we consider $u_1 = 0.096$ eV, $u_0 = 0.05952$ eV for the local moiré potential, $\hbar v/a = 2.13$ eV, and $\lambda_1 = 9$ meV nm, $\lambda_2 = 18$ meV nm and $\lambda_3 = 0$ for the nonlocal moiré potential [107]. The obtained results show again good agreement with the TB results with relaxation. Improvements in the continuum model could be further obtained by accounting for the local distortions of the AA, AB, and DW regions, which introduce periodic pseudomagnetic magnetic fields [105,108,109].

The most notable effect remains the gap opening between the remote and narrow bands induced by relaxation. Moreover, the lattice relaxation increases the energy separation between the valence and conduction narrow bands, and broadens the width of the narrow bands, as also shown in Fig. 6. The lattice relaxation also introduces a pronounced electron-hole asymmetry in the TB results. The DOS peak in the conduction band is larger than that in the valence band, although both peaks exhibit nearly equal magnitudes at $\theta = 0.93^\circ$ and $\theta = 1.6^\circ$ [75]. The asymmetry between the DOS peaks associated with the narrow bands, as well as its evolution with twist angle, is consistent with recent experimental observations in

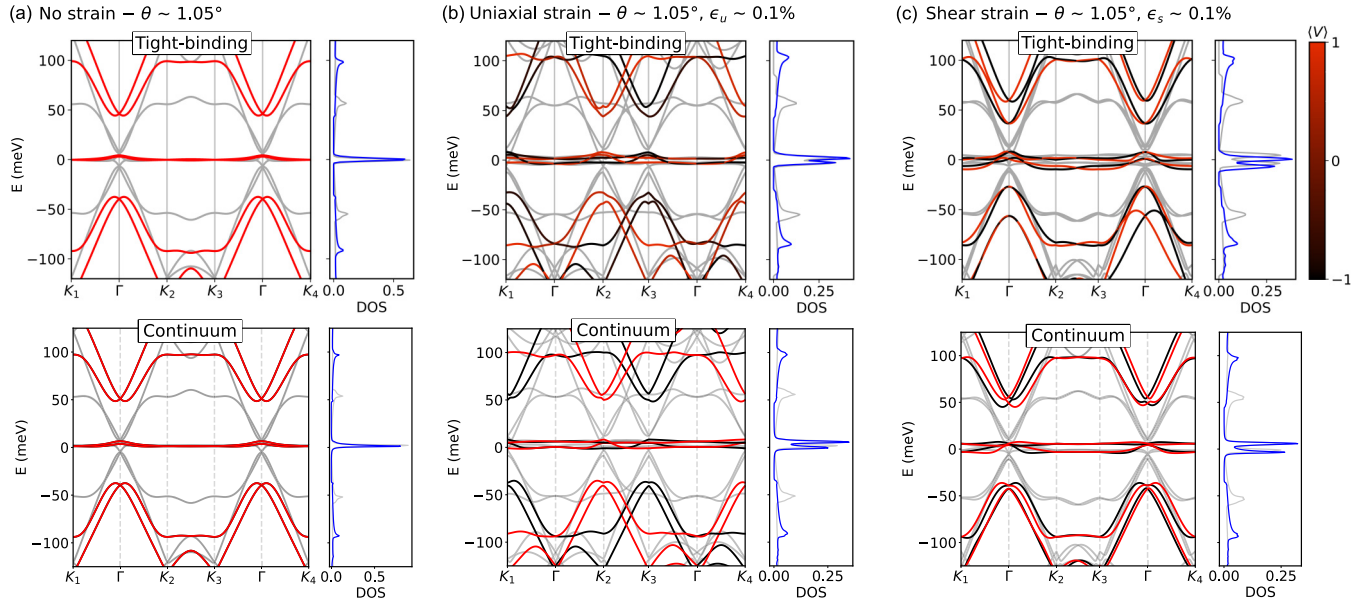


FIG. 5. Band structure and DOS for relaxed TBG with $\theta = 1.05^\circ$ and (a) no strain, (b) uniaxial strain $\epsilon_u = 0.1\%$, and (c) shear strain $\epsilon_s = 0.1\%$. The band structure and DOS of rigid cases are plotted with gray dots. The colors in the band structure are the same as in Fig. 3. Note that, in the plots, the energy range in the relaxed case is almost two times larger than the energy range of the rigid case in Fig. 3.

which similar behavior was reported as the twist angle and strain were varied in the same device [46]. The continuum model effectively captures the particle-hole asymmetry only when the nonlocal moiré potential is taken into account [75]. Interestingly, we find that the gap between the remote conduction and valence bands remains nearly constant under strain, while the separation between the remote and narrow bands decreases as strain increases, reflecting their broadening.

Since the main effect of the nonlocal moiré potential is to introduce a small particle-hole asymmetry, from here on we simplify the continuum model by keeping only the local moiré potential [17,87]. This approximation aligns with the motivation of the continuum model, which aims to provide a minimal model that captures the main features seen in the TB band structures [12,15]. Although our results below can be directly extended to include the effect of the nonlocal moiré potential, we expect this to only slightly change quantitatively the strain-dependence behavior, without affecting our main conclusions.

E. Narrow bands with strain and twist

In line with the TB results, the continuum model reflects that the strain effectively increases the bandwidth of the narrow bands around the magic angle. Nevertheless, there is always a minimum bandwidth depending on the twist and strain. Thus, one can still identify potential twist and strain configurations at which electronic correlations could be maximized. Here, we shall particularly focus on the identification of the twist angle at which the bandwidth of the narrow bands is minimum.

Figure 7 shows the bandwidth evolution as a function of the twist angle θ and the uniaxial strain magnitude ϵ , with different directions ϕ , for the relaxed configuration of continuum model parameters. In general, we observe that the twist

angle at which the bandwidth is minimum tends to shift in the presence of strain. The shift is nonuniform and depends non-trivially on the strain direction. Thus, we observe that as the strain magnitude increases, the magic angle tends to increase when $\phi = 0^\circ$, but it tends to decrease when $\phi = 30^\circ$. For shear strain, one obtains a similar behavior as in Fig. 7, only that the effect is stronger for the same strain magnitude, and the dependence on the strain direction is shifted [cf. Eq. (8)].

Remarkably, the minimum bandwidth always seems to follow a linear dependence on the strain magnitude [20]. We have checked that this behavior persists even without the strain fields [75]. The main difference then is that the bandwidth evolution becomes almost insensitive to the strain direction, but scales linearly with the strain magnitude. Such linear dependence of the bandwidth is roughly due to the linear dependence of the moiré vector on the strain strength [see Eq. (11)], which introduces the strain effect through the moiré potential given by Eq. (25).

It should be noted that under strain, a minimum bandwidth does not necessarily correlate to a higher DOS. This is because with strain, the narrow bands are not, in general, uniformly flat over the whole mBZ. A band at a particular twist and strain configuration can have, for instance, a larger bandwidth than at other configuration, but yet be flatter over a wider region of the mBZ. Consequently, the configuration with higher bandwidth would still have higher vHs. In this sense, a minimum bandwidth should only be considered as an indicator for the appearance of strong electronic correlations.

Although a nonzero strain tends to increase the bandwidth, it is crucial that such an increase depends on the twist angle. Since most samples are, at least, likely to inherit some kind of random strain [4,10,110,111] (e.g., due to their fabrication method), which can vary from sample to sample, our results highlight that the notion of *magic angle* is intrinsically connected to the experimental conditions of the system.

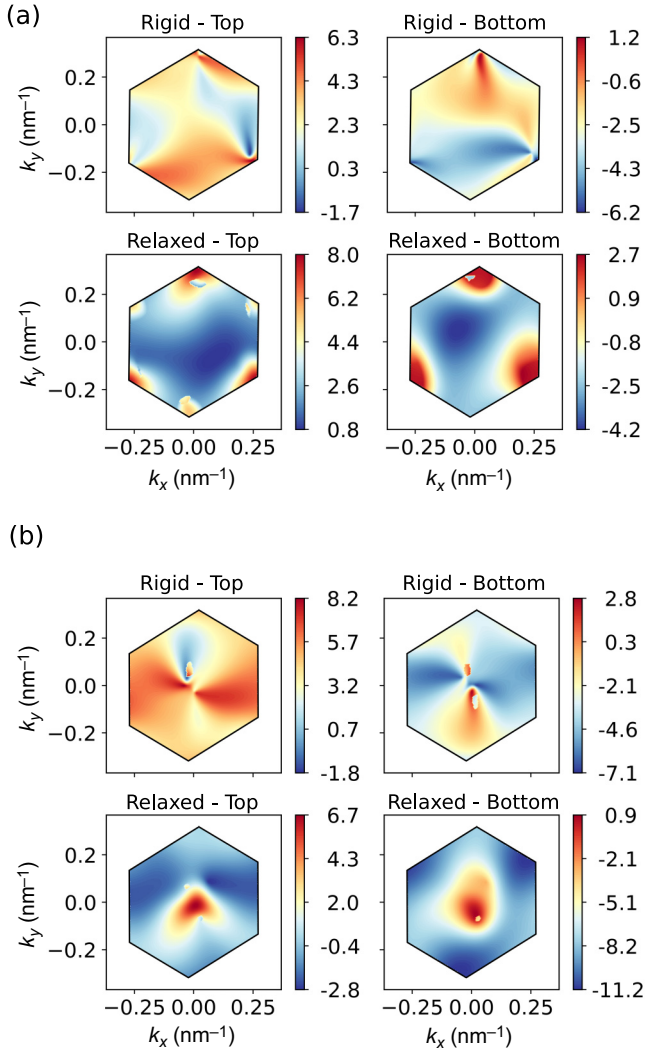


FIG. 6. Comparison of energy map of the top and bottom narrow bands (tight-binding results) between relaxed and rigid TBG with $\theta = 1.05^\circ$ and (a) uniaxial strain $\epsilon_u = 0.1\%$ and (b) shear strain $\epsilon_s = 0.1\%$. The mBZ is illustrated with black line. The color represents the energy with unit meV. We only show the energy map of narrow bands from valley K in the mBZ, which are identified by the valley operator.

IV. STRAIN AND ELECTROSTATIC INTERACTIONS

Our analysis so far has neglected the role of electron-electron interactions in the system. However, these interactions are actually crucial in the narrow band regime due to the quenching of the kinetic energy. In this section, we will address, in particular, the role of the electrostatic interactions within the continuum model, as accounted by the Hartree potential [59–61]. Our main interest will be the effect of electrostatic interactions on the bandwidth and charge density of the twisted and strained bilayer configurations.

The Hartree interaction is the direct (classical) interaction of an electron with the surrounding charge density:

$$V_H(\mathbf{r}) = \int d\mathbf{r}' v_C(\mathbf{r} - \mathbf{r}') \delta\rho(\mathbf{r}'), \quad (32)$$

where $v_C(\mathbf{r} - \mathbf{r}')$ is the bare Coulomb potential and $\delta\rho(\mathbf{r}')$ is the electronic charge density with respect to CNP. Replacing the plane-wave expansion of the Bloch states in TSBG leads to

$$V_H(\mathbf{r}) = \sum_{\mathbf{G} \neq 0} V_H(\mathbf{G}) e^{-i\mathbf{G} \cdot \mathbf{r}}, \quad (33)$$

$$V_H(\mathbf{G}) = \frac{v_C(\mathbf{G})}{A_c} \sum_{\mathbf{k}, \mathbf{G}'} \sum_{n, \eta, i} u_{n, \mathbf{k}, \eta, i}^*(\mathbf{G}' + \mathbf{G}) u_{n, \mathbf{k}, \eta, i}(\mathbf{G}'), \quad (34)$$

where $u_{n, \mathbf{k}, \eta, i}(\mathbf{G})$ are the Fourier coefficients of the band, valley/spin, and layer/sublattice indices n, η, i , respectively, and $v_C(\mathbf{G})$ is the Fourier transform of the bare Coulomb potential (see the Supplemental Material [75] for details). We consider a gated configuration of two metallic plates [112], for which $v_C(\mathbf{G}) = e^2 \tanh(d|\mathbf{G}|)/2\epsilon_0\epsilon_r|\mathbf{G}|$, where d is the distance between the two metallic plates and ϵ_r is the relative primitivity of the system. For the numerical calculations, we set $d = 40$ nm. Note that the $\mathbf{G} = 0$ term in $V_H(\mathbf{r})$ is neglected because it is canceled by the background positive charge (jellium model) [59, 113].

In unstrained TBG, the moiré pattern is perfectly triangular, and the largest Fourier components of the Hartree potential correspond to the first six reciprocal vectors of equal magnitude [59, 60]. Owing to the C_3 symmetry, each reciprocal vector contributes equally to the charge density and the Hartree potential, which therefore follow the same spatial profile [60]. Under strain, however, the moiré pattern becomes distorted and loses its triangular symmetry [21, 41], making the contributions from different Fourier components inequivalent. As a result, the Hartree potential is no longer proportional to the charge density. In our numerical calculations, we therefore include all Fourier components $V_H(\mathbf{G})$ within the reciprocal moiré vectors of the continuum model.

The Hartree potential is diagonal in the valley/spin and sublattice/layer flavors, with matrix elements [114]

$$\langle \mathbf{k} + \mathbf{G}' - \mathbf{G}, \eta', i' | \hat{V}_H | \mathbf{k} + \mathbf{G}', \eta, i \rangle = \delta_{\eta\eta'} \delta_{ii'} V_H(\mathbf{G}). \quad (35)$$

Since the Hartree potential depends on the occupied Bloch states from CNP, the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}_H$ is solved self-consistently, for different filling factors, up until convergence.

Figure 8 shows the numerical results for the evolution of the band structure and density of states, from CNP ($\nu = 0$), to a filling of $\nu = +2$ (two electrons per moiré unit cell), for different dielectric constants ϵ_r . The results correspond to $\theta = 1.05^\circ$ with no strain (top panels), and uniaxial strain with magnitude $\epsilon = 0.1\%$ and direction $\phi = 30^\circ$ (bottom panels). In both cases, we observe that as the dielectric constant diminishes and the Hartree potential increases, the band structure is strongly reshaped [59–61, 115].

Interestingly, by comparing the nonstrain with the strain case, we observe that the interacting band structures end up having similar bandwidths, despite having quite different single-particle bandwidth. This is because the Hartree potential diminishes as the bare active bands increase their bandwidth, essentially due to the decrease in the quenching of the kinetic energy. As a result, under strain there is a competition between the increase of the noninteracting bandwidth and the decrease of the Hartree potential. The synergy

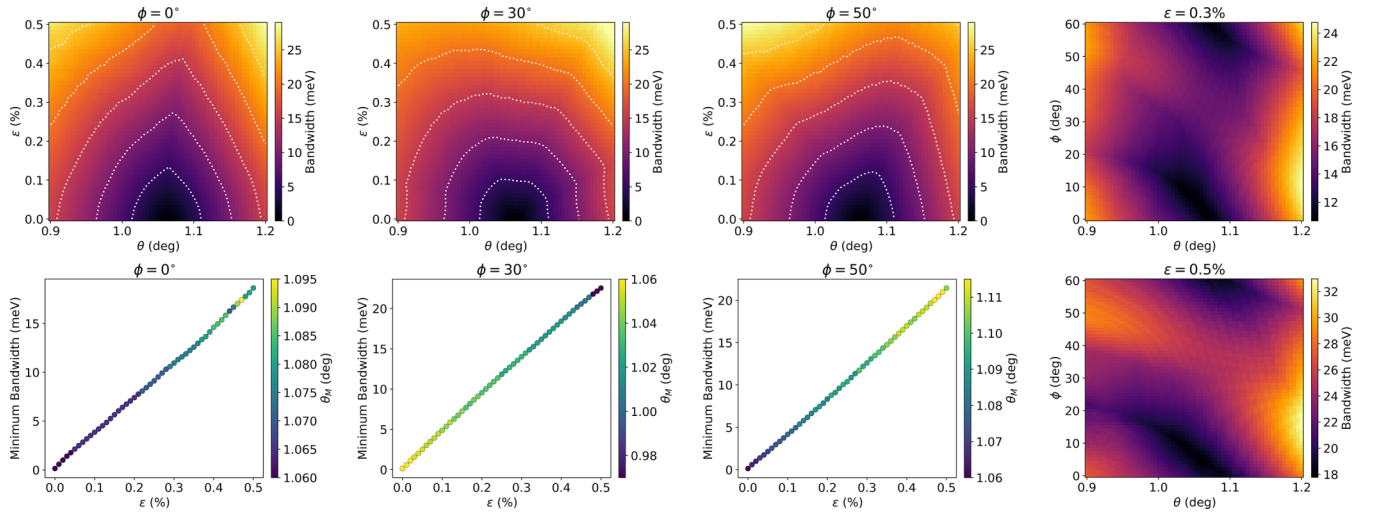


FIG. 7. Numerical continuum model results for the bandwidth evolution in the top narrow band, as a function of the twist angle θ and (1) uniaxial strain magnitude ϵ along fixed directions $\phi = 0^\circ, 30^\circ, 50^\circ$; white dotted lines indicate constant bandwidths from 5 to 25 meV, in steps of 5 meV. (2) Strain direction for fixed magnitudes $\epsilon = 0.3\%, 0.5\%$. The first three bottom panels show the minimum bandwidth at θ_M (right colorbar) as a function of the strain magnitude ϵ , following an almost linear relation. All the results correspond to the relaxed configuration with parameters $\hbar v/a = 2.13$ eV, $u_1 = 0.096$ eV, and $u_0 = 0.05952$ eV.

between both effects determines the effective bandwidth under strain and electrostatic interactions. It may actually be that, under strain, the net bandwidth becomes comparable, or even smaller, than the one corresponding to the no-strain scenarios.

As the strain increases, the Hartree effect not only weakens but also evolves into a nearly uniform energy shift. In other

words, it changes from a non-rigid shift in the unstrained case, to an almost rigid (and small) shift at larger strains. This behavior indicates that the charge density across different momentum points becomes increasingly uniform as strain grows. Figure 9 illustrates this transition from nonrigid to rigid behavior, for the case of uniaxial strain. While the

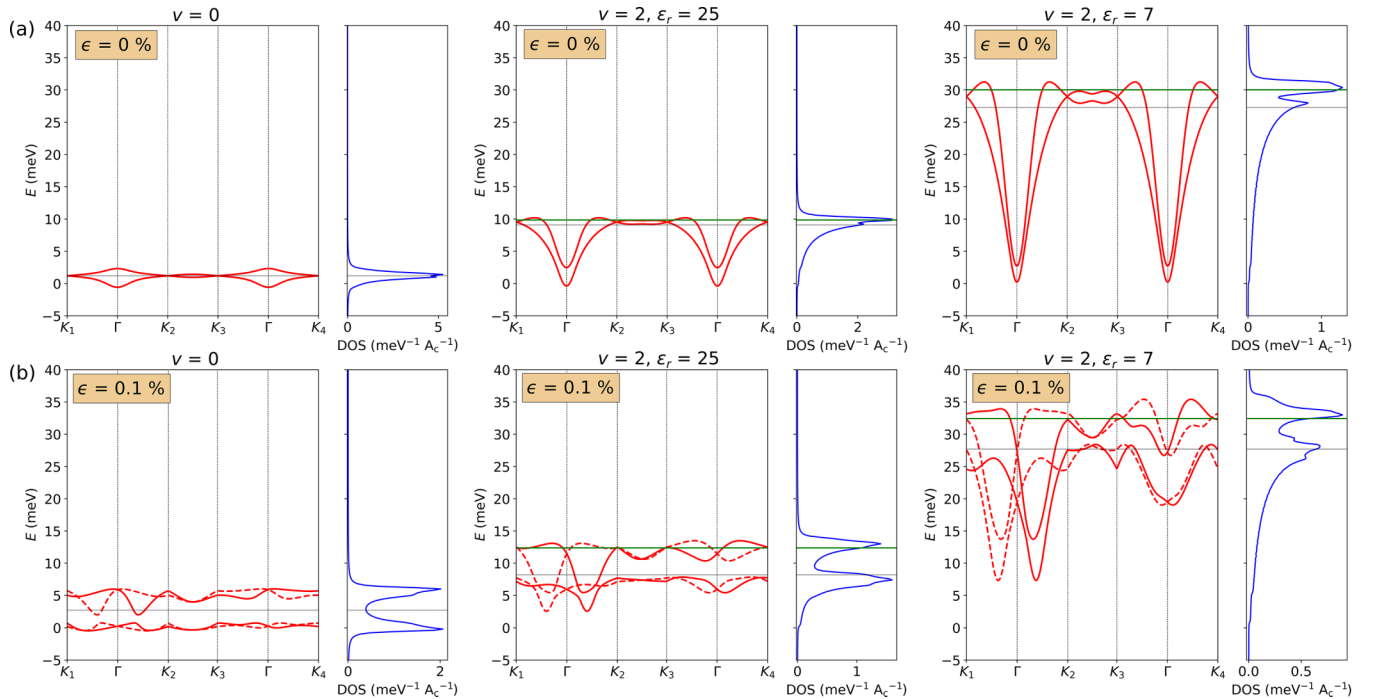


FIG. 8. Evolution of the band structure and DOS as a function of the electrostatic interactions (self-consistent Hartree), from the noninteracting case at charge neutrality (filling $\nu = 0$), to a filling $\nu = 2$ with different dielectric constants ϵ_r . Panel (a) shows the results for the no-strain case at $\theta = 1.05^\circ$, while panel (b) shows the results for $\theta = 1.05^\circ$ and uniaxial strain with magnitude $\epsilon = 0.1\%$ and direction $\phi = 30^\circ$. In all cases, the horizontal gray and green lines indicate the CNP and the Fermi level, respectively. In the band structures, the solid and dashed lines correspond to the K and K' valleys. All the results are for the relaxed configuration with continuum model parameters $\hbar v/a = 2.13$ eV, $u_1 = 0.096$ eV, and $u_0 = 0.05952$ eV.

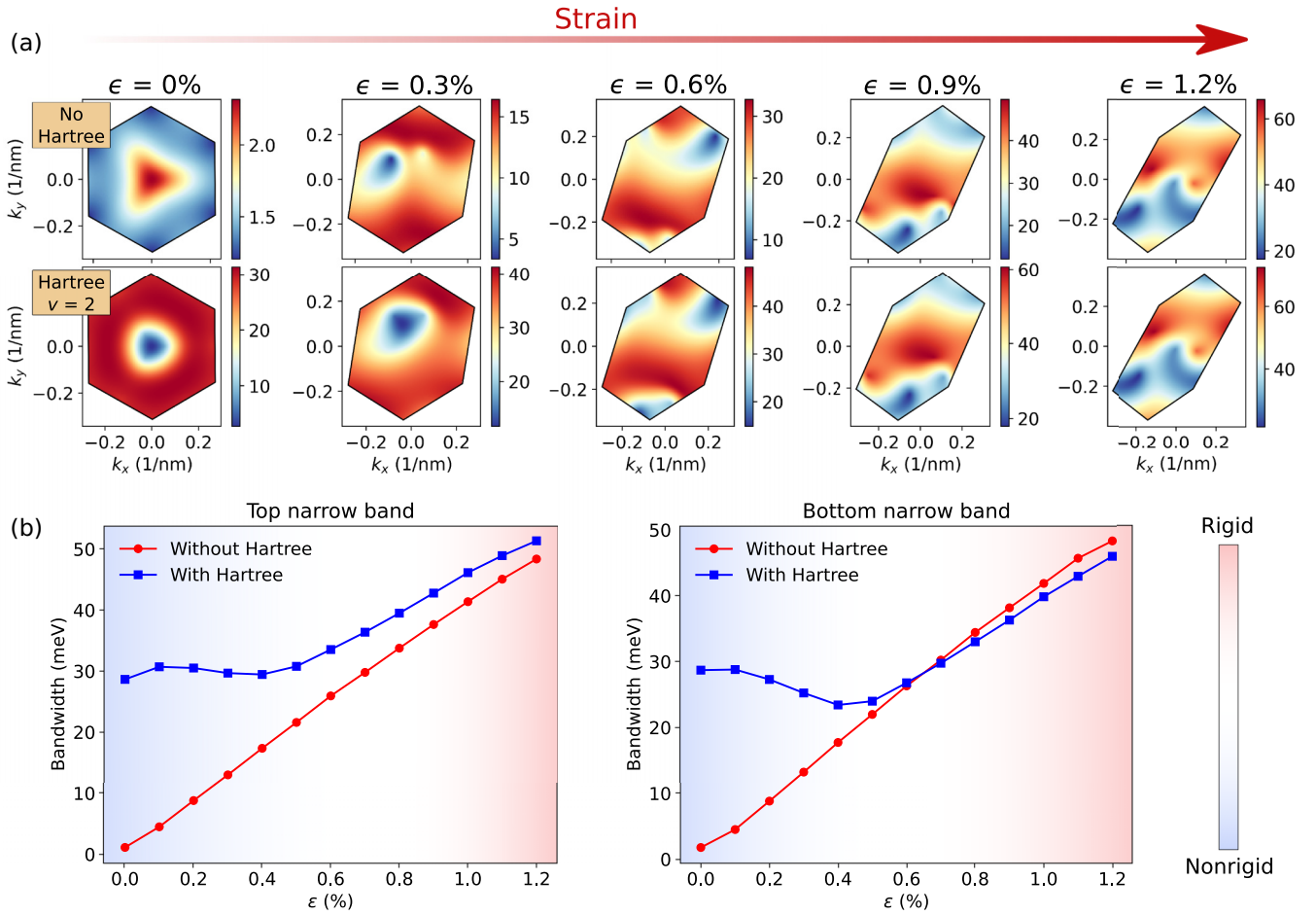


FIG. 9. Evolution from a nonrigid to a rigid Hartree effect as the strain increases. Panel (a) shows the continuum model density plot of the top narrow band for $\theta = 1.05^\circ$ and uniaxial strain with direction $\phi = 20^\circ$ and increasing strain magnitudes ϵ . The top and bottom density panels show, for each strain magnitude, the bands without Hartree and with Hartree (filling $\nu = 2$ and $\epsilon_r = 7$), respectively. Panel (b) shows the bandwidth in the top and bottom narrow bands, with and without Hartree, as a function of the uniaxial strain magnitude ϵ with direction $\phi = 20^\circ$; other parameters as in panel (a). The colormap indicates, schematically, the nonrigid to rigid transition as the strain increases and the bandwidths become similar.

noninteracting and interacting bands differ noticeably at low strain, they become nearly identical at higher strain values, implying that the Hartree potential becomes effectively negligible. The strain threshold for this transition depends nontrivially on the strain direction (and, more generally, on the strain type). It also varies with the filling factor because of the asymmetric Hartree renormalization of the conduction and valence bands, depending on whether the system is electron or hole doped.

Besides the local Hartree potential, within mean field the electrons also experience the nonlocal (exchange) Fock potential that accounts for correlations due to the Pauli principle [114]. The Fock potential modifies quantitatively the renormalization of the bands [60], but its main effect is to induce polarized broken symmetry phases. Previous works have shown that under particular strain configurations, the Fock potential can stabilize different orders, such as the so-called Kramers intervalley coherent order, or the incommensurate Kekulé spiral order [50,64,65,107]. These results, however, were obtained under particular combinations of twist and strain (e.g., only uniaxial strain). Although a detailed account of strain-induced broken symmetry phases is beyond the

scope of this paper, our Hartree results point out that different combinations of twist and strain could potentially lead to a plethora of competing orders.

V. BAND TOPOLOGY WITH STRAIN

The strain-induced reshaping of the electronic properties in TSBG is expected to influence the valley-dependent topology of the band structure. Previous studies have indeed reported a rich topological phase diagram arising from the interplay between twist and strain, both in transition metal dichalcogenides (TMDs) [20] and in bilayer graphene [84,116]. However, a detailed analysis of how the topology of the narrow bands in TSBG evolves with different types of strain is still lacking.

Since strain preserves time-reversal symmetry, the Chern numbers of opposite valleys remain equal in magnitude and opposite in sign, yielding an overall zero Chern number, i.e., a topologically trivial system. Nevertheless, each valley can still host nontrivial topology. A clear signature of such valley topology, even without breaking time-reversal symmetry, is the nonlinear Hall effect [117,118], which can be used to

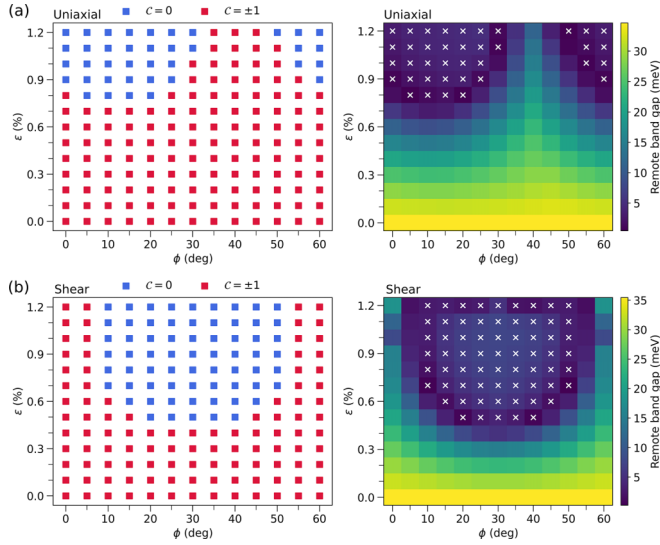


FIG. 10. Strain-induced topology evolution of the narrow bands, for the noninteracting case at $\theta = 1.05^\circ$ with (a) uniaxial heterostrain and (b) shear strain. In each case, the top left panel shows the Chern number in the top and bottom narrow bands as a function of the strain direction ϕ and magnitude ϵ . For all parameters, $C = +1(-1)$ for the top (bottom) bands. The top right panel shows the gap between the top narrow bands and the remote bands. The minimum gap, at which it closes and then reopens, corresponds to the topological transitions $|C| = 1 \rightarrow 0$ in panel (a); the white crosses indicate the regions where the narrow bands are trivial ($C = 0$).

probe the topological character of the narrow bands [119]. In what follows, we therefore focus on the valley-resolved topology of the TSBG band structure.

We study the topology evolution of the bands by computing the Chern number

$$C_n = \frac{1}{2\pi} \int \Omega_n(\mathbf{k}) \cdot d\mathbf{k}, \quad (36)$$

where $\Omega_n(\mathbf{k}) = i\langle \partial_{\mathbf{k}} \psi_{n\mathbf{k}} | \times | \partial_{\mathbf{k}} \psi_{n\mathbf{k}} \rangle$ is the Berry curvature of the n -band Bloch states $\psi_{n\mathbf{k}}$, $d\mathbf{k}$ is a reciprocal-space surface vector, and the integration is over a moiré unit cell. To obtain C_n numerically, we use the Fukui-Hatsugai-Suzuki method [120], considering different strain parameters. For comparison, we analyze separately both the noninteracting and the interacting cases with electrostatic interactions. All the results are obtained using the continuum model for the relaxed configuration. The Chern numbers are computed for the top and bottom narrow bands by introducing a small mass term $\sim m\sigma_z$ in the TSBG Hamiltonian that breaks the inversion symmetry and opens a gap at the Dirac points.

A. Noninteracting case

Figure 10 shows the results for the noninteracting case at $\theta = 1.05^\circ$ under uniaxial and shear strain with different directions ϕ and magnitudes ϵ . When interaction effects are neglected, the two narrow bands retain opposite Chern numbers of equal magnitude, so their total Chern number remains zero. In the absence of strain, the upper and lower narrow bands are topological with valley Chern numbers of $+1$ and -1 , respectively. Upon introducing strain, a topolog-

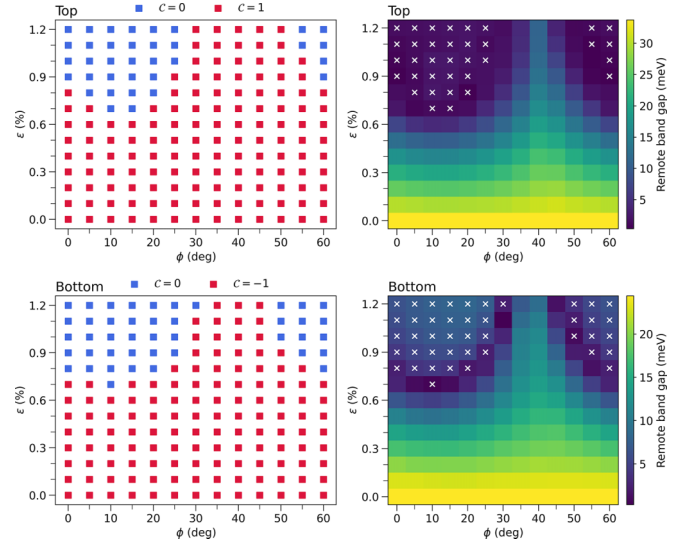


FIG. 11. Strain-induced topology evolution of the top and bottom narrow bands with electrostatic interaction (self-consistent Hartree potential), at $\theta = 1.05^\circ$ with uniaxial heterostrain, for a filling of $\nu = +2$ electrons per moiré unit cell and dielectric constant $\epsilon_r = 7$. The top (bottom) panel shows the Chern number in the top (bottom) narrow band, and their corresponding gap to the remote bands, as a function of the uniaxial strain direction ϕ and magnitude ϵ ; the white crosses in the remote band gap indicate where the narrow band is trivial ($C = 0$). Due to the electrostatic interactions, the topological transitions $|C| = 1 \rightarrow 0$ at which the remote band gap closes and reopens are different for each narrow band, leading to strain configuration at which only one band is topological (or trivial).

ical transition to trivial narrow bands ($C = 0$) occurs when the gap between the narrow and remote bands closes and reopens. This behavior arises because the strain increases the bandwidth of the narrow bands and simultaneously shifts the remote bands to lower energies (see Fig. 5). The critical point at which the gap closes depends nontrivially on the strain magnitude and direction, and, in general, also on the twist angle. Interestingly, the noninteracting band topology is preserved up to relatively large strain magnitudes ($\epsilon \sim 2\%$). The obtained topological transition could be realized with a recent strain technique that generates a position-dependent strain by bending the TBG across a nanoridge [121].

The touching between the narrow and the remote bands that triggers the topological transition is further accompanied by a transfer of charge density. Figure 12 shows this transfer of charge density $\rho_{\mathbf{k}}(\mathbf{r})$ for uniaxial strain (noninteracting case), at the momentum point $\mathbf{k}$ of minimum (direct) gap between the narrow and remote bands. As clearly seen, the charge density of the topological band ($C = 1$) is directly transferred to the remote band after the gap closes and the narrow band becomes trivial ($C = 0$). This charge transfer behavior occurs, in general, for any kind of twist and strain that induces a remote gap closing. The dependence on the specific type of strain is reflected in the profile of the charge density transferred (e.g., its symmetries) and the specific twist and strain parameters at which the topological transition takes place. For biaxial strain, for instance, the system retains the C_3 symmetry and the topological transition involves the transfer of ringlike

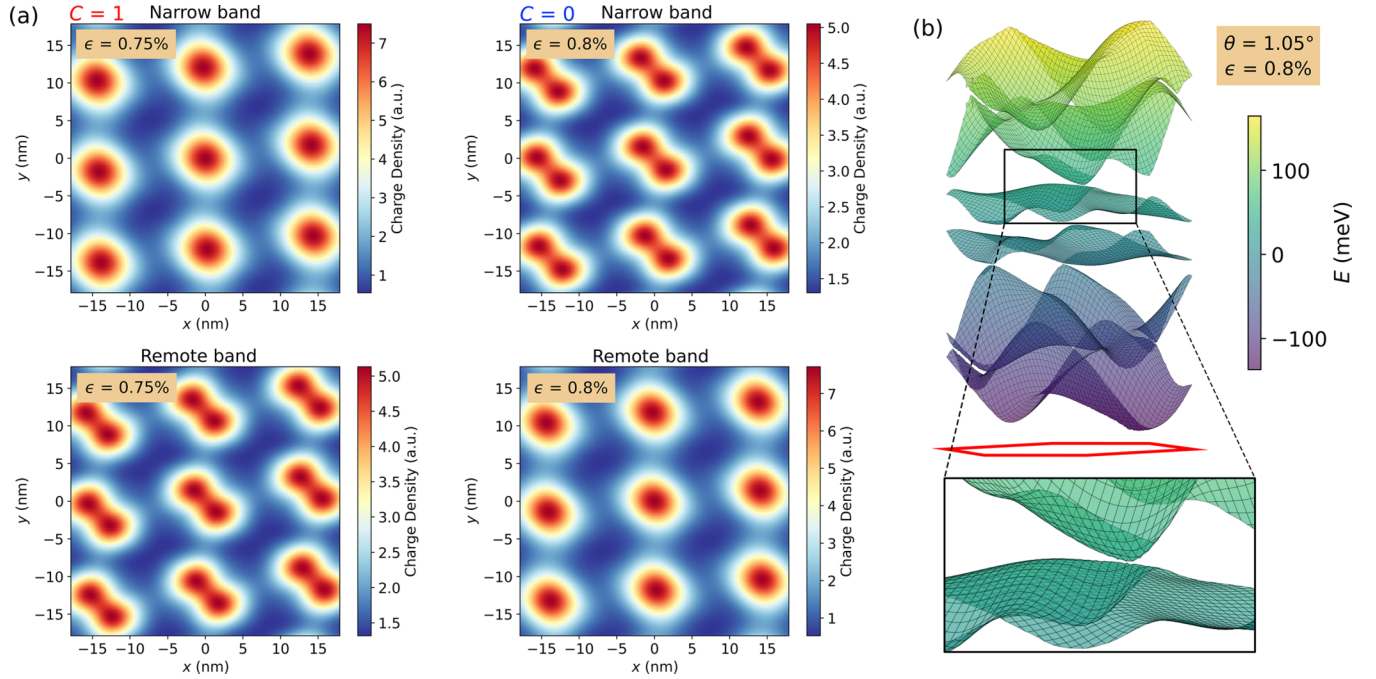


FIG. 12. (a) Charge density $\rho_k(\mathbf{r})$ in the top narrow band and the closest remote band, at the momentum point $\mathbf{k}$ of minimum direct gap between them, for twist angle $\theta = 1.05^\circ$ and uniaxial strain at $\phi = 20^\circ$, with magnitudes $\epsilon = 0.75\%$ and $\epsilon = 0.8\%$. The transition from a topological ($C = 1$) to trivial ($C = 0$) narrow band takes place between the two strain magnitudes (cf. Fig. 10). When the transition occurs, there is a charge density transfer from the top to the remote band. Panel (b) shows the noninteracting three-dimensional band structure for the uniaxial strain magnitude $\epsilon = 0.8\%$. The enlarged inset highlights the minimum gap between the top narrow band and the remote band, at which the charge transfer takes place.

to AA-centered charge densities between the top and remote bands [75].

The strain-induced topological transitions are connected to changes in the Berry curvature [122], which reverses its momentum dependence before and after the transition [75]. With strain the Berry curvature exhibits, in general, three distinct peaks, but only one having a larger magnitude [84,116,123–126]. The largest peak in the Berry curvature occurs around the momentum point where the narrow and remote bands close their gap. Thus, the peaks of the Berry curvature, and by extension of the Berry dipole, directly reflect the point where the narrow and remote bands touch and the topology changes. Since the strain breaks the symmetries of the system, the peaks in the Berry curvature are in general distributed nonuniformly in the moiré Brillouin zone (their position depending on the twist and strain).

B. Interacting case

Figure 11 shows the topology evolution of the narrow bands after including electrostatic interactions. In contrast to the noninteracting case, we now see that by increasing the strain magnitude the topology of the top and bottom narrow bands becomes asymmetrical. That is, there are now strain configurations for which the sum of the top and bottom band Chern numbers is not zero. This is because for any nonzero filling the Hartree potential reshapes the top and bottom bands asymmetrically (cf. Fig. 8). In general, for positive fillings ν (electron doped) the bottom narrow band is more strongly

renormalized, and vice versa for negative fillings ν . This leads to different strain parameters at which the gap with the remote bands closes and then reopens, and therefore, wider strain regimes in which only one band is topological. Compared to the noninteracting case of Fig. 10, we particularly see that the Hartree potential shrinks and increases, respectively, the regimes where the bottom and top bands are topological. Since the Hartree potential is practically symmetric with respect to charge neutrality [59,60], the regime in which only one band is topological is reversed when the system is hole doped ($\nu < 0$).

It is interesting to compare the strain with other perturbations in their capacity to modify the topology of the narrow bands. Table I lists the topology effect of four common perturbations in TBG: strain, Hartree (electrostatic interactions), substrate, and displacement field. For a fixed twist angle (e.g., the magic angle), only a strain [84,116] or a substrate [114] can, by itself, modify the topology of the central narrow bands. In contrast, the topology of the narrow bands cannot be changed by means of solely electrostatic interactions [59,60] or a displacement field [127,128]. Note that when two or more of the perturbations act in conjunction, the topology can always change (e.g., strain with Hartree, or Hartree with displacement field, and so on).

Topology changes in the narrow bands, by means of any of the listed perturbations in Table I, pose a restriction on topological heavy fermion models of the narrow bands in TSBG [49,129,130], as they rely on the topological nature of the bands.

TABLE I. Possible perturbations and their effect on being able to change the topology of the narrow bands in twisted bilayer graphene. The four perturbations are assumed to act on TBG at a fixed twist angle (e.g, the magic angle $\theta = 1.05^\circ$), with a small mass term $\sim \sigma_z m$ that opens a gap at the Dirac points. The topological nature of the bands is taken with respect to transitions between nonzero and zero valley Chern numbers in the top and bottom narrow bands. The Hartree potential is assumed to be for fillings between $-4 \leq \nu \leq 4$. Nonlisted perturbations involving two or more effects (e.g., strain and electrostatic interactions) can always change the topology of the narrow bands.

Perturbation	Topology change	References
Strain	✓	[84,116], this work
Hartree	×	[59,60]
Substrate	✓	[114]
Displacement field	×	[127,128]

VI. CONCLUSION

In summary, we studied the combined effects of twist and strain in bilayer graphene using atomistic tight-binding and strain-extended continuum models. Strain reshapes the moiré geometry, broadens the narrow bands, splits the vHs, lifts valley degeneracy, and shifts the Dirac points within the mBZ. The shear strain introduces stronger distortion of both the geometrical and electronic properties. Specifically, under the same strain strength, the shear type induces a larger vHs separation than the uniaxial strain, in agreement with recent experimental results [46,48]. Moreover, the strain direction is crucial: It controls both the bandwidth and the valley-resolved topology, and shifts the twist angle that minimizes the bandwidth.

A continuum model with strain-induced scalar and gauge fields reproduces the atomistic spectra and the strain-driven topological transitions that occur when the gap to the remote bands closes and reopens. Including electrostatic (Hartree) interactions, we found nonrigid spectral shifts at low strain that evolve toward an almost rigid shift at higher strain; the interaction mainly reshapes the bands without reversing the strain-induced broadening. These results show that strain pro-

vides a practical knob to control band structure and valley topology in moiré graphene.

ACKNOWLEDGMENTS

We thank Christophe De Beule, Mikito Koshino, and Eduardo V. Castro for fruitful discussions. Z.Z. thanks Wei Li for the discussion in the 2DSPM conference in San Sebastián, which inspired the initial idea of this work. IMDEA Nanociencia acknowledges support from the “Severo Ochoa” Programme for Centres of Excellence in R&D (CEX2020-001039-S/AEI/10.13039/501100011033) financed by MICIU/AEI/10.13039/501100011033 and from NOVMOMAT, Grant No. PID2022-142162NB-I00, funded by MCIN/AEI/ 10.13039/501100011033 and by “ERDF A way of making Europe”. F.E. acknowledges support from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 101210351. Z.Z. acknowledges support from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 101034431 and from the “Severo Ochoa” Programme for Centres of Excellence in R&D (CEX2020-001039-S/AEI/10.13039/501100011033). P.A.P. acknowledges funding by Grant No. JSF-24-05-0002 of the Julian Schwinger Foundation for Physics Research. S.Y. acknowledges funding from the National Natural Science Foundation of China (Grants No. 12425407 and No. 12174291) and the Natural Science Foundation of Hubei Province, China (Grant No. 2023BAA020). Numerical calculations presented in this paper have been performed in the Supercomputing Center of Wuhan University.

Z.Z. and F.E. supervised the project. D.W. performed the tight-binding calculations with the help of Z.Z. F.E. performed the continuum calculations. All authors discussed the results. F.E., D.W., and Z.Z. cowrote the manuscript with inputs from all the authors.

The authors declare no competing interests.

DATA AVAILABILITY

The data and codes that support the findings of this article are not publicly available. They are available from the authors upon reasonable request.

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