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# All Magic Angles in Twisted Bilayer Graphene are Topological

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We show that the electronic structure of the low-energy bands in the small angle-twisted bilayer graphene consists of a series of semi-metallic and *topological* phases. In particular we are able to prove, using an approximate low-energy particle-hole symmetry, that the gapped set of bands that exist around *all* magic angles have nontrivial topology stabilized by a magnetic symmetry, provided band gaps appearing at fillings of  $\pm 4$  electrons per Moiré unit cell. The topological index is given as the winding number (a  $\mathbb{Z}$  number) of the Wilson loop in the Moiré BZ. Furthermore, we also claim that, when the gapped bands are allowed to couple with higher energy bands, the  $\mathbb{Z}$  index collapses to a *stable*  $\mathbb{Z}_2$  index. The approximate, emergent particle-hole symmetry is essential to the topology of graphene: when strongly broken, non-topological phases can appear. Our paper underpins topology as the crucial ingredient to the description of low-energy graphene. We provide a 4-band short range tight-binding model whose 2 lower bands have the same topology, symmetry, and flatness as those of the twisted bilayer graphene, and which can be used as an effective low-energy model. We then perform large-scale (11000 atoms per unit cell, 40 days per  $\mathbf{k}$ -point computing time) *ab-initio* calculations of a series of small angles, from  $3^\circ$  to  $1^\circ$ , which show a more complex and somewhat different evolution of the symmetry of the low-energy bands than that of the theoretical Moiré model, but which confirms the topological nature of the system.

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Twisted bilayer graphene (TBG) is an engineered material consisting of two layers of graphene, coupled via van-der-Waals interaction and rotated relative to each other by some twist angle  $\theta$ . This material exhibits rich single and many-body physics [1–4]. Recently, it was suggested that for  $\theta_e \sim 1.1^\circ$ , charge gaps appear at fillings of  $\pm 4$  electrons per Moiré unit cell. Importantly, another charge gap at  $-2$  was also detected, and conjectured to be a “Mott gap” [5, 6]. If true that the “Mott” state appears, this represents the first many-body phase in zero-field graphene. Upon gating the sample, zero resistivity was observed at low temperatures within a range of carrier density near the Mott gap. The superconductivity in TBG is *conjectured* to be unconventional [7–12]. TBG could be a new platform for the study of strong correlation physics [13–17]. The observed single-particle charge gaps at fillings  $\pm 4$  are consistent with the prediction of an earlier theoretical model in Ref. [18], which we call the Moiré band model (MBM). In MBM, the two valleys at  $K$  and  $K'$  in the graphene Brillouin zone (BZ) decouple. In each valley, the electronic bands of TBG are obtained by coupling the two Dirac cones in the two layers offset in momentum by the angle twist. The model predicts the vanishing of the Fermi velocity at half-filling for certain twist angles called the “magic angles”, labeled as  $\theta_{mi}$  with

$i$  integers. The predicted first (largest) magic angle is  $\theta_{m1} \sim 1.05^\circ$ , close to the experimental  $\theta_e$ , and therefore the experimental observation of the narrow bands and “Mott physics” may be related to the vanishing Fermi velocity.

In this paper, we show, by exhaustive analytical, numerical and *ab-initio* methods, that nontrivial band topology is prevalent in TBG *near every magic angle*, given band gaps appearing at  $\pm 4$ . We prove that in the MBM for each valley, as long as direct band gaps exist between the middle two bands (not counting spin) and the rest, the two bands possess nontrivial band topology protected by the symmetry  $C_2T$ , a composite operation of twofold rotation and time-reversal [19–21]. The nontrivial topology is diagnosed both from irreducible representations (irreps) of magnetic groups at high-symmetry momenta as well as from the winding number of Wilson loops. The proof for arbitrary  $\theta$  exploits an approximate particle-hole (PH) symmetry in the original MBM; without invoking this symmetry, or if the symmetry is strongly broken, the zero energy bands do not necessarily need to be topological. When the PH symmetry is broken (softly, in the MBM), the statement is proved for  $\theta_{m1} \geq \theta \geq \theta_{m6}$  via explicit calculations. We conjecture that the fragile  $\mathbb{Z}$  topological index of the two middle bands collapses to a *stable*  $\mathbb{Z}_2$  index when more

bands are considered.

The nontrivial band topology obstructs the building of a two-band tight-binding model for one valley with correct symmetries and finite range of hopping. In order to capture the symmetry, dispersion and topology of the Moiré bands, we—for the first time—write down a four-band tight-binding (TB) model defined on the Moiré superlattice with short range hopping. The TB model offers an anchor point for the study of correlation physics in TBG, when interactions are projected to its lower two bands. We test the validity of MBM and of the symmetry eigenvalues used to obtain our TB model by performing large scale first principles calculations very close to  $\theta_{m1}$ . Each  $k$  point we computed takes about 30-40 days for  $\theta \sim \theta_{m1}$ . Different from the MBM, we find that the gap at Moiré  $K$  point due to the inter-valley coupling of graphene changes non-monotonically as  $\theta$  decreases. This (along with graphene buckling) could explain the decrease in conductivity at half filling observed in experiments. If this gap is ignored, the DFT bands have the same topology with the MBM and TB model.

We now analyze the symmetries of the one-valley MBM. (Please see Section 2 of [22] for a short review of MBM.) Due to the vanishing of the  $K$  to  $K'$  inter-valley coupling, any symmetry that relates  $K$  to  $K'$  in the original layer is hence not present in the one-valley model: time reversal,  $C_{6z}$  and  $C_{2y}$  are absent, but  $C_{3z}$ ,  $C_{2x}$ , and  $C_{2z}T$  remain, which generate the magnetic space group (MSG)  $P6'2'2$  (#177.151 in the BNS notation [23]). Spin-orbit coupling is neglected in the MBM. For the phase at  $\theta \gtrsim \theta_{m1}$  in MBM, where the two bands near charge neutrality point are disconnected from other bands (A-phase in Fig. 1(a)) the irreps of the two bands are calculated to be  $\Gamma_1 + \Gamma_2$ ,  $M_1 + M_2$  and  $K_2 + K_3$  at  $\Gamma$ ,  $M$  and  $K$  points, respectively. (See Table I for the definitions of irreps [24]). Compared to the irreps of elementary band representations [25–27] (EBRs), which represent the atomic limits, listed in Table 1 of Ref. [22], we conclude that these two bands (dubbed 2B-1V for “two-band one-valley”) cannot be topologically trivial: they cannot be decomposed into sum of a positive number of atomic insulators. If we allow coefficients to be negative, we obtain this decomposition: 2B-1V =  $s@2c + p_z@1a - s@1a$ . Here  $s@2c$  represents the band formed by the  $s$  orbital at the honeycomb lattice,  $p_z(s)@1a$  represents the band formed by the  $p_z(s)$  orbital at the triangular lattice. The negative integer indicates that 2B-1V at least host a “fragile” topology [25, 27, 28]; namely, one cannot construct exponentially localized Wannier functions unless they are coupled to some other atomic bands.

As the twist angle decreases away from  $\theta_{m1}$  in the MBM, the band structure and the irreps at high-symmetry momenta experience non-monotonous changes, but “magic angles”—where the Fermi velocity at half-filling vanishes—reappear periodically. In Fig. 1,

	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$M_1$	$M_2$	$K_1$	$K_2K_3$		
$E$	1	1	2	$E$	1	1	$E$	1	2
$2C_3$	1	1	-1	$C'_2$	1	-1	$C_3$	1	-1
$3C'_2$	1	-1	0				$C_3^{-1}$	1	-1

TABLE I. Character table of irreps at high symmetry momenta in magnetic space group  $P6'2'2$  (#177.151 in BNS settings) [24]. The definitions of high symmetry momenta are given in Table 1 of Ref. [22]. For the little group of  $\Gamma$ ,  $E$ ,  $C_3$ , and  $C'_2$  represent the conjugation classes generated from identity,  $C_{3z}$ , and  $C_{2x}$ , respectively. The number before each conjugate class represents the number of operations in this class. Conjugate class symbols at  $M$  and  $K$  are defined in similar ways.

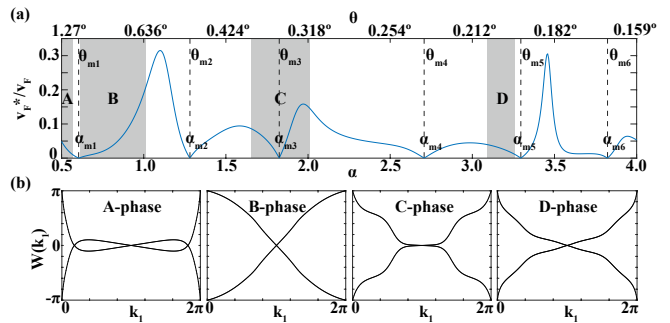


FIG. 1. (a) Fermi velocity at the charge neutrality point of the MBM plotted as a function of the twist angle. The dimensionless parameter  $\alpha = w/(2v_F|\mathbf{K}|\sin(\frac{\theta}{2}))$  uniquely determines the band structure of the MBM (up to a scaling);  $w$  is the inter-layer coupling,  $v_F$  is the Fermi velocity of single layer graphene,  $|\mathbf{K}|$  is the distance between  $\Gamma$  and  $K$ , and  $\theta$  is the twist angle. (See Ref. [18] or Section 2 of Ref. [22] for more details.) In this plot we set  $w = 110\text{meV}$ ,  $v_F|\mathbf{K}| = 19.81\text{eV}$ . The gapped regions,  $\Theta_a$ , where the two bands near charge neutrality point are fully disconnected from all other bands are shadowed with grey, and labeled as A, B, C, D. The magic angles, where the Fermi velocity vanishes, are marked by dashed lines. By numerical calculation we find that  $\alpha_{m1} \approx 0.605$  ( $\theta_{m1} \approx 1.05^\circ$ ),  $\alpha_{m2} \approx 1.28$  ( $\theta_{m2} \approx 0.497^\circ$ ),  $\alpha_{m3} \approx 1.83$  ( $\theta_{m3} \approx 0.348^\circ$ ),  $\alpha_{m4} \approx 2.71$  ( $\theta_{m4} \approx 0.235^\circ$ ),  $\alpha_{m5} \approx 3.30$  ( $\theta_{m5} \approx 0.193^\circ$ ),  $\alpha_{m6} \approx 3.82$  ( $\theta_{m6} \approx 0.167^\circ$ ). (b) The Wilson loops of the four gapped phases have the same winding number, 1.

we show the evolution of the Fermi velocity as function of twist angle  $\theta$ . As a function of  $\theta$ , the middle two bands are not always separated by a (direct) gap at all momenta: there are four gapped intervals, denoted as  $\Theta_a$ , where the middle two bands form a separate group of bands, shaded by grey in Fig. 1. While  $\theta_{m3} \in \Theta_a$ ,  $\theta_{m1, m2, m4, m5, m6} \notin \Theta_a$ . Therefore, the topology is ill-defined for the middle two bands in the MBM at higher magic angles. However, for any  $\theta \in \Theta_a$ , as well as for smaller angles, we show below that 2B-1V is topologically nontrivial.

Besides the  $P6'2'2$  symmetry, the MBM also has an approximate PH symmetry. In the limit of zero rotation of the Pauli matrices of the spin between the

two graphene layers, this symmetry is exact—one of the approximations used in Ref. [18]. As we discuss in Section 2 of Ref. [22], this PH symmetry is *unitary* and it *anti-commutes* with  $C_{2x}$ . The symmetry is crucial in proving a theorem for TBG. We numerically show that our results, understood in light of the approximate PH symmetry, hold for the general case [29]. First we show that in the presence of the approximate PH symmetry, for  $\theta \in \Theta_a$  2B-1V has *at least* nontrivial fragile topology. The explicit full proof is given in Sections 2 and 4 of Ref. [22]. The irreps at K and K' of 2B-1V are always the same as the irreps at K and K' in single layer graphene. For the irreps of 2B-1V at  $\Gamma$  and M, one uses that the PH symmetry operator anti-commutes with  $C_{2x}$  but commutes with the other generators of  $C_{2z}T$  and  $C_3$ . Due to these relations, the upper and the lower irreps have opposite  $C_{2x}$  eigenvalues and hence form  $\Gamma_1 + \Gamma_2$ . Similarly, the irreps at M are forced to be  $M_1 + M_2$ . The bands at any  $\theta \in \Theta_a$  have the same irreps at all high-symmetry momenta as those for  $\theta \gtrsim \theta_{m1}$  (A-phase in Fig. 1(a)). They then have the same EBR decomposition as the A-phase and we know that the 2B-1V again has fragile topology. The fragile topology can be proved from another perspective. In Section 4 of Ref. [22], we prove a lemma relating the winding of the Wilson loop eigenvalues of any 2B-1V model to the irreps at high-symmetry momenta, similar to index theorems in Ref. [30–32]. Applying the lemma to the irreps of 2B-1V at any  $\theta \in$  any gapped interval, we find the winding to be  $\pm 1 \pmod 3$ , *i.e.*, nontrivial.

The irreps cannot, by themselves, distinguish if the winding is even or odd. For the first four gapped phases, we calculate the Wilson loop of 2B-1V, and find its winding to always be  $\pm 1$ . This suggests something stronger: we *conjecture* that 2B-1V has in fact a stable  $\mathbb{Z}_2$  topological index protected by  $C_{2z}T$ . To see this, one realizes that the homotopy group of gapped Hamiltonians in 2D is given by  $\pi_2[O(N_{occ} + N_{unocc})/O(N_{occ} \oplus N_{unocc})] = \mathbb{Z}_2$  for  $N_{unocc,occ} > 2$  and  $= \mathbb{Z}$  for  $N_{occ} = 2$  where the latter is nothing but the winding number of Wilson loop eigenvalues. Adding trivial bands to the lowest two bands maps one element in  $\mathbb{Z}$  to one  $\mathbb{Z}_2$  following the simple rule  $z_2 = z \pmod 2$ , *i.e.*, odd windings are stable to superposition of trivial bands (see Section 4 of Ref. [22]). The collapse from  $\mathbb{Z}$  classification to  $\mathbb{Z}_2$  classification when more bands are considered has been discussed in Ref. [33], and the  $\mathbb{Z}_2$  index is identified as the second Stiefel-Whitney class.

Having proved the topological nature of the one-valley model. We note that the two-valley model is just two copies of the one-valley model. As shown in Section 2 of Ref. [22], the irreps of the 4 bands near charge neutrality are the same as those of two atomic insulators. If we break the valley quantum number by considering the inter-valley coupling, a small gap is opened at the K point, and the four bands are now Wannierizable.

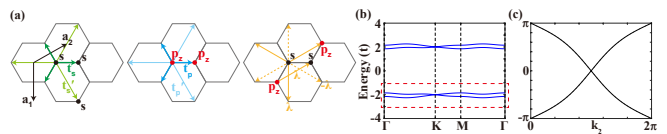


FIG. 2. The four-band tight-binding model for one valley. The *lower* two bands have identical irreps and Wilson loop winding of the gapped middle two bands in the one-valley MBM. (a) The tight-binding model. The energy splitting between  $s$  and  $p_z$  is  $\Delta$ . The hopping parameters  $t_{s,p}$ ,  $t'_{s,p}$ ,  $\lambda$  are all in general complex numbers. (b) The band structure. (c) The Wilson loop of the lower two bands. (b) and (c) are calculated with the parameters  $t_s = t_p = t$ ,  $t'_s = t'_p = -\frac{1}{3}t$ ,  $\lambda = \frac{2}{\sqrt{27}}t$ , and  $\Delta = 0.15t$ . As discussed in Section 5 of Ref. [22], such parameters are chosen to flatten the band width.

We now build short-range hopping models with the correct symmetries and topology, that should be used as toy-models for the two topological graphene bands. Due to the topological obstruction, a two-band short range model with the correct symmetry that simulates 2B-1V is excluded [14, 34]. However, we can successfully build a tight-binding 4-band, 1 valley lattice model with short range hopping parameters, which has 2 bands separated by a band gap from another 2 bands: either of these two bands is a model for the 2B-1V. We here give the strategy for building this model, and leave the details in Section 5 of Ref. [22]. We showed that the irreps ( $\Gamma_1 + \Gamma_2$ ,  $M_1 + M_2$ , and  $K_2K_3$ ) of the middle two bands in one-valley MBM, can only be written as a difference of irreps of atomic insulators:  $s@2c + p_z@1a - s@1a$ . We now reinterpret these irreps differently: from Table 1 in Ref. [22] we see that they can be thought as forming one disconnected branch of the composite bands formed by the sum of  $s$  and  $p_z$  orbitals sitting on the honeycomb lattice ( $2c$ ). This understanding gives us an ansatz for building the TB model. We start with two independent orbitals ( $s$  and  $p_z$ ) at the honeycomb lattice, which give the irreps  $2\Gamma_1$ ,  $2M_1$ ,  $K_2K_3$ , and  $2\Gamma_2$ ,  $2M_2$ ,  $K_2K_3$ , respectively. We then mix the two EBR's, undergo a phase transition, and decompose the bands into two new branches, each of which has the irreps  $\Gamma_1 + \Gamma_2$ ,  $M_1 + M_2$ , and  $K_2K_3$  — the correct representations of 2B-1V. By this method the tight binding model reproduces the irreps of the middle two bands. What is left is to reproduce the correct Wilson loop winding (in principle it may wind  $3n \pm 1$  times.) Heuristically, the number of phase transitions gives the winding of the Wilson loop. Since the winding of the Wilson loop is 1 in the 2B-1V model, only one phase transition separates this phase from the phase described by the two orbitals with a gap between them. By this strategy we obtain the hoppings shown in Fig. 2. Our TB model reproduces both the correct irreps, Wilson loop winding and flat dispersion.

Our proofs of topology in low energy TBG are based on the simplified MBM. To give them any credibility, we now

must relate our predictions to the realistic calculations of twisted bilayer graphene with negligible spin-orbit coupling. We perform a series of *ab-initio* calculations for  $i \in \{6, 10, 16, 23, 30\}$  where  $i$  denotes the commensurate twist angle by the formula  $\theta_i = \arccos \frac{3i^2+3i+0.5}{3i^2+3i+1}$  [35]. In our calculations, the distance between the two layers is set to be 3.35Å. Full band structures are given in Section 6 of [22]. Our *ab-initio* calculations show two remarkable features different from the MBM: **1.** the PH symmetry breaking is larger. **2.** the gap at the  $K$  point of the Moiré BZ is tiny but exists.

In Fig. 3(a), we show the evolution of the *ab-initio* energy bands at  $\Gamma$  explicitly. The realistic TBG has two graphene valleys. Thus the time-reversal symmetry is recovered and the realistic TBG has a higher symmetry group than  $P6'2'2$ . However, to keep the notations consistent with the one-valley results, we still label the bands by the irreps of  $P6'2'2$  (by forgetting the time-reversal symmetry). The gray line stands for the 2-fold  $2\Gamma_2$  band and the red line stands for the 2-fold  $2\Gamma_1$  band. The two blue lines stand for two different 4-fold  $2\Gamma_3$  bands. The energies at the  $\Gamma$  point are not PH symmetric: the gap between the lower  $2\Gamma_3$  and  $2\Gamma_2$  bands is much smaller than that between the higher  $2\Gamma_3$  and  $2\Gamma_1$  bands. A metallic phase occurs for the middle 4 bands for  $16 < i < 30$ , in which the middle 4 bands are not separated from others. In Fig. 3(b), we calculate the gap at the Moiré  $K$  point as a function of the twist angles ( $\theta_i$ ). We find the gap at  $K$  always exists and varies non-monotonically as changing theta. In the MBM, no energy difference is expected between two  $K_2K_3$  representations coming from different valleys. However, in *ab-initio* calculations of TBG without lattice warping, this is not the case. Due to numerical difficulties, we only obtain the gap for  $i = 6, 10, 16$  and  $23$ . We conjecture that the gap at  $K$  is not negligible for an extremely small angle. Since the experimental data suggests that the gap is small, we are left with the conclusion that effects not introduced in our *ab-initio* such as lattice relaxation and/or graphene lattice warping, are important and render the gap at the  $K$  point much smaller.

In conclusion, we have performed a complete and exhaustive study of the TBG band structure and showed that the low energy bands are always topological, as long as the lowest two bands are gapped from the rest. We then provided short-range toy tight-binding models for the low energy TBG, which should (with atomic orbitals matching the charge density of a triangular lattice) be used to study the effects of correlations in graphene. We then checked our results by performing a large set of *ab-initio* calculations, and presented the areas of agreement and disagreement with the simple, continuum model, as well as possible solutions to these disagreements.

Our work underpins topology as the fundamental

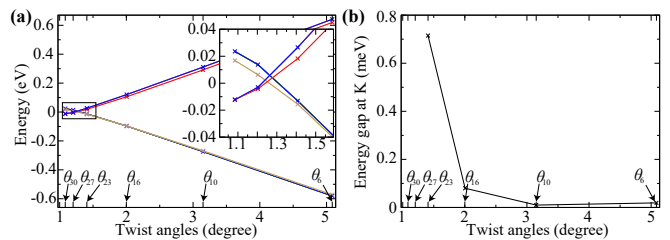


FIG. 3. Electronic band structures with different commensurate twist angles  $\theta_i$ . (a) The *ab-initio* electronic band structures clearly show the breaking of partial-hole symmetry. The bands change non-monotonically as decreasing  $\theta$ . The inset is the zoomin of the blackbox area. The two blue bands indicate two  $2\Gamma_3$  bands; the gray band is the  $2\Gamma_2$  band; the red band is the  $2\Gamma_1$  band. (b) The gap at  $K$  at charge neutrality as a function of the twist angle.

property of the low energy bands of TBG. Here we briefly discuss a few possible effects in the strong correlation physics that may arise from the band topology. When the interaction is smaller than the gap between the 2B-1V and other bands, an efficient way to study the interacting phase is to project the interaction term to the 2B-1V low-energy space. However, since exponentially decaying symmetric Wannier functions are obstructed in the 2B-1V, the symmetric Wannier functions have to be power-law decaying and the projected interaction will become effectively long-range, though the original interaction is short-range. Novel symmetry-breaking phases and collective modes can appear due to this effective long-range interaction. Another nontrivial effect arising from the band topology is the large superfluid weight in the superconducting phase. In Ref. [36] the authors showed that when a flat band with nonzero spin Chern number becomes superconducting, the superfluid weight must be larger than a topological lower bound. In Ref. [37], we show that similar effects also happen in TBG: with certain pairing, the superfluid weight in the superconducting phase of the fragile 2B-1V has a lower bound given by the winding number of the Wilson loop.

*Note.* During the extended period of time that passed while obtaining our *ab-initio* results, Ref. [14] has also predicted that the bands at half filling are fragile topological. The differences between our papers are: our paper contains *ab-initio* results essential in confirming the nature of the bands, uses the PH symmetry to *prove* all low-energy bands in TBG at *any* angle are topological. Our paper does not present conjectures or proofs about the Mott phase of TBG. After our paper was posted, Ref. [38] proved that the  $C_2T$  fragile phase with nontrivial  $\mathbb{Z}_2$  index became Wannierizable after adding atomic bands. This conclusion is not inconsistent with ours since stable index does not necessarily implies non-Wannierizability. After a very brief discussion with us, the authors of Ref. [38] posted a version 2 of their paper which identifies

a stable index (referred as the second Stiefel-Whitney index). After Ref. [38] appeared, Ref. [39] presented an elaborate study on the Stiefel-Whitney index and its relation with Wilson loop.

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