Incommensurability-induced sub-ballistic narrow-band-states in twisted bilayer graphene

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Abstract

We study the localization properties of electrons in incommensurate twisted bilayer graphene for small angles, encompassing the narrow-band regime, by numerically exact means. Sub-ballistic states are found within the narrow-band region around the magic angle. Such states are localized in momentum-space and follow non-Poissonian level statistics, in contrast with their ballistic counterparts found for close commensurate angles. Transport results corroborate this picture: for large enough systems, the conductance of samples with fixed width decreases with the system size in the longitudinal direction for incommensurate angles within the sub-ballistic regime. Our results show that incommensurability/quasiperiodicity effects are of crucial importance in the narrow-band regime. The incommensurate nature of a general twist angle must therefore be taken into account for an accurate description of magic-angle twisted bilayer graphene.

Narrow-band electronic systems are natural platforms to search for exotic physics. Otherwise modest perturbations can here attain energies comparable to the bandwidth, yielding a non-perturbative reorganization of the eigenstates into phases of matter often very different from their parent state. Recently, twisted bilayer graphene (tBLG) has emerged as a paradigmatic system displaying this mechanism. When the twist angle between the layers approaches the so-called magic angle, $\theta \approx 1.1^\circ$, extremely narrow, nearly flat, bands appear at low energies [1–6]. In this regime, superconductivity [7] and correlated insulating phases [8] were observed around integer electronic fillings, pointing to relevant electron-electron interactions [9]. The similarities with the cuprates [10] sparked redoubled interest in these effects, which emerge here in a simpler, cleaner and highly tunable system, where all ingredients can potentially be easily isolated and understood. This triggered intense theoretical [11–27] and experimental [28–37] research.

Due to the high degree of sample-purity, models of tBLG typically assume a Fermi gas with a flat-band dispersion as a starting point [11–13, 18, 21, 23–25, 38, 39]. This is a major difference with respect to the cuprates, as disorder is intrinsic to doped Mott insulators [40] and has even been observed to increase the critical temperature [41]. Nonetheless, in [42, 43], localization has been predicted for the recently observed ‘dodecagonal graphene quasicrystal’ [44, 45], a tBLG with $\theta = 30^\circ$. This phenomenon is due to the quasiperiodic nature of the system for incommensurate values of $\theta$. Incommensurability was also shown to induce quantum phase transitions in two-dimensional (2D) models [46], including the so-called chiral limit of tBLG for moderate twist angles ($\theta \approx 9^\circ$), yielding a critical ‘magic-angle semimetallic’ state with a multifractal momentum-space wave function. For more realistic models of tBLG, the proximity to commensurate angles with small unit cells, has been shown to imprint sharp conductance signatures [47]. However,
for small angles, $\theta \lesssim 3^\circ$, these features seem to be washed away, in accordance with the general belief underlying continuous models [14].

Incommensurability can doubtlessly induce localization [48–50] or multifractallity in 2D [46]. However, at this point, it is not clear how the commensurate/incommensurate nature of the tBLG structure affects the properties of eigenstates in the small-angle narrow-band regime. As in tBLG several energy scales are comparable, understanding the role played by incommensurability is essential to devise effective interacting models able to faithfully capture their competition.

In this letter we address the effects of incommensurability/quasiperiodicity in the nature of the narrow-band states and on the transport properties of tBLG, neglecting electron–electron interactions. We employ a number of numerically exact methods to show that incommensurate angles induce momentum-space delocalization of the narrow-band states, whereas for commensurate angles eigenstates are ballistic with a localized momentum-space wave function. The presence of a sub-ballistic regime is corroborated by finite-size scaling analysis of the conductance which decreases with system size for incommensurate structures, while saturating for commensurate ones.

1. Model and methods

We study a model of tBLG with the tight-binding Hamiltonian

$$H = -t \sum_{l, (r_{l,α}, r_{l,β}), (r_{l',α}, r_{l',β})} c_{l,α}^\dagger(r_{l,α}) c_{l',β}(r_{l',β}) + \sum_{|r_{l,α} - r_{l',β}| < 2} t_{1}(r_{1,α} - r_{2,β}) c_{l,α}^\dagger(r_{l,α}) c_{2,β}(r_{2,β}) + \text{h.c.},$$

(1)

where the first term describes the nearest-neighbor intralayer hopping $t$ [51], and $l = 1, 2$ is the layer index. The second term models the interlayer hopping, with $r_{l,α}$ the in-plane position in layer $l$ and sublattice $α = A, B$. The interlayer hopping $t_{1}(r)$ is parameterized in terms of Slater–Koster parameters used in [52–54]:

$$r_{1}^2 = r_{V_{pp}}(r_{\Delta}) + r_{V_{pp}}(r_{\Delta})$$

where $r_{\Delta} = \sqrt{d_{1}^2 + d_{2}^2}$, $V_{pp}(r) = t_{1} \exp\left((d_{l} - r)/\delta\right)$, $V_{pp}(r) = -t_{1} \exp\left((d_{l} - r)/\delta\right)$, $d_{l} = 0.142$ nm is the C–C distance, $d_{1} = 0.335$ nm is the distance between layers and $\delta = 0.1844$, with $d_{1} = 0.246$ nm the monolayer constant. We used $t = 2.7$ eV and $t_{1} = 0.48$ eV. For the calculations presented hereafter, energy and length scales are measured in units of $t$ and $a$, respectively.

Interlayer hoppings were considered only among atoms with in-plane distance $r < \Lambda$. For a small cutoff, $\Lambda \sim d$, the narrow-band angle, $\theta_{0}$, is very sensitive to relative translations of the layers. This effect washes-away for larger $\Lambda$. To mitigate finite-size effects we set $\Lambda = 2.6d$, above which this effect is already insignificant.

A tBLG lattice with periodic boundary conditions can be defined by the integers $(m, n, r)$, where $(m, r)$ are coprime numbers that determine the commensurate twist angle $\theta(m, r)$ [3], and $n$ is the linear number of supercells in the system, i.e. the lattice contains $n^{2}$ supercells. The superlattice basis vectors, the commensurate twist angle $\theta(m, r)$ [3], and the number of moiré pattern cells $N_{m}(n, r)$ as a function of the integer tuples are given in the supplemental material (SM) (available online at stacks.iop.org/2DM/9/011001/mmedia) [55].

We follow a well established method that consists of approximating an infinite incommensurate structure (here characterised by twist angle $\theta_{0}$) by a sequence of approximants with increasing lattice size (here taken to be $n = 1$ structures with $\theta(m, r) \approx \theta_{0}$) [56]. An approximant structure may encompass many moiré cells (for $r \neq 1$), its unit cell coincides with the size of the system.

Commensurate structures are obtained by taking $n > 1$ and a finite-size scaling analysis is performed by increasing $n$ with fixed $(m, r)$. The main advantage of this method is to eliminate boundary effects, present for open systems, by always considering closed boundary conditions [57].

To characterize the system's eigenstates near the narrow-band energies, we used Krylov–Schur exact diagonalization (ED) with shift-invert [58, 59]. To further mitigate finite-size effects, we average all relevant quantities with respect to a phase-twist we introduce in the boundary conditions and to a random relative stacking translation, $\delta_{1}$, between the two layers. We approximate the density of states (DOS) by binning the energies, $\rho(E) = N(E)/\Delta EN$, where $N(E)$ is the number of states inside the bin centered around energy $E$ and width $\Delta E$, and $N$ is the total number of sites. We also study the eigenstates’ momentum-space localization properties through the momentum-space inverse participation ratio (IPR) [60],

$$I_{k} = \left(\sum_{k,α} |\Psi_{l=1, k,α}|^{2}\right)^{-2} \sum_{k,α} |\Psi_{l=1, k,α}|^{4},$$

(2)

where $\Psi_{l=k,α}$ is the eigenstate amplitude in layer $l$ momentum $k$ and sublattice $α$. Note that we restrict the sum in $I_{k}$ to the unrotated layer, $l = 1$, without loss of generality (alternatively we could have chosen the rotated layer or both). For wavefunctions localized in momentum-space, $I_{k} \sim L^{0}$, where $L$ is the linear system size [61], whereas a $I_{k} \sim L^{-\nu}$, with $\nu > 0$, indicates momentum-space delocalization. We checked that the real-space inverse participation ratio always scales with $L^{-\nu}$, signaling no real-space localization (see SM [55]). Therefore, $I_{k} \sim L^{-\nu}$, with $\nu > 0$, indicates the presence of sub-ballistic states.
To complement the eigenstate’s analysis, we study the statistics of the energy levels through the quantity $r_{st} = \langle \Delta E \rangle_{EE_{st}}$, where $r_{st}$ is defined as $r_{st} = \min(\Delta E_i, \Delta E_{i+1})/\max(\Delta E_i, \Delta E_{i+1})$, with $\Delta E_i = E_i - E_{i-1}$ (for ordered levels $E_i > E_{i-1}$) and where the average, $\langle \rangle_{EE_{st}}$, is first performed over all the eigenvalues within an energy window $E_w$ for each realization and then over $N_r$ realizations of boundary twists and stacking shifts. The relevant known values [62] for $r_{st}$ are: (a) $r_{st}^{\text{Poisson}} \approx 0.39$ if the spacings follow a Poisson distribution; (b) $r_{st}^{\text{GUE}} \approx 0.6$ for the Gaussian unitary ensemble (GUE), when the Hamiltonian breaks time-reversal symmetry (here due to twisted boundary conditions). Case (a) applies when the wavefunction is localized in some basis: this includes ballistic (momentum-space localized) or insulating (real-space localized) states. Case (b) applies when the wavefunction is delocalized in any basis and when the energy levels satisfy a random matrix theory description.

Finally, we analyze transport properties by computing the conductance, $G$. We considered two semi-infinite stripes of single-layer graphene that overlap within a region of fixed width and variable length, $\sim L$. The graphene leads are rendered metallic by doping (see SM [55] for more details).

2. Commensurate vs. incommensurate

We start by providing a general overview on the differences between commensurate and incommensurate structures around the first magic-angle. Figures 1(a) and (b), depict the DOS and $I_k$ of incommensurate structures for different energies and angles with a fixed number of moiré cells $N_M = 48$. As expected, a narrow-band occurs for the magic-angle $\theta_0 \approx 1.09^\circ$, close to the merging of two van-Hove singularities (VHS) present at larger $\theta$. Remarkably, figure 1(b) shows that $I_k$ becomes very small for energies within the narrow-band. This is not observed for commensurate structures, as justified below.

Figures 1(c) and (d) show $r_{st}$ and $I_k$ averaged within the energy window represented by the horizontal dashed lines in figure 1(a), both for incommensurate ($r = 9, 12, 15; n = 1$) and commensurate ($r = 1; n = 7, 9$) structures. As expected for ballistic states, for commensurate angles, $r_{st}$ follows Poisson statistics and $I_k$ is independent of the system size. Conversely, for incommensurate angles: (a) $r_{st}$ raises above the Poisson value within a finite interval of (incommensurate) angles, reaching a maximum value for $\theta = \theta_0$; (b) For the same interval of angles, $I_k$ scales down with system size, reaching a minimum for $\theta = \theta_0$. Outside this regime, $I_k$ becomes $L$-independent and approaches the value obtained for commensurate structures (figure 1(d)).

These results suggest that, as a function of $\theta$, there is a ‘collision’ of energy bands around $\theta_0$, with subsequent band inversion. We confirm such phenomena when the narrow band regime is tuned by changing the amplitude of $t_L$ (see [55]). It is plausible that the same happens when changing $\theta$. 
for fixed \( t_\perp \), but a similar analysis is prevented within our setup by changes in system size with \( \theta \). Within this picture, the narrow-band regime corresponds to the collision area where states from the two hands become highly mixed (as seen by \( \mathcal{I}_k \)) and their energy levels repel (as seen by \( r_{st} \)). Moreover, at least a finite portion of the states inside the considered energy window have sub-ballistic properties within a finite interval of angles that we now explore in more detail.

### 3. Sub-ballistic regime

We provide an energy resolved and finite-size scaling analysis. Figure 2 shows two angles chosen in order to observe merged VHS in figure 2(a), and a minimal bandwidth in figure 2(b).

Figures 2(c), (d) and (e), (f) depict, respectively, \( \mathcal{I}_k \) and \( r_{st} \) averaged over the shaded energy windows of figures 2(a) and (b). The results do not change significantly if smaller energy windows are considered. The approximant series was chosen to ensure a monotonic approach to the desired incommensurate angle upon increasing system size (see [55]), and we ensure an overall angle variation in the series below 10\(^{-6}\). States with different scaling behaviors arise at different energies. Typically, when \( \rho(E) \) is larger, the \( \mathcal{I}_k \) is smaller and decreases faster with system size. The latter correlates with a faster scaling of \( r_{st} \) towards the GUE value. For instance, for energies corresponding to the larger DOS observed in figure 2(b), \( \mathcal{I}_k \) reaches its smallest value, scaling as \( \mathcal{I}_k \sim L^{-1}, L^{-2} \). The insets in (c) and (d) contain the quantity \( \chi_k = -d\log \mathcal{I}_k / d\log L \), computed by fitting the data points (\( \log L, \log \mathcal{I}_k \)), considering only points with \( L \geq L_{\text{min}} \). Complete information on the data used in figures (a)–(f) can be found in table S1 in [55].

Outside the narrow-band region, states are ballistic (\( r_{st} = r_{st}^{\text{Poisson}} \) and \( \mathcal{I}_k \sim L^0 \)) even in regions with a highly suppressed DOS. An example is given in figure 2(f) for the states within the shaded area in the inset of figure 2(b).

Finally, for angles above and below the narrow-band regime in figure 2, but still within the sub-ballistic range, states exhibiting non-ballistic properties are also observed. However, their limiting behavior is less conclusive (see [55]).

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**Figure 2.** (a), (b) DOS for incommensurate structures of different sizes, for the angles marked in figure 1(c). The inset in (b) shows a log-scale plot of \( \rho(E) \) for a wider energy range. (c)–(f) Average \( r_{st} \) and \( \mathcal{I}_k \) for a small energy window around selected energies, indicated by the shaded areas in (a), (b) along with marker on top, as a function of the linear system size \( L \propto N^{1/2} \) (the largest systems correspond to \( N \gtrsim 10^6 \), see [55]). The dotted and dashed lines in (c) and (d) correspond respectively to \( \mathcal{I}_k \sim L^{-1}, L^{-2} \). The insets in (c) and (d) contain the quantity \( \chi_k = -d\log \mathcal{I}_k / d\log L \), computed by fitting the data points (\( \log L, \log \mathcal{I}_k \)), considering only points with \( L \geq L_{\text{min}} \). Complete information on the data used in figures (a)–(f) can be found in table S1 in [55].
Figure 3. (a), (b) Finite-size scaling analysis of the conductance for commensurate, $\theta_c$, and incommensurate, $\theta_{ic}$, angles near $\theta_{ft}$: (a) is for $E = 0.084$, inside the narrow band; while (b) is for $E = 0.06$, outside. The error bars correspond to the error of the average conductance computed for 25 different stackings between the graphene layers (see SM [55]). (c) DOS for $\theta_c$ and $\theta_{ic}$. Inset: log-scale plot for a wider energy range. (d), (e) Finite-size analysis of $I_k$ and $r_{st}$, averaged on small energy windows [shaded areas in (c) around $E = 0.06$ and $E = 0.084$, with widths $\Delta E = 10^{-2}$ and $2 \times 10^{-4}$] for $\theta_c$ and $\theta_{ic}$ (see table S2 in [55]). For $E = 0.06$, the DOS is small and a larger energy window is used to increase statistics. Plot markers are used in the scaling analysis of (d) and (e). Dotted and dashed lines in (d) correspond respectively to $I_k \sim L^{-1}$, $L^{-2}$.

4. Conductance

In order to understand the consequences of the sub-ballistic states in transport, we computed the conductance, $G$, using the Kwant package [63]. Unfortunately, for the parameters above, finite-size effects are too severe to draw systematic conclusions (see SM [55]), as the largest systems attainable contain only $N_M \sim 10^2$ moiré cells. To mitigate finite-size effects by increasing the number of moiré cells simulated, we increased the interlayer coupling to $t_\perp = 1.9$ eV, a well-known procedure for shifting the narrow-band regime to larger angles ($\theta_0 \sim 4.4^\circ$, in this case), with smaller period moiré patterns [1–3]. Representative conductance results for $t_\perp = 1.9$ eV are given in figures 3(a) and (b), together with an ED analysis in figures 3(c)–(e). In figure 3(a), $G(L)$ is computed for an energy within the narrow band. In the commensurate case, $G(L)$ converges with $L$ as expected. Conversely, it decreases with $L$ in the incommensurate case, hinting sub-ballistic transport. For smaller $L$, the conductance is very similar in both cases, showing that large enough systems are crucial to observe incommensurability effects in the conductance. On the other hand, ED captures a sub-ballistic behavior even for the smaller systems used: a small, $L$-decreasing $I_k$ and GUE statistics are observed in figures 3(d) and (e).

For energies outside the narrow-band, where the DOS is very small (see inset in figure 3(c)), the ED and conductance results are very similar for commensurate and incommensurate angles (figures 3(b) and (d)), suggesting that incommensurability effects become unimportant.

5. Discussion

We studied the eigenstate localization and transport properties of tBLG for commensurate and incommensurate angles around the first magic angle. For a finite interval of incommensurate angles, encompassing the narrow-band regime, eigenstate delocalization in momentum-space is concomitant with non-Poisson energy level statistics and with a decrease of the conductance with system size. This is compatible with sub-ballistic transport and contrasts with commensurate angles, or with angles away from the narrow-band region, where transport is ballistic. Moreover, the scaling of $I_k$ with system size seem to indicate diffusive behavior, although the results from conductance scaling are unclear with the available system sizes. The present results indicate that the scenario of a ‘magic angle semimetal’ with momentum-space delocalized wave functions, proposed in [46] for a model of moderate angle chiral tBLG, extends to models of incommensurate tBLG.
with twist angles close to the experimentally relevant magic angle $\theta \approx 1.1^\circ$.

Our results have major implications for the low energy properties of tBLG as, in the narrow-band regime, incommensurability alone breaks down a Bloch wave description even for perfectly clean samples. In particular, an analysis of the influence of correlations should equally account for the incommensurate nature of tBLG. These effects have been overlooked in the vast majority of theoretical studies on tBLG, namely the ones starting from continuum models [1–3]. Our findings may also be relevant to the enhanced, linear temperature resistivity observed in tBLG at the magic angle [64, 65]. Even though we restricted the study to small angle tBLG, we anticipate that the present results also apply to other systems with concomitant narrow-bands and incommensurability: tBLG at large angles [66], double bilayers [67–69], twisted bilayers of transition metal dichalcogenides [70, 71]. We also note that even though our model does not account for lattice relaxation, recent experimental results showed that near the magic-angle, both the relaxed and unrelaxed structures are stable, being possible to change between them by applying a STM tip pulse [72]. Moreover, even in the relaxed case, the narrow-band is still present [73] and may even be narrower [74] with incommensurability effects possibly enhanced.

As single-particle localization can give rise to many-body localization once interactions are included [75, 76], we expect the single-particle properties here reported to also play an important role once interactions are considered.

Finally, we checked that our results are robust to relatively strong Anderson-like disorder, of the order of the narrow-band’s width (see [55]), for the studied system sizes (that are much smaller than the finite disorder-induced localization length). Interestingly, commensurate structures are more fragile and, at stronger disorder, their localization properties approach those of disorder-free incommensurate structures.

**Data availability statement**

The data that support the findings of this study are available upon reasonable request from the authors.

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**References**

[1] Lopes Dos Santos J M B, Peres N M R and Castro Neto A H 2007 Graphene bilayer with a twist: electronic structure Phys. Rev. Lett. 99 256802
[2] Bistritzer R and MacDonald A H 2011 Moiré bands in twisted double-layer graphene Proc. Natl Acad. Sci. USA 108 12233–7
[3] Lopes Dos Santos J M B, Peres N M R and Castro Neto A H 2012 Continuum model of the twisted graphene bilayer Phys. Rev. B 86 155449
[4] De Trambly Laisserrière G, Mayou D and Magaud L 2010 Localization of Dirac electrons in rotated graphene bilayers Nano Lett. 10 804–8
[5] Suáez Moroll E, Correa J D, Vargas P, Pacheco M and Barticevic Z 2010 Flat bands in slightly twisted bilayer graphene: tight-binding calculations Phys. Rev. B 82 121407
[6] Shallcross S, Sharma S, Kandelaki E and Pankratov O A 2010 Electronic structure of turbostratic graphene Phys. Rev. B 81 165105
[7] Cao Y, Fatemi V, Fang S, Watanabe K, Taniguchi T, Kaxiras E and Jarillo-Herrero P 2018 Unconventional superconductivity in magic-angle graphene superlattices Nature 556 43–50
[8] Cao Y et al 2018 Correlated insulator behaviour at half-filling in magic-angle graphene superlattices Nature 556 80–84
Balents L, Dean C R, Efetov D K and Young A F 2020 Superconductivity and strong correlations in moiré flat bands Nature, Phys. 16 725–33
Bednorz J G and Müller K A 1986 Possible high Tc superconductivity in the Ba-La-Cu-O system Z. Phys. B 64 189–93
Kang J and Vafek O 2018 Symmetry, maximally localized Wannier states and a low-energy model for twisted bilayer graphene narrow bands Phys. Rev. X 8 031088
Zou L, Po H C, Vishwanath A and Senthil T 2018 Band structure of twisted bilayer graphene: emergent symmetries, commensurate approximants and Wannier obstructions Phys. Rev. B 98 085435
Po H C, Zou L, Vishwanath A and Senthil T 2018 Origin of Mott insulating behavior and superconductivity in twisted bilayer graphene Phys. Rev. X 8 031089
Tamopolsky G, Kruchkov A J and Vishwanath A 2019 Origin of magic angles in twisted bilayer graphene Phys. Rev. Lett. 122 106405
Haddadi F, Wu Q S, Kruchkov A J and Yazyev O V 2020 Moiré flat bands in twisted double bilayer graphene Nano Lett. 20 2410–5
Song Z, Wang Z, Shi W, Li G, Fang C and Andrei Bernevig B 2019 All magic angles in twisted bilayer graphene are topological Phys. Rev. Lett. 123 086401
Carr S, Fang S, Jarillo-Herrero P and Kaxiras E 2018 Pressure dependence of the magic twist angle in graphene superlattices Phys. Rev. B 98 085144
Chen C, Castro Neto A H and Pereira V M 2020 Correlated states of a triangular net of coupled quantum wires: implications for the phase diagram of marginally twisted bilayer graphene Phys. Rev. B 101 165431
Cea T, Walet N R and Guinea F 2019 Electronic band structure and pinning of fermi energy to van hove singularities in twisted bilayer graphene: a self-consistent approach Phys. Rev. B 100 205113
Po H C, Watanabe H and Vishwanath A 2018 Fragile topology and Wannier obstructions Phys. Rev. Lett. 121 126402
Koshino M, Yuan N F Q, Koresutne T, Ochi M, Kuroki K and Fu L 2018 Maximally localized Wannier orbitals and the extended Hubbard model for twisted bilayer graphene Phys. Rev. X 8 031087
Po H C, Zou L, Senthil T and Vishwanath A 2019 Faithful tight-binding models and fragile topology of magic-angle twisted bilayer graphene Phys. Rev. B 99 195455
Kennes D M, Lischner J and Karrasch C 2018 Strong correlations and d + id superconductivity in twisted bilayer graphene Phys. Rev. B 98 241407
Peltonen T J, Ojaerji R and Heikila T 2018 Mean-field theory for superconductivity in twisted bilayer graphene Phys. Rev. B 98 220504
Isobe H, Yuan N F Q and Fu L 2018 Unconventional superconductivity and density waves in twisted bilayer graphene Phys. Rev. X 8 041041
Calderón M J and Bascones E 2020 Interactions in the 8-orbital model for twisted bilayer graphene Phys. Rev. B 102 155149
Cea T and Guinea F 2020 Band structure and insulating states driven by coulomb interaction in twisted bilayer graphene Phys. Rev. B 102 045107
Chung T F, Xu Y and Chen Y P 2018 Transport measurements in twisted bilayer graphene: electron–phonon coupling and Landau level crossing Phys. Rev. B 98 035425
Yankowitz M, Chen S, Polshyn H, Zhang Y, Watanabe K, Taniguchi T, Graf D, Young A F and Dean C R 2019 Tuning superconductivity in twisted bilayer graphene Science 363 1059–64
Lu X et al 2019 Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene Nature 574 653–7
Jiang Y, Lai X, Watanabe K, Taniguchi T, Haule K, Mao J and Andrei E Y 2019 Charge order and broken rotational symmetry in magic-angle twisted bilayer graphene Nature 573 91–95
Sharpe A L, Fox E J, Barnard A W, Finney J, Watanabe K, Taniguchi T, Kastner M A and Goldhaber-Gordon D 2019 Emergent ferromagnetism near three-quarters filling in twisted bilayer graphene Science 365 605–8
Kerenyi A et al 2019 Maximized electron interactions at the magic angle in twisted bilayer graphene Nature 572 95–100
Choi Y et al 2019 Electronic correlations in twisted bilayer graphene near the magic angle Nat. Phys. 15 1174–80
Xie Y, Lian B, Jack B, Liu X, Chiu C L, Watanabe K, Taniguchi T, Andrei Bernevig B and Yazdani A 2019 Spectroscopic signatures of many-body correlations in magic-angle twisted bilayer graphene Nature 572 101–5
Tomarkin S L, Cao Y, Demir A, Watanabe K, Taniguchi T, Jarillo-Herrero P and Ashoori R C 2019 Electronic compressibility of magic-angle superlattices Phys. Rev. Lett. 123 046601
Serlin M, Tschirhart C L, Polshyn H, Zhang Y, Zhu J, Watanabe K, Taniguchi T and Young A F 2020 Intrinsic quantized anomalous Hall effect in a moiré heterostructure Science 367 900–3
Haule M, Andrei E Y and Haule K 2019 The Mott-semiconducting state in the magic angle bilayer graphene Phys. Rev. B 101 085130
Yuan N F Q and Fu L 2018 Model for the metal-insulator transition in graphene superlattices and beyond Phys. Rev. B 98 045103
Pan S H et al 2001 Microscopic electronic inhomogeneity in the high-Tc superconductor Bi2Sr2CaCu2O8+δ Nature 413 282–5
Leroux M et al 2019 Disorder raises the critical temperature of a cuprate superconductor Proc. Natl Acad. Sci. USA 116 16969–75
Moon P, Koshino M and Son Y W 2019 Quasicrystalline electronic states in 30° rotated twisted bilayer graphene Phys. Rev. B 99 165430
Park M J, Kim H S and Lee S 2019 Emergent localization in dodecagonal bilayer quasicrystals Phys. Rev. B 99 245401
Yao W et al 2018 Quasicrystalline 30° twisted bilayer graphene as an incommensurate superlattice with strong interlayer coupling Proc. Natl Acad. Sci. USA 115 6928–33
Ahn S J et al 2018 Dirac electrons in a dodecagonal graphene quasicrystal Science 361 782–6
Fu Y, König E J, Wilson J H, Chou Y Z and Piseri J H 2020 Magic-angle semimetals npj Quantum Mater. 5 71
Olyaei H Z, Amorim B, Ribeiro P and Castro E V 2020 Ballistic charge transport in twisted bilayer graphene (arXiv:2007.14498)
Huang B and Vincent Liu W 2019 Moiré localization in two–dimensional quasiperiodic systems Phys. Rev. B 100 144202
Szabo A and Schneider U 2019 Mixed spectra and partially extended states in a two-dimensional quasiperiodic model Phys. Rev. B 101 014205
Rossignolo M and Dell’Anna L 2018 Localization transitions and mobility edges in coupled Aubry–André chains Phys. Rev. B 99 054211
We also tested models with intralayer hoppings up to third nearest neighbors and observed that the results remained qualitatively unaffected up to the expected shift in the energy of the Dirac points and a slight change in the narrow band angle θθθθ
Seesupplementalmaterial,whichincludes[55,79,80],for: details on finite-size scaling method used for exact diagonalization results and additional information on these results; Results on band inversion; technical details on the computation of momentum-space inverse participation ratio; technical details and additional results on conductance [56]. This method was originally proposed in [77]. See also [78] for an example of a recent application [57]. It is important to advert that the study of momentum-space localization in infinite systems requires closed boundary conditions, which motivate the construction of approximant structures previously described. For open boundaries, one-dimensional edge defects are sufficient to induce momentum-space delocalization even for commensurate structures [58].

Hernandez V, Roman J E and Vidal V 2005 SLEPc: a scalable and flexible toolkit for the solution of eigenvalue problems ACM Trans. Math. Softw. 31 351

Balay S et al 2019 PETSc Web Page (available at: www.mcs.anl.gov/petsc)

Guinea F and Walet N R 2019 Continuum models for twisted bilayer graphene: effect of lattice deformation and hopping parameters Phys. Rev. B 99 205134

Wobst A, Ingold G L, Hänggi P and Weinmann D 2002 From ballistic motion to localization: a phase space analysis Eur. Phys. J. B 27 11–14

In fact, \( L \) is the linear size of the rhombus used to compute \( T_n \), which is proportional to \( N^{1/4} \); this size is what sets the resolution for the computation of \( T_n \), see SM [55] for details.

As a result, the ratio of consecutive level spacings in random matrix ensembles follows a power law, with an exponent close to the value of the GUE prediction.

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Pal H K, Spitz S and Kindermann M 2019 Emergent Geometric Frustration and Flat Band in Moiré Bilayer Graphene Phys. Rev. Lett. 123 186402

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