Floquet-Engineered Topological Flat Bands in Irradiated Twisted Bilayer Graphene

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We propose a tunable optical setup to engineer topologically nontrivial flat bands in twisted bilayer graphene under circularly polarized light. Using both analytical and numerical calculations, we demonstrate that nearly flat bands can be engineered at small twist angles near the magic angles of the static system. The flatness and the gaps between these bands can be tuned optically by varying laser frequency and amplitude. We study the effects of interlayer hopping variations on Floquet flat bands and find that lattice relaxation favors their formation. Furthermore, we find that, once formed, the flat bands carry nonzero Chern numbers. We show that at currently known values of parameters, such topological flat bands can be realized using circularly polarized UV laser light. Thus, our work opens the way to creating optically tunable, strongly correlated topological phases of electrons in moiré superlattices.

Introduction.—Despite the simplicity of its structure, graphene and its multilayers have proven to support a remarkable diversity of electronic behaviors [1–3]. Among such systems, twisted bilayer graphene (TBG) has shown some of the most surprising properties. When rotated relative to one another, two graphene layers form a moiré pattern, which, even in the absence of true commensuration, may be treated to a good approximation as a Bravais lattice with a large unit cell [4–10]. The possibility of unusual electronic states in this system has long been appreciated, in part because the electronic structure supports van Hove singularities at relatively low energy [11–21]. More recently, the potential for these systems to support extraordinarily flat bands at “magic” twist angles [9, 10, 22] has been verified experimentally, and the system demonstrated to display interaction physics in the forms of Mott insulating behavior and superconductivity [23, 24]. The implications of this single-particle structure for collective electron states is now an area of intense investigation [25–42]. While there has been significant progress, a complete understanding of the physical origin of the magic angle flatness remains elusive [43–58]. In particular, magic angles are obtained at mechanically fine-tuned values, which cannot be changed once a sample is prepared [59].

In this paper, we demonstrate that TBG as a platform for correlated electronic states is enriched by circularly polarized light impinging on the system. In particular, this offers a highly controllable optical setup to engineer topological flat bands over a range of small twist angles away from the magic angle, and allows in situ optical tuning of the flat band structure in TBG. Moreover, we show that these Floquet flat bands are gapped, separated from each other and other bands by sizable energy gaps, and have nonzero Chern numbers. This combination of properties – extreme flatness, gaps, and non-vanishing Chern numbers – makes these bands near-perfect analogs of Landau levels, the energy spectrum of two-dimensional electrons in a static magnetic field. This offers the potential that electrons in this setting can support states akin to those found in the fractional quantized Hall effect [60, 61], stabilized by repulsive interactions among the electrons. Indeed, such “Floquet fractional Chern insulators” have been argued to be present in honeycomb lattices subject to circularly polarized light [62]. As we explain below, TBG is special in that the large size of the moiré unit cell allows the flat Chern band to emerge at
relatively low excitation energies relative to that needed to induce topological behavior in more microscopic honeycomb lattices such as single layer graphene [63, 64]. (This possibility was recently explored in driven TBG at larger twist angles [65], where no flat bands were observed.) Thus, our work shows that irradiated TBG represents an extremely attractive setting to search for fractional Chern insulators and other correlated electron states.

Setup and model.—Our setup is illustrated in Fig. 1(a). A circularly polarized laser beam with vector potential $\mathbf{A}(t) = A(\cos \Omega t, \sin \Omega t)$ and frequency $\Omega$ is directed normal to the TBG. In the context of single layer graphene and related systems, time-dependent perturbations have been found to modify the electronic properties in ways that allow behaviors inaccessible to the bare materials to emerge [63, 64, 66–88]. Provided the driving potential does not break the translational symmetry of the lattice, the spectrum can be labeled by the crystal momentum $\mathbf{k}$, which falls within the same Brillouin zone as that of the static system. The dynamics of the temporally periodic Hamiltonian $H_F(t) = H_0(t + 2\pi/\Omega)$ is governed by the Floquet-Schrödinger equation $[H_F(t) - i\hbar \partial_t] |\psi_{ks}(t)\rangle = \epsilon_{ks} |\psi_{ks}(t)\rangle$, and supports quantum states characterized by the Floquet bands of quasienergies $\epsilon_{ks}$, labeled by $s$, whose values fall into a “Floquet zone” of size $\hbar \Omega$. The corresponding Floquet modes $|\psi_{ks}(t)\rangle$ are also periodic and furnish a basis for the solutions of the time-dependent Schrödinger equation, $|\psi_{ks}(t)\rangle \equiv e^{-i\epsilon_{ks}t/\hbar} |\phi_{ks}(t)\rangle$.

For sufficiently large frequency, we can model the low-energy dynamics of irradiated twisted bilayer graphene following Bistritzer and MacDonald [9] and treat the interlayer hopping in an effective long-wavelength approximation. In the position basis, $H(t) = \begin{pmatrix} h_{\theta/2}(t) & T \\ T^\dagger & h_{-\theta/2}(t) \end{pmatrix}$, where $h_{\theta/2}(t) = v_F[-i\hbar \nabla - e\mathbf{A}(t)] \cdot \sigma_{\theta/2}$, with rotated Pauli matrices $\sigma_{\theta/2} = e^{-i\theta/4}(\sigma_x, \sigma_y) e^{i\theta/4}$ and Fermi velocity $v_F$, is the low-energy Dirac Hamiltonian of one of the valleys of a single graphene sheet twisted by angle $\theta/2$. The interlayer tunneling matrix $T = \sum_{n=1}^3 T_n e^{-i k_n \mathbf{q}_n \cdot \mathbf{r}}$, with $T_n = w_{AA} \sigma_0 + w_{AB} q_n \cdot \sigma_{\pi/2}$, (2) where the unit vectors $\mathbf{q}_1 = (0, -1)$, $\mathbf{q}_{2,3} = (\pm \sqrt{3}/2, 1/2)$ encode the tunneling $w_{AA}$ and $w_{AB}$ between the AA- and AB-stacked regions of the twisted bilayer graphene. Here, $k_0 = 8\pi \sin(\theta/2)/3a$ is the wavevector of the moiré pattern and $\alpha$ is the Bravais lattice spacing of graphene.

In our numerical calculations, we have taken parameter values $a = 2.4$ Å, $h v_F / a = 2.425$ eV, and $w_{AB} = 112$ meV based on experimental observations. We study the Floquet spectrum and compare to the static situation as a function of $u \equiv w_{AA}/w_{AB}$, the twist angle $\theta$ [or equivalently $\alpha \equiv w_{AB}/h v_F k_0 = 1.1 \times 10^{-2}/2 \sin(\theta/2)$], the laser frequency $\Omega$ and the electric field amplitude $E = \Omega A$.

Topological Floquet flat bands.—For sufficiently high frequencies, we may find the Floquet spectrum from an effective static Floquet Hamiltonian $H_F \approx \mathcal{P} + \delta H_F$, where $\mathcal{P} = H^{(0)}$, $\delta H = [H^{(-1)}, H^{(1)}]/\hbar \Omega$, and $H^{(n)} = \int_0^1 e^{-2i\pi n\tau} H(2\pi\tau/\Omega) d\tau$ are the Fourier components of the periodic Hamiltonian. In our setup, $\mathcal{P}$ is the Hamiltonian of the static system found by setting $\mathbf{A} = 0$, which supports flat bands at a series of magic angles. The leading term at high frequencies is spatially uniform and is given by

$$\delta H_F = \frac{(ev_F A)^2}{\hbar \Omega} \sigma_z \otimes 1.$$  (3)

Note that $v_F$ here is the Fermi velocity of single layer graphene, which is considerably larger than the Fermi velocity for Dirac points of the static moiré lattice under flat band conditions. This relatively large coefficient allows non-trivial physics in the irradiated system to emerge with only moderate laser amplitudes.

For $u = 0$, $\mathcal{P}$ is chiral symmetric under the chiral operator $\sigma_z \otimes 1$; thus, $\{\mathcal{P}, \delta H_F\} = 0$. Since the zero energy states of $\mathcal{P}$ can be chosen to be eigenstates of the chiral operator, they remain eigenstates of $H_F$ in the presence of $\delta H_F$ but acquire a finite energy $\pm (ev_F A)^2/2\hbar$. In the chiral limit, $\mathcal{P}$ has two degenerate absolutely flat bands [64], $\mathcal{P}|\psi_{k\pm}\rangle = 0$. Therefore, the Floquet spectrum will also have two absolutely flat bands with a finite central gap $\epsilon_{g1} = 2(ev_F A)^2/\hbar \Omega$. For $u > 0$, this gap is modified but we expect that it will be nearly linear in $\Omega^{-1}$ for large frequencies. This is indeed what we find in our numerical solutions shown in Fig. 1(b).

In contrast to the static situation, these Floquet flat bands have nonzero Chern numbers. One way to see this is that $\delta H_F$ acts the same way on both layers, so that the gap at the moiré $K$ and $K'$ points have the same pattern of time-reversal symmetry breaking. Therefore, the total Chern number of the gapped flat bands must be nonzero. A more explicit way to show this result is to use the solutions for the absolute flat bands in the chiral limit $u = 0$ [54]. The $K$ dependence of the entire band is given by the same Siegel theta function, confirming the same gap is produced at moiré $K$ and $K'$ points. Since these points are Dirac points of the central bands for all values of $\alpha$ (with zero velocity at the magic angles), the total Chern number is the sum of the two Chern numbers of the gapped Dirac points, i.e. $C_{\pm} = \pm (1/2 + \frac{1}{2}) = \pm 1$.

Due to time-reversal symmetry breaking by the circularly polarized laser field, the Chern number at the other valley of the single layer graphene must also have the same sign. To see this concretely, one may note that an appropriate Bistritzer-MacDonald model for the
other valley may be obtained by an inversion \( x \to -x \) in Eq. (1), or, equivalently, by changing the sign of terms proportional to \( \sigma_x \) prior to the \( \pm \theta/2 \) rotation. This has the effect of changing the sign of \( \delta H_F \) generated at high frequency in Eq. (5), thus producing a Floquet gap at the other valley with the opposite sign. This sign reversal is a consequence of time-reversal breaking. For a momentum path surrounding a moiré \( K \) or \( K' \) point, the line integral of the Berry’s connection also receives an extra minus sign due to spatial inversion. The net effect of this is to induce the same Chern number in the moiré band of the graphene at the other valley. Thus, including the spin degeneracy factor, the central Floquet bands acquire a nontrivial Chern number \( C = \pm 4 \).

The Chern numbers are stable away from the chiral limit \( u > 0 \) as long as the bulk gap remains open. As we show below, there is indeed a finite gap over a wide range of parameters which, in particular, includes the range of experimentally relevant values.

**Numerical results.—** We have solved the Floquet-Schrödinger equation for our model Hamiltonian 1) and calculated the Chern numbers 59) associated with the Floquet bands numerically. In Fig. 2(a), we show the bandwidth of the two central bands for the equilibrium (static) and the irradiated system for laser frequency \( \hbar \Omega = 6 \) eV and electric field \( E = 2 \times 10^4 \) kV/cm. For the whole range of interlayer tunneling ratio \( 0 \leq u \leq 1 \), the static system shows flat bands at magic angle close to the chiral limit (\( u = 0 \)) value \( \theta \approx 1.08^\circ \) corresponding to \( \alpha \approx 0.586 \). We also note the appearance of flat bands at lower twist angles \( \theta \approx 0.93^\circ \) (\( \alpha \approx 0.68 \)) in a range \( u > 0.8 \) that are unrelated to those appearing in the chiral limit. Interestingly, evidence of such flat bands has recently been observed in experiment 50).

For the irradiated case illustrated in Fig. 2(b), two central Floquet flat bands, formed around the value of the magic angle in the chiral limit, are apparent. Several trends are noteworthy in this case: (i) Flat bands are observed over a wider range of twist angles, which, in the chiral limit, we estimate to be \( 1.01^\circ \lesssim \theta \lesssim 1.13^\circ \). (ii) These bands become even flatter for smaller values of \( u \), leading to ultraflat bands, with bandwidths smaller than those in the equilibrium case by one or two orders of magnitude, over a range \( u \lesssim 0.2 \). (iii) The flat bands at the lower twist angle (larger \( \alpha \)) are also narrower than their static counterparts. (iv) The bands for smaller \( \alpha \) have stable Chern numbers \( C = \pm 1 \) per valley and per spin (total Chern number \( C = \pm 4 \)) over a wide region, including the chiral limit; however, the flat bands at larger \( \alpha \) are trivial due to a gap closing that separates the two regions.

Band gaps for the Floquet spectrum are illustrated in Fig. 3. The gap between the two central Floquet bands, \( \epsilon_{g1} \), remains non-vanishing in the entire range of parameters shown. The gap \( \epsilon_{g2} \) between the central bands and the next Floquet band is about an order of magnitude larger than \( \epsilon_{g1} \), which means the central Floquet bands can be taken as reasonably flat and isolated. Note that the \( \epsilon_{g2} \) gap closes for smaller twist angles just before the second flat band region appears.

**Experimental considerations.—** In contrast to the static case, irradiated TBG offers an electron platform in which a filled flat band has non-trivial topology, in principle allowing for analogs of fractional quantum Hall states – fractional Chern insulators 62) – supporting quasiparticles of fractional charge and statistics. The parameters needed to produce this platform should be within experimentally realizable parameters. For example, both the frequencies in the UV range and dynamical electric fields \( \sim 10^4 \) kV/cm used in our calculations are in ranges that are accessible by currently available laser technology 63).

Our results are computed over a range of the parameter \( u \), which physically represents the ratio of tunneling amplitudes between layers for sites on the same sublattice (AA tunneling) to ones on opposite sublattices (AB
Because the lowest energy configuration for graphene bilayers involves AB stacking, a lattice-relaxed system will naturally have larger regions of AB alignment relative to AA alignment, suggesting $u < 1$. Fits to experimental data yield $0.7 < u < 0.9$ (shown by horizontal bars in Figs. 2 and 3). In this range, the width of central the Floquet bands near the largest magic angle ($\theta \approx 1.08^\circ$) is $\delta \theta \approx 3$ meV, while the second region of narrow bands at $\theta \lesssim 1^\circ$ has a width $\delta \theta \approx 2$ meV. Note that both these widths are smaller than our calculated width for the static system near $\theta \approx 0.93^\circ$, for which clear signatures of interacting flat band physics have been observed.

The possibility of observing interacting topological flat band physics at the largest magic angle is further supported by the relative isolation of flatbands from bands above and below; for $u \sim 0.8$, the gap between the central bands is of order $\epsilon_{g1} \approx 4$ meV, while the separation from bands above and below are of order $\epsilon_{g2} \approx 30$ meV. Thus experiments at temperatures at or below $\sim 10$ K will avoid thermal excitations into these bands.

A striking feature of our results is that the situation improves notably as $u$ decreases, as is apparent in Figs. 2 and 3. It should be possible to adjust $u$ by judicious choices of substrate or by application of pressure. Both can increase the interlayer coupling, therefore increasing the sizes of the lower energy AB regions at the expense of the AA regions. At small $u$, the bandwidth of the central Floquet bands can become extremely small, falling well below that of the static system at the same parameters. Moreover, the range of angles for which the bandwidth is anomalously small increases notably, which in principle relaxes some of the challenges associated with producing samples with finely tuned twist angles.

Static TBG has already proven to be a remarkable host for correlated, interacting electron physics. The application of time-dependent fields offers a way of further enriching this system, by introducing non-trivial topology into the flat band. Thus, irradiated TBG may well prove to be a unique host for exotic, gapped quantum electron states with unusual quasiparticles, without the need for magnetic fields to stabilize them.

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