Prediction of novel ‘magic’ angles and correlations for twisted bilayer graphene in a perpendicular electric field

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At certain angles of rotation called ‘magic angles’ twisted bilayer graphene features almost flat bands. The resulting strong correlations drive the system to novel phases which have been observed in experiments recently. A complete understanding of the ‘magic’ angle physics—both at the single-particle as well as the many-particle level—is still missing, and the search is ongoing. Here, we identify a new set of ‘magic’ angles, where locally flat bands with a variety of possible many-body instabilities arise, but where the single-particle problem admits an exact solution. This occurs in the presence of an external perpendicular electric field at multicritical Lifshitz points. At these angles, which can be quantified exactly, the central band features a monkey saddle, resulting in strong electronic correlations.

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When two graphene layers are rotated with respect to each other, beautiful moiré patterns appear. Such systems, commonly called twisted bilayer graphene (TBG), host fascinating electronic properties both at the single-particle as well as at the many-particle level. They manifest nontrivial commensuration physics [1], topological states [2], and quantum fractals [3], to name a few. A particularly intriguing phenomenon occurs at twist angles smaller than about 1°, when the interlayer coupling becomes nonperturbative [4]: almost flat bands emerge at a set of angles termed ‘magic angles’ [4]. The quenched kinetic energy at these angles results in novel, correlated phases. Recent experiments have found both Mott-like and superconducting phases in such systems [5, 6], which has spurred frenetic activity in this field [7, 55]. Despite much progress, a complete understanding of the origin of the flat bands at ‘magic’ angles is still missing. This has impeded a systematic study of correlations as well.

In this Letter we show that a new set of ‘magic’ angles, distinct from those reported so far, arise in TBG in the presence of a perpendicular electric field. These angles are also defined by locally flat bands leading to strong correlations, but they admit an exact solution, facilitating exploration of those correlations. The novel ‘magic’ angles occur at multicritical Lifshitz points, where the central band features a monkey saddle. Such a feature leads to an instability to either s-wave superconductivity, charge-density wave, spin-density wave, or ferromagnetism, depending on details of the electron-electron interaction [54]. These new ‘magic’ angles are defined purely geometrically in terms of distances on the hexagonal lattice and we find them using a number theoretic approach [57].

Realistic fermionic systems displaying a monkey saddle point are rare—only a few have been discussed in the literature so far: Majorana excitations of SU(2)-invariant spin liquids on the triangular lattice [58] and Bernal bilayer graphene in a perpendicular field. The advantage with twisted graphene bilayers is that the energy scale of the monkey saddle can be enhanced by about two orders of magnitude over that of their Bernal-stacked counterparts. This strongly enhances interactions and brings the temperature required for observing the predicted correlations [56] into a range readily accessible in experiments. Moreover, because the predicted ‘magic’ angles depend on the applied electric field, this strongly correlated physics can be observed without extraordinary control of the twist angle itself.

A graphene bilayer with relative twist angle Θ and interlayer bias energy V due to the perpendicular electric field is described by a Hamiltonian

\[
\begin{pmatrix}
H_1 & H_\perp \\
H_\perp & H_2
\end{pmatrix},
\]

where \(H_1 = v \mathbf{σ} \cdot \mathbf{k}\) and \(H_2 = v \mathbf{σ} \cdot \mathbf{k} + V\) are Dirac Hamiltonians for each individual layer and \(H_\perp\) is the interlayer coupling. Here, we combine Pauli matrices \(σ_x\) and \(σ_y\) into a vector \(σ = (σ_x, σ_y)^T\) and we write the Hamiltonian only for a single valley for simplicity. The interlayer Hamiltonian then has the form

\[
H_\perp(\mathbf{r}) = \frac{γ}{3} \sum_{j=0}^{2} e^{i \mathbf{q}_j \cdot \mathbf{r}} \begin{pmatrix}
1 & e^{-2πi j/3} \\
1 & 1
\end{pmatrix}.
\]

The coupling energy \(γ\) is on the order of 300 meV [59]. The vectors \(\mathbf{q}_j = K_0 - K_j\) are differences between the K-vectors \(K_0\) and \(K_j\) in the two layers, respectively, and have length \(q_j = 8\pi \sin(\delta/2) / (3\sqrt{3}a)\) with \(a = 1.42\) Å.

The interlayer Hamiltonian Eq. (2) is not translationally invariant and thus breaks momentum conservation. This makes the theory of a twisted graphene bilayer much harder than that of a Bernal stacked bilayer. The Hamiltonian of the twisted bilayer in our approximation, however, is periodic in real space with the period of the...
moiré pattern and thus does conserve crystal momentum. In an extended Brillouin zone scheme, the momenta of moiré pattern and thus does conserve crystal momentum.

After a gradient expansion, momenta \( q \) direction of the moiré pattern of the bilayer is the hexagon bounded by corners at \( \pm q_j \), shown in Fig. 1. The nonperturbative limit of a graphene bilayer without interlayer bias is reached when the interlayer coupling energy \( \gamma \) becomes of order \( v q_j \). Then the interlayer coupling energy \( \gamma \) is able to overcome the kinetic energy cost of a change of the electron momentum by \( q_j \). A complete analytical understanding of this limit has remained elusive to date. However, very rich phenomenology has been discovered numerically, including the mentioned ‘magic’ angles. [4].

In the biased bilayer a different nonperturbative limit can be reached: consider bias energies \( V_{2n+1,l} = v Q_{2n+1,l} \), where \( Q_{2n+1,l} \) is the magnitude of the momentum of a point \( Q_{2n+1,l} \) on the lattice of Fig. 2 that is connected to \( \Gamma \) by a shortest path of \( 2n + 1 \) links. The index \( l \) appears because in general there will be several such momentum magnitudes. Because of the \( C_3 \) symmetry of the lattice, there are \( 3n \) lattice points of that magnitude, with integer \( m \). At such bias energies interlayer tunneling events connecting \( Q_{2n+1,l} \) to \( \Gamma \) thus couple states of equal intralayer energy and such processes are resonant. They are nonperturbative even when the bias energy \( V = V_{2n+1,l} + \delta V \) deviates by \( \delta V \) from its resonant value, as long as \( \delta V \lesssim (\gamma / v q)^{2n} \). We take this limit, while keeping at the same time \( \gamma \ll v q \), such that all other interlayer processes (corresponding to points on the lattice Fig. 2 with distance to \( \Gamma \) different from \( Q_{2n+1,l} \)) are perturbative. We remark that in this limit, \( \delta V \lesssim \gamma (\gamma / v q) \) and \( \gamma \ll v q \), the gaps in AB/BA-stacked regions are not able to localize the wavefunctions into a chiral network. This makes this limit fundamentally different from the one taken in Ref. [60].

In our limit \( \delta V \lesssim \gamma \ll v q \) and for momenta near the \( \Gamma \)-point of the SBZ, the only low-energy degrees of freedom are the two sublattice amplitudes of an electron on layer 1 with momentum near \( \Gamma \) and \( 3n \) amplitudes for an electron to have momentum and intralayer energy near the resonant values \( Q_{2n+1,l} \) and 0, respectively, on layer 2. We obtain a low-energy theory of the twisted bilayer by a Schrieffer-Wolff transformation of the Hamiltonian Eq. 1 with low-energy space defined by those \( 3m + 2 \) amplitudes. In our limit \( \gamma \ll v q \) we may moreover expand this effective Hamiltonian in the small parameter \( \zeta = \gamma / v q \) and we truncate this expansion at the lowest non-trivial order in \( \zeta \). For the first resonance \( V_{1,1} \) we find this way a low-energy Hamiltonian

\[
H_{\text{eff}} = \begin{pmatrix}
0 & (v k_x + i v k_y) & e^{-i 2 \frac{\pi}{3} \Omega} & 0
\end{pmatrix},
\]

where \( \Omega = \gamma \sqrt{1 + \frac{\gamma^2}{2}} \) and \( \hat{q}_j \) denotes a unit vector in direction of \( q_j \). Effective low-energy theories for other resonant spaces are found in the same way and have Hamiltonians of dimension \( 3m + 2 \). In particular, many momenta \( Q_{2n+1,l} \) with \( n > 0 \) also have \( m = 1 \). We will refer to them below as “3-stars.” After a gradient expansion, their low-energy Hamiltonians have the same form as Eq. 3, only with renormalized values of all constants, including the resonant bias \( V_{2n+1,l} \) and the \( \hat{q}_j \), due to virtual interlayer processes.

While nonperturbative, as a five-dimensional matrix, \( H_{\text{eff}} \) has indeed exact analytic solutions in terms of spec-

![FIG. 1: (Color online) All momenta attainable from \( \Gamma \) by repeated application of \( H_{\text{eff}} \). They form a hexagonal lattice in the extended zone scheme. The SBZ is indicated in green (light gray).](image)
Intriguingly, our low-energy theory Eq. 3 predicts a set of ‘magic’ angles with flattened band for biased bilayers just as predicted in Ref. [1] for unbiased ones. Those are the angles where perfect resonance, that is $\delta V = 0$, is achieved in Eq. (3). Electrons at the band center then have zero velocity and infinite mass. This sort of localization is protected by the symmetries of the system: In addition to its $C_3$ symmetry, $H_{\text{eff}}$ at resonance also has a chiral symmetry involving space inversion:

$$\mathcal{PS}: \mathbf{k} \mapsto -\mathbf{k}, \quad \psi \mapsto S\psi,$$

where

$$S = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (5)$$

changes the sign of energies,

$$S^\dagger H_{\text{eff}} (-\mathbf{k}) S = -H_{\text{eff}} (\mathbf{k}). \quad (6)$$

Moreover, $H_{\text{eff}}$ has a low-energy band which, near $k = 0$, is isolated from all other bands. This is implied by its $k = 0$, $\delta V = 0$ eigenvalues that separate into a singlet at energy $\varepsilon = 0$ and two doublets at $\varepsilon = \pm \sqrt{3}\Omega$. Because of its $C_3$ symmetry, that low-energy band is bound to have zero velocity at $k = 0$. Moreover, the chiral/inversion symmetry $\mathcal{PS}$, which precludes even powers in an expansion of the dispersion relation around $k = 0$, implies infinite mass of the charge carriers. The lowest term in an expansion of the dispersion relation of $H_{\text{eff}}$, Eq. (3), at $\delta V = 0$ is of order three in $k$ and takes the form of a monkey saddle:

$$\varepsilon = \frac{v^3}{120^2} \left( k_x^3 - 3\sqrt{3}k_x^2k_y - 3k_xk_y^2 + 3\sqrt{3}k_y^3 \right). \quad (7)$$

Our exact solution to the low-energy physics of this system in the regime we considered allows us to not only predict the existence of these ‘magic’ angles, but also give an exhaustive list of their exact values. First, we recall that Eq. (3) describes the low-energy physics at resonance with all 3-stars. Therefore, a flattened band arises at all angles that have perfect resonance with a 3-star. On the other hand, one can see readily that isolated, flattened bands do not exist at resonance with stars that have $m > 1$: The effective Hamiltonians for the corresponding resonant spaces at $k = 0$ have rank 4, but dimension $3n + 2 > 5$. Therefore they have zero velocity and infinite mass. This sort of localization is protected by the symmetries of the system: In addition to its $C_3$ symmetry, $H_{\text{eff}}$ at resonance also has a chiral symmetry involving space inversion:

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the radii of all 3-stars on the hexagonal lattice. This can be done using a number theoretic approach outlined in Ref. [4]: one represents points on the hopping lattice Fig. 2 by the numbers corresponding to those points in the complex plane. The answer to our question is then found by prime factorization in the ring of those numbers.

We find in this way that a twisted bilayer has infinitely many resonances with $m = 1$ that occur at values of the bias voltage

$$V = h\nu_F |\mathbf{q}_1| \prod_j m_j^{\mu_j}, \quad (8)$$

where $\mu_j$ are arbitrary positive integers and the $m_j$ are primes $\equiv 2 \pmod{3}$. See Supplemental Material at [] for a derivation of Eq. (8) using the results of Ref. [57]. At a given bias voltage $V$ there are accordingly infinitely many ‘magic’ angles

$$\delta \Theta = 2 \arcsin \frac{3\sqrt{3}V a}{4h\nu_F \prod_j m_j^{\mu_j}}.$$ 

Fig. 2 depicts the lowest energy band of the system at resonance with the first 3-star. This figure is generated with a converged truncation of the full Hamiltonian Eq. (1) rather than the effective theory Eq. (3). Its “monkey saddle” with zero gradient and curvature at $k = 0$ is evident. Closer inspection shows that at resonance the system is at a multicritical Lifshitz point: the crossing of two transition lines in the space of bias voltage versus chemical potential (each line identifying a Lifshitz transition between Fermi surfaces topologically equivalent to a single circle and to three circles, respectively). This is the same mechanism by which monkey saddles appear also in the dispersion of Bernal bilayers with a perpendicular field [59]. Differently from that case, however,
at nonzero $\delta V$ on the space-dependence of the electron-electron interaction. Such pair of non-nested monkey saddles has been predicted in Ref. [56] to have a many-body instability protected by the symmetries our effective theory, as assumed in the renormalization group analysis of Ref. [56] into immediate experimental reach.

The regime $\delta V \lesssim \gamma \ll vq$ requires bias voltages $V \approx vq > \gamma$ and cannot be reached experimentally in a graphene bilayer at small rotation angle, where $\gamma \approx 300\,\text{meV}$ [59]. We propose two ways to reach this limit. The first one is in a heterostructure that has an h-BN layer sandwiched between two graphene layers [61]. Since h-BN is an insulator, such a configuration at low-energies effectively acts as a graphene bilayer with reduced interlayer coupling. Density functional theory calculations of the bandstructure of such systems [62] predict an effective coupling of order $\gamma \approx 20\,\text{meV}$ between the graphene layers [63]. Therefore, our limit in such sandwiches is reached at experimentally attainable bias voltages $V \gtrsim 100\,\text{meV}$. Insertion of additional h-BN layers further reduces the required bias fields. The second way to achieve the limit $\delta V \lesssim \gamma < vq$ is by choosing a rotation angle near $\theta = 38.21^\circ$. In that case the dominant interlayer coupling is of higher order and the above results apply with reduced interlayer coupling $\gamma \approx 7\,\text{meV}$ and $q = \sqrt{3}\delta K$ [63].

The monkey saddle of Fig. 3 has the cubic form assumed in the renormalization group analysis of Ref. [56] up to energy scale $\gamma$. In the proposed twisted sandwich of a single h-BN layer between two graphene layers scaling can thus be observed up to energies of order $20\,\text{meV}$, which is about two more orders of magnitude than in Bernal graphene bilayers [56]. This strongly enhances many-body interactions and brings the predictions of Ref. [56] into immediate experimental reach.

In conclusion, we have identified a new set of ‘magic’ angles in twisted graphene bilayers in the presence of a perpendicular electric field. Unlike in the unbiased case, the system admits an exact solution at these angles. The band structure becomes locally flat with a pair of non-nested “monkey saddles” and many-body instabilities as discussed in Ref. [56]. The perpendicular field gives great experimental control and allows observation of this physics across a wide range of twist angles by tuning the field to multicritical Lifshitz points. The resulting correlations can be observed at temperatures about two orders of magnitude higher than in previously proposed realizations [56].

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This agrees with the order of magnitude of both the energies of the relevant orbitals in the B and N atoms and the mediated coupling by virtual hopping function overlap between carbon atoms in the two layers expected direct graphene-to-graphene coupling by wavefunction overlap between carbon atoms in the two layers.

\[ \gamma_{gh} \approx -\gamma_{BN} \approx -\frac{16}{\varepsilon_N} \text{eV}, \]

\[ \gamma_{gh}^\prime \approx -\frac{25}{\varepsilon_B} \text{eV} \text{ is the coupling between a graphene layer and the h-BN layer and} \]

\[ \gamma_{gh} \approx -\frac{1}{\varepsilon_N} \gamma_{BN} \approx -\frac{50}{\varepsilon_B} \text{eV are the energies of the relevant orbitals in the B and N atoms} \text{.} \]

This agrees with the order of magnitude of both the expected direct graphene-to-graphene coupling by wavefunction overlap between carbon atoms in the two layers and the mediated coupling by virtual hopping onto a B or a N atom \( \gamma \approx \gamma_{gh}^\prime BN/\varepsilon_B + \gamma_{gh} BN/\varepsilon_N \) (here, \( \gamma_{gh} BN \approx 0.25 \text{eV} \) is the coupling between a graphene layer and the h-BN layer and \( \varepsilon_B \approx 3.16 \text{eV}, \varepsilon_N \approx -1.50 \text{eV} \) are the energies of the relevant orbitals in the B and N atoms).