Magic-angle semimetals

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(Dated: September 14, 2018)

We introduce and characterize a class of “magic-angle” semimetal models and, as an application, propose multiple cold atomic quantum emulators of twisted bilayer graphene. The models are defined in one to three dimensions and contain momentum space nodes as well as an incommensurate quasiperiodic potential. With both numerical and analytical tools, we demonstrate an undiscovered link between magic-angle phenomena and a single-particle eigenstate quantum phase transition. At criticality, we report a nonanalytic behavior of the density of states, the appearance of flatbands, and wave functions which Anderson delocalize in momentum space displaying a multifractal scaling spectrum. We outline the necessary conditions for magic-angle semimetals and construct effective Hubbard models on superlattices by computing Wannier states, which demonstrates that the effective interaction scale is dramatically enhanced across the single-particle transition. As a result, we argue that the eigenstate quantum criticality is unstable towards the inclusion of interactions. All sufficient ingredients of our proposal are available in present day cold atomic laboratories for which the magic-angle effect can be exploited to induce strong correlations in quantum degenerate gases.

Introduction. Since the discovery of quantum phases of matter, particularly strongly correlated phases, there has been a need to fundamentally understand and control them. In particular, engineering band structures with non-trivial topological wave functions has achieved success in creating and controlling novel quantum phases in a variety of systems such as doped strong spin-orbit insulators, ultracold atoms and photonics with artificial gauge fields, electronics with topological circuit Lagrangians, semiconducting multilayer heterostructures, and dynamically driven Floquet systems. However, the ability to design band structures that, in the presence of interactions, reliably create unconventional superconductors through strong correlations has remained out of reach.

The discovery of a correlated insulator and accompanying superconducting phases in graphene heterostructures revolutionized this field of quantum engineering. New, strongly interacting, solid state systems can now be engineered with a rather weakly correlated two-dimensional semimetal (graphene). Qualitatively, the Moiré pattern at certain magic angles of twisted bilayer graphene (TBG) graphene heterostructures creates flat bands out of two-dimensional Dirac cones. We show that in arbitrary dimension quasiperiodicity generically, and in a universal fashion, creates flat bands in nodal, semimetallic, band structures due to a previously unnoticed single particle quantum phase transition (QPT)—what we call the “magic angle” in analogy to TBG. Near this transition we demonstrate the existence of strong correlations by computing Wannier states within a series of band gaps; these lead to a Hubbard model with a dramatically increased interaction scale. We therefore argue that the single particle quantum critical state is unstable towards the inclusion of interactions, which form a Mott insulator at half filling.

Crucially, our findings are independent of many of the system’s details and, therefore, demonstrate the existence of a wide multitude of engineered, strongly-coupled quantum systems which we call magic-angle semimetals. To demonstrate this, we classify the family of these models with symmetry protected nodes as well as introduce and solve a series of models; most of which can be straightforwardly realized with existing ultracold atom and trapped ion experimental setups. Thus, we propose a simple route to emulate the phenomena of magic-angle TBG in a wide variety of quantum many body systems.

“Magic-angle semimetals”. The whole class of magic-angle semimetal models are governed by Hamiltonians of...
FIG. 1. An incommensurate quasiperiodic potential generically drives an eigenstate quantum phase transition from a semimetal (SM) to metal (M). a. For many models, the velocity at the Dirac node $v$ decreases with the strength of the potential $W$ until it reaches $v=0$ at the transition, $W_c$; this is an indication of the flattening of the bands. In some cases an intermediate metallic phase (2D cases shown in inset) separates a reentrant semimetal with a reversed helicity (depicted by the Dirac cones). b. We construct a phase diagram in terms of potential strength $W$ and quasiperiodic modulation $Q$ by computing the density of states at zero energy $\rho(0)$; analytical perturbative results [Eq. (3)] for the first magic-angle transition near $Q=\pi$ is represented by the green dashed line. Higher transitions are indicated by the white dotted lines. Cuts along the dashed white lines are presented in Fig. 2.e.d. c. An infinite number of semimetal minibands form as the transition is approached. We construct exponentially localized Wannier states on the first four minibands (see Fig. 3) leading to a model with an effective, strongly renormalized space dispersion $E(k)$, see Figs. 1–3, leading to exotic many-body states. Importantly, these effects occur generically under the necessary condition that the quasiperiodic potential respects the symmetries which protect the semimetallic touching points (see supplement [33]).

Effective models. A variety of effective models illustrate our proposal. For concreteness, we formally introduce the following, a 2D tight-binding Hamiltonian of “perfect” spin-orbit coupling (SOC) on a square lattice (we fix the bare lattice spacing to unity and $\hbar=1$)

$$\hat{T} = \sum_{r,\mu=x,y} \frac{it}{2} c^{\dagger}_{\mu} \sigma_\mu c_{\mu+r+\hat{\mu}} + \text{h.c.},$$

$$\hat{V} = W \sum_{r,\mu=x,y} \cos(Qr_\mu + \phi_\mu) c^{\dagger}_{\mu} c_{\mu r},$$

(2)

where $\sigma_\mu$ are the Pauli matrices, $r$ is the position on the lattice, $c_\mu$ are two-component spinors of fermionic annihilation operators (at the single particle level, they can also be bosonic), and $\phi_\mu$ is a phase offset typically averaged over. The kinetic part $\hat{T}$ has a momentum-space dispersion $E_0(k) = \pm t \sqrt{\sin^2 k_x + \sin^2 k_y}$ with four Dirac nodes and a velocity $v_0 = t$, see Fig. 2a. The role of the twist angle and interlayer hopping in TBG is replaced by the incommensurate wavevector $Q$ and potential strength $W$, respectively. Unless otherwise stated, $Q = 2\pi/\sqrt{3}$ where $\rho$ is the golden ratio, and in numerical simulations we employ rational approximants, $Q_n = 2\pi F_{n-2}/F_n$, where the system size $L = F_n$ is given by the $n$th Fibonacci number [32].

In addition to Eq. (2) we have studied a multitude of other 1D-dimensional models in an incommensurate potential: the $\pi$-flux model and the honeycomb model in 2D, a 3D variant of Eq. (2) (studied previously in Ref. [32]), and a 1D long range hopping model with a power-law dispersion $E = -t \ln |\cos k|^{\sigma}$ with $\sigma < 1$ (this corresponds to a hopping $t_{ij} \sim |i-j|^{-(1+\sigma)}$ for $|i-j| \gg 1$ [34]—in this 1D case, $v$ is not a velocity) [33]. Each of these models generates flat bands and magic-angle
FIG. 2. Panels a, b: DOS $\rho(E)$ in units of $(tL^2)^{-1}$ averaged over 300 realizations of $\phi_x, \phi_y$ and random twisted boundary conditions \[33\]. The gray (yellow) shading represents the number of states in the first (second) miniband and matches the area of the small squares around each Dirac point produced by either a honeycomb optical lattice \[35, 36\] or artificial gauge fields \[37, 38\], whereas the 1D model we consider can be realized using trapped ions \[40\]. The 3D variant of Eq. (2) is theoretically possible to implement \[41, 42\], but has not been experimentally realized yet. In each of these experimental setups, quasiperiodic potentials can then be realized, e.g. by additional lasers \[43\], programmable potentials \[44\], or a digital mirror device \[45\].

Single-particle spectrum and velocity renormalization. We first discuss the spectral characteristics of magic-angle semimetals probed through the DOS, defined as $\rho(E) = L^{-d} \sum_i \delta(E - E_i)$ where $E_i$ is the $i$th eigenenergy. At weak quasiperiodic modulation the semimetal is stable, i.e. $\rho(E)$ vanishes at zero energy with the same power law as in the limit of $W = 0$, while hard spectral gaps and Van-Hove singularities develop at finite energy. For Weyl and Dirac Hamiltonians the low-$|E|$ DOS obeys $\rho(E) \sim |v|^d |E|^{d-1}$, and as $W$ increases, the $(d-1)$st derivative of the DOS $\langle \rho^{(d-1)}(0) \rangle \propto 1/|v|^d$ increases, see Fig. 2a for the model Eq. (2). These weak coupling features may be understood at the level of perturbation theory.

We find that gaps appear at finite energy due to the hybridization of degenerate spin states a distance $Q$ away in momentum space \[32\], see the gray lines in Fig. 2a, inset. This process “carves out” a square around each Dirac cone which contains $2(\pi - Q)\sqrt{2}\tau_1^2$ states. For the chosen $Q$, a second gap is numerically observable at larger $W$, see Fig. 2b, which corresponds to a fourth order Umklapp scattering and generates a miniband of $2(4Q - 3\pi \sqrt{2})\sqrt{2}\tau_1^2$ states per cone. For a given incommensurate $Q$ (along with the distance between nodes), there is an infinite sequence of relevant orders in perturbation theory that open up gaps near zero energy, forming minibands; this is in contrast to the commensurate case when this sequence is finite. For $Q = 2\pi/\varphi^2$, it is given by half the even Fibonacci numbers $F_{2n}/2$, which is the sequence $1, 4, 7, 12, 305, \ldots$ (see supplement \[33\] for proofs).

The renormalization of the velocity can be analytically determined using fourth-order perturbation theory by integrating out states at Manhattan distance $Q$ and $2Q$ from each Dirac point \[17, 33\]. In terms of the dimensionless coupling constant $\alpha = W/|2t\sin(Q)|$ for Eq. (2) this yields

$$v(W) = \frac{1 - 2\alpha^2[1 - \cos(Q)] + \alpha^4[16 + 2 + 1/\cos(Q)]}{1 + 4\alpha^2 + \alpha^4[16 + 2 + 1/\cos(Q)]^2}.$$

The root of the numerator captures the first magic-angle transition line well when $Q > \pi/2$ and is only inaccurate for the transition line not adiabatically connected to $W = 0$ at small $Q$, see Fig. 1b. For reentrant semimetallic phases, Eq. (3) indicates the reversal of the Berry phase, consistent with the inversion of miniband states in 3D \[32\].

To go beyond perturbation theory, we compute the DOS using the numerically exact kernel polynomial method (KPM), on sufficiently large system sizes across a range of models of various dimensions. At a critical $\alpha = \alpha_c \approx 1$ the DOS becomes non-analytic and a metallic spectrum with finite $\rho(0)$ develops for $\alpha > \alpha_c$, see Fig. 2b. In particular, for $d > 1$ and fixed $Q$, $\rho(E) \sim |W - W_c|^{-\beta}|E|^{-d-1}$ implying the velocity $v(W) \sim |W - W_c|^{\beta/d}$. Surprisingly, we find $\beta \approx 2$ across a broad range of models, $Q$ values, and dimensions \[32, 33\], in agreement with perturbation theory in 2D. This exponent also agrees with similar results in TBG \[17, 18\].
indicating that this phenomenon is within the same universality class. In 1D this magic-angle effect also exists but is modified by the form of the dispersion such that \( \rho(E) \sim |W - W_0|^{-\beta} |E|^{1/\sigma-1} \), and for the case \( \sigma = 1/3 \) we find \( \beta = 4.0 \pm 0.8 \). This velocity renormalization for a multitude of models is plotted in Fig. 1b, here \( v(W) \) is determined by computing the twist dispersion of the energy using exact diagonalization and agrees with the calculation of \( \rho^{(d-1)}(0) \), see \[32\].

**Critical single-particle wave functions:** Critical properties across the magic-angle transition appear not only in the spectrum but also in the eigenfunctions near \( E = 0 \) \[32\], see Figs. 2a–d. We show that magic-angle semimetals are intimately linked to the physics of Anderson transitions in momentum space, and we conjecture this to be true for TBG due to universality.

We compute the low energy wavefunctions using exact diagonalization on small system sizes and Laukczos for large \( L \) reaching up to \( L = 610 \). Qualitatively, we find that the structure of the wave functions in the semimetallic phase is stable and adiabatically connected to the ballistic \( W = 0 \) limit, with isolated ballistic spikes in momentum space, see Fig. 2a. In contrast, the form of the wave functions is completely different in the metallic state, see Fig. 2b, as it appears delocalized both in momentum and real space with non-trivial structure \[33\].

Finally, in the reentrant semimetal, the wave functions are again ballistic, see Fig. 2c. Crucially, in all models that we studied, the positions of the transitions in the spectral properties of the DOS coincide with the transitions of the wave functions characteristics within numerical resolution, see Figs. 2d–d.

In order to quantify the eigenstate QPTs of the wave functions, we generalize the multifractal wave function analysis \[31\] to momentum space. We define the inverse participation ratio of the energy eigenstates in momentum space \[32\], \( \psi(\mathbf{k}) \) at a given energy \( E \)

\[
\mathcal{I}_M(q, L) = \sum_{\mathbf{k}} |\psi(\mathbf{k})|^2 q \sim L^{-\tau_M(q)},
\]

(4)

We can now apply properties of the scaling exponent \( \tau_M(q) \), typically used to analyze real space localization, to eigenstates in momentum space. It monotonically increases [obeying \( \tau_M(0) = -d \) and \( \tau_M(1) = 0 \)] and distinguishes delocalized wave functions \( \tau_M(q = q(d - 1)) \) from exponentially localized peaks \( \tau_M(q > 0) = 0 \) and critical states with non-marginal “multifractal” \( \tau_M(q) \). A variant of multifractal states, which are called “frozen,” display \( \tau_M(q > q_c) = 0 \) for a given \( q_c \in (0, 1] \); their peak height is system size independent, as in standard localized states, but show multifractal correlations in their tails \[31\]. We employ the standard binning technique (varying the binning size \( B \)) to numerically extract the scaling exponents \( \tau_M(q) \) in systems of a given finite size, see supplement \[33\] for details.

The scaling analysis of \( J_M(q, L) \), presented in Figs. 2e–f for Eq. (2), discloses three phases of distinct wavefunction structures in momentum space. A frozen spectrum \( \tau_M(q) \) occurs in the two semimetal regimes of smallest \( W \) and sufficiently large \( W \). In sharp contrast, the function \( \tau_M(q) \) unfreezes in the metallic phase with finite \( \rho(0) \).

Surprisingly, throughout the metallic phase the spectra appear to be weakly multifractal in both momentum and real space \[33\], we find \( \tau_M(q) \approx 2(q - 1) - 0.25q(q - 1) \) (in the region \( |q| < 1 \) and within the limits of our numerical precision) in Fig. 2f. The observation of similar behavior in all models that we investigated \[33\] corroborates the interpretation of the magic-angle phenomenon as one of eigenstate quantum criticality and generalizes the quasiperiodic 3D Weyl semimetal to diffusive metal QPT \[32\] to arbitrary dimensions. In two dimensions we do not find any signatures of diffusion (consistent with the marginality of two dimensions \[33\]) and in one dimension the semimetal transitions directly to an Anderson insulator \[33\]. Lastly, when \( d > 1 \) and \( W \) is much larger than the magic-angle transition, all investigated models undergo Anderson localization in real space.

**Wannier functions, Hubbard model.**—We now turn to the interparticle interaction term \( \hat{U} \) in the Hamiltonian in Eq. (1). In order to illustrate how the appearance of flatbands enhances correlations, we construct a series of emergent Hubbard models near the magic-angle transition for Eq. (2) at \( \phi_\mu = \pi/2 \) supplemented by

\[
\hat{U} = U \sum_{\mathbf{r}} n_{\mathbf{r}} \uparrow n_{\mathbf{r}, \downarrow},
\]

(5)

with \( n_{\mathbf{r}} = c_{\mathbf{r}}^\dagger c_{\mathbf{r}} \).

In contrast to the previous discussion, we take systems that are not perfectly incommensurate in order to build translationally invariant Hubbard models. In particular, we still use the rational approximants \( Q_n = 2\pi F_{n-2}/F_n \), only now we take the size of the system \( L = mF_n \) for some integer \( m \), effectively taking the thermodynamic limit in \( L \) before the limit of pure quasiperiodicity \( Q_n \to Q \). This is reminiscent of Moiré lattices used to model TBG, and similarly, we can unambiguously define a supercell of size \( \ell = F_n \) and isolate bands in \( \ell \)-space. In particular, these bands are intimately related to the hierarchy of minibands derived with perturbation theory: when \( \ell = F_{3a_1+b} \) for integers \( a \) and \( b \), the gap for the lowest \( |E| \) band opens at order \( F_{3a_1}/2 \) in perturbation theory \[33\] (for \( \ell = F_{3a_1} \), the Dirac nodes gap at order \( F_{3a_1}/2 \)). This allows us to systematically study each miniband opening.

To build the Hubbard models, we perform approximate joint diagonalization on the position operators \( \langle \hat{x}_\mu \rangle \) projected (with projection operator \( P \)) onto a given band \( \hat{X}_{\beta, m} \equiv P \hat{x}_\mu P \) in order to determine the Wannier states \[49\] (for details and code, see \[33\]).

As a clear example, when \( W = 0.5t \) and \( (\ell, m) = (13, 8) \), we see a clear band around \( E = 0 \) in Fig. 3a, and we find Wannier centers in a well defined grid (Fig. 3b) corresponding to exponentially localized Wannier states (Figs. 3c–d). The projected Hamiltonian has the approximate form of Eq. (2) with a renormalized \( U_{\text{eff}} \), \( t_{\text{eff}} \), and \( W_{\text{eff}} = 0 \). With this approach, we can identify successive gaps leading up the metallic transition from either side
along with dramatic enhancements of interactions, which reach up to a massive $U_{\text{eff}}/t_{\text{eff}} \sim 4100U/t$ for the fourth miniband with supercell $\ell = 377$, as shown in Fig. 1c. This can also been shown analytically using a one step renormalization group calculation, which yields the divergence $U_{\text{eff}}/t_{\text{eff}} \sim U(1/\ell)^{d-1}Z^2/v \sim 1/|W-W_c|$, ($\sqrt{Z}$ is the wave function renormalization) [33]. Due to finite size, the apparent location of $W_c$ can artificially shift, therefore in Fig. 1c we use $W_c = W_c \sin Q_{\text{eff}}$ where $W_c$ is the transition point when $n \to \infty$. In the supplement we present the data for a large set of $(\ell, m)$ corroborating our findings [33].

Away from $E = 0$, nearly flat (semimetallic) bands can form well before the magic-angle transition with similarly large $U_{\text{eff}}/t_{\text{eff}}$, see Fig. 2a, and near the transition, multiorbital Hubbard models [50] also appear [33].

Summary and experimental implications. We introduced a class of magic-angle semimetals of which twisted bilayer graphene is the most prominent representative. Employing a combination of numerical and analytical methods we have demonstrated the general appearance of a single-particle quantum critical point at which, simultaneously, (i) the kinetic energy vanishes universally, (ii) a non-zero density of states appears at zero energy, and (iii) the wave functions display delocalization and multifractality in momentum space. Lastly, in the presence of interactions we demonstrated that this eigenstate criticality leads to a strongly correlated Hubbard model by computing Wannier states on a superlattice.

We conclude with the experimental relevance of our theoretical findings. As mentioned, all sufficient ingredients for cold atomic emulation of the magic-angle phenomenon, i.e. semimetals in a quasiperiodic potential, are available in present day cold atomic laboratories. In addition to any spectroscopic measurements that probe the density of states (e.g. radiofrequency spectroscopy [51]), we propose the analysis of wavepacket dynamics as an indicator of magic-angle physics and numerically predict a non-monotonic behaviour of the wave function spreading as a function of $W$ [33] in the parameter regime with multiple magic angles. Moreover, our work opens an entirely novel experimental protocol for realizing strong correlations by first cooling the gas to quantum degeneracy and then applying a quasiperiodic potential to create flat bands (without the need to cool the system in a Mott insulator phase).

Regarding experimentally realized twisted graphene heterostructures, it has not been obvious whether incommensurability is an important ingredient. Quasiperiodic effects rely upon weakly detuned processes at which the total transferred momentum wraps the Brillouin zone. In contrast, the momentum transfer induced by scattering off a small angle superstructure is minute. Therefore—it is often concluded—both effects of incommensurability and intervalley scattering are negligible as processes in higher order perturbation theory. However, since by definition $\alpha \sim 1$ at the magic angle, the argument of parametric suppression of high order processes is questionable and incommensurate effects are therefore in principle possible in TBG. Furthermore, analogous to the continuous phase boundary in Fig. 1, the physics of small angles directly connects to large, incommensurate twists [52–54]. Of course, the amplification of interaction effects as a consequence of non-analytic DOS persists independently of strict or approximate incommensuration, but perfect eigenstate criticality involves Anderson delocalization in momentum space which only exists for perfect incommensuration. While any rational approximant leads to a rounding of the QPT (akin to finite size effects in usual transitions), our paper promotes eigenstate quantum criticality as the ultimate origin of flatbands in magic-angle semimetals, including twisted bilayer graphene.

Acknowledgements We thank I. Bloch, P.-Y. Chang, P. Coleman, M. Foster, Y. Komijani, A. M. Rey, and D. Vanderbilt for useful discussions. We also thank S. Gopalakrishnan and D. Huse for collaborations on related work and for insightful discussions. J.H.W. and J.H.P. acknowledge the Aspen Center for Physics where some of this work was performed, which is supported by National Science Foundation Grant No. PHYS-1607611. E.J.K. was financially supported by the U.S. Department of Energy, Basic Energy Sciences, grant number DE-FG02-99ER45790. This work was supported by the Caltech Institute for Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation and the Air Force Office for Scientific Research (J.H.W.). Y.-Z.C. was supported in part by a Simons Investigator award to Leo Radzihovsky and in part by the Army Research Office.
under Grant Number W911NF-17-1-0482. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Office or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein. The authors acknowledge the Beowulf cluster at the Department of Physics and Astronomy of Rutgers University, The State University of New Jersey, and the Office of Advanced Research Computing (OARC) at Rutgers, The State University of New Jersey (http://oarc.rutgers.edu) for providing access to the Amapel cluster and associated research computing resources that have contributed to the results reported here.

[1] S.-Y. Xu, Y. Xia, L. A. Wray, S. Jia, F. Meier, J. H. Dil, J. Osterwalder, B. Slomski, A. Bansil, H. Lin, R. J. Cava, and M. Z. Hasan, Science 332, 560 (2011).
[2] J. Dalibard, F. Gerbier, G. Juzeliūnas, and P. Řehberg, Rev. Mod. Phys. 83, 1523 (2011).
[3] T. Ozawa, H. M. Price, A. Amo, N. Goldman, M. Hafezi, L. Lu, M. Rechtsman, D. Schuster, J. Simon, O. Zilberberg, et al., arXiv preprint arXiv:1802.04173 (2018).
[4] M. Aidelsburger, S. Nascimbene, and N. Goldman, arXiv preprint arXiv:1710.00851 (2017).
[5] C. H. Lee, S. Imhof, C. Berger, F. Bayer, J. Brehm, L. W. Molenkamp, T. Klisieki, and R. Thomale, Communiqué Physics 1, 39 (2018).
[6] A. Burkov and L. Balents, Phys. Rev. Lett. 107, 127205 (2011).
[7] I. Belopolski, S.-Y. Xu, N. Koirala, C. Liu, G. Bian, V. N. Strocov, G. Chang, M. Neupane, N. Alidoust, D. Sanchez, et al., Science advances 3, e1501692 (2017).
[8] N. H. Lindner, G. Refael, and V. Galitski, Nature Physics 7, 490 (2011).
[9] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, et al., Nature 556, 80 (2018).
[10] G. Chen, L. Jiang, S. Wu, B. Lv, H. Li, K. Watanabe, T. Taniguchi, Z. Shi, Y. Zhang, and F. Wang, arXiv preprint arXiv:1803.01985 (2018).
[11] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, Nature 565, 43 (2018).
[12] M. Yankowitz, S. Chen, H. Polshyn, K. Watanabe, T. Taniguchi, D. Graf, A. F. Young, and C. R. Dean, arXiv preprint arXiv:1808.07865 (2018).
[13] K. Kim, A. DaSilva, S. Huang, B. Fallahazad, S. Larentis, T. Taniguchi, K. Watanabe, B. J. LeRoy, A. H. MacDonald, and E. Tutuc, Proc. Natl. Acad. Sci. 114, 201620140 (2017).
[14] J. C. W. Song, A. V. Shytov, and L. S. Levitov, Phys. Rev. Lett. 111, 266801 (2013).
[15] P. Wu, T. Lovorn, E. Tutuc, and A. MacDonald, arXiv preprint arXiv:1804.03151 (2018).
[16] G. Trambly de Laissardiere, D. Mayou, and L. Magaud, Nano letters 10, 804 (2010).
[17] R. Bistritzer and A. H. MacDonald, Proc. Natl. Acad. Sci. 108, 12233 (2011).
[18] J. L. dos Santos, N. Peres, and A. C. Neto, Phys. Rev. B 86, 155449 (2012).
[19] G. Li, A. Luican, J. L. Dos Santos, A. C. Neto, A. Reina, J. Kong, and E. Andrei, Nature Physics 6, 109 (2010).
[20] I. Brihuega, P. Mallet, H. González-Herrero, G. Trambly de Laissardière, M. M. Ugeda, L. Magaud, J. M. Gómez-Rodríguez, F. Yndurain, and J.-Y. Veuillen, Phys. Rev. Lett. 109, 196802 (2012).
[21] Y. Kim, P. Herlinger, P. Moon, M. Koshino, T. Taniguchi, K. Watanabe, and J. H. Smet, Nano letters 16, 5053 (2016).
[22] B. Padhi, C. Setty, and P. W. Phillips, arXiv preprint arXiv:1804.01101 (2018).
[23] H. C. Po, L. Zou, A. Vishwanath, and T. Senthil, arXiv preprint arXiv:1803.09742 (2018).
[24] N. F. Q. Yuan and L. Fu, Phys. Rev. B 98, 045103 (2018).
[25] J. Kang and O. Vafek, arXiv preprint arXiv:1805.04918 (2018).
[26] C. Xu and L. Balents, Phys. Rev. Lett. 121, 087001 (2018).
[27] B. Lian, Z. Wang, and B. A. Bernevig, arXiv preprint arXiv:1807.04382 (2018).
[28] J. F. Dodaro, S. A. Kivelson, Y. Schattner, X. Q. Sun, and C. Wang, Phys. Rev. B 98, 075154 (2018).
[29] T. M. Wolf, O. Zilberberg, I. Levkivskyi, and G. Blatter, arXiv preprint arXiv:1805.10670 (2018).
[30] C. Janot, Quasicrystals: A Primer, Monographs on the physics and chemistry of materials (OUP Oxford, 2012).
[31] E. Kaxiras and P. Jarillo-Herrero, Nature 556, 80 (2018).
[32] J. H. Pixley, J. H. Wilson, D. A. Huse, and S. Gopalakrishnan, Phys. Rev. Lett. 120, 207604 (2018).
[33] Supplementary Materials to this publication.
[34] M. Gärttner, S. Syrzanov, A. Rey, V. Guraire, and L. Radzihovsky, Phys. Rev. B 92, 041406 (2015).
[35] L. Tarruell, D. Greif, T. Uehlinger, G. Jotzu, and T. Esslinger, Nature 483, 302 (2012).
[36] G. Jotzu, M. Messer, R. Desbuquois, M. Lebrat, T. Uehlinger, D. Greif, and T. Esslinger, Nature 515, 237 (2014).
[37] M. Aidelsburger, M. Lohse, C. Schweizer, M. Atala, J. T. Barreiro, S. Nascimbène, N. R. Cooper, I. Bloch, and N. Goldman, Nature Physics 11, 162 EP (2014).
[38] L. Huang, Z. Meng, P. Wang, P. Peng, S.-L. Zhang, L. Chen, D. Li, Q. Zhou, and J. Zhang, Nature Physics 12, 540 (2016).
[39] Z. Wu, L. Zhang, W. Sun, X.-T. Xu, B.-Z. Wang, S.-C. Ji, Y. Deng, S. Chen, X.-J. Liu, and J.-W. Pan, Science 354, 83 (2016).
[40] P. Richerme, Z.-X. Gong, A. Lee, C. Senko, J. Smith, M. Foss-Féig, S. Michalakis, A. V. Gorshkov, and C. Monroe, Nature 511, 198 (2014).
[41] K. Sun, W. V. Liu, A. Hemmerich, and S. Das Sarma, Nature Physics 8, 67 EP (2011).
[42] J.-H. Jiang, Phys. Rev. A 85, 033640 (2012).
[43] T. Dubček, C. J. Kennedy, L. Lu, W. Ketterle, M. Soljačić, and H. Buljan, Phys. Rev. Lett. 114, 225301 (2015).
[44] M. Schreiber, S. S. Hodgman, P. Bordia, H. P. Lschen, M. H. Fischer, R. Vosk, E. Altman, U. Schneider, and I. Bloch, Science 349, 842 (2015).
[45] J. Smith, A. Lee, P. Richerme, B. Neyenhuis, P. W. Hess, P. Hauke, M. Heyl, D. A. Huse, and C. Monroe, Nature Physics 12, 907 (2016).
[46] C. Weitenberg, M. Endres, J. F. Sherson, M. Cheneau, P. Schau, T. Fukuhara, I. Bloch, and S. Kuhr, Nature 471, 319 (2011).
[47] E. Abrahams, P. Anderson, D. Licciardello, and T. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).
[48] T. Devakul and D. A. Huse, Phys. Rev. B 96, 214201 (2017).
[49] N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Rev. Mod. Phys. 84, 1419 (2012).
[50] H. C. Po, L. Zou, T. Senthil, and A. Vishwanath, arXiv preprint arXiv:1808.02482 (2018).
[51] J. Gaebler, J. Stewart, T. Drake, D. Jin, A. Perali, P. Pieri, and G. Strinati, Nature Physics 6, 569 (2010).
[52] H. K. Pal, S. Spitz, and M. Kindermann, arXiv preprint arXiv:1803.07060 (2018).
[53] W. Yao, E. Wang, C. Bao, Y. Zhang, K. Zhang, K. Bao, C. K. Chan, C. Chen, J. Avila, M. C. Asensio, et al., Proc. Natl. Acad. Sci. 201720865 (2018).
[54] S. J. Ahn, P. Moon, T.-H. Kim, H.-W. Kim, H.-C. Shin, E. H. Kim, H. W. Cha, S.-J. Kahng, P. Kim, M. Koshino, Y.-W. Son, C.-W. Yang, and J. R. Ahn, Science, aar8412 (2018)
I. Models

In this section we define the models which we analyzed. The tight-binding Hamiltonians of models dubbed “perfect” spin orbit coupling (SOC) are given by

\[
\hat{T}_{SOC} = \sum_{r,\mu} \left[ \frac{it}{2} c_r^{\dagger} \sigma_\mu c_{r+\hat{\mu}} + h.c. \right],
\]  
\[
\hat{V}_{SOC} = W \sum_{r,\mu} \cos(Qr_\mu + \phi_\mu) c_r^{\dagger} c_r.
\]

where \(t\) is the hopping matrix element, and \(W\) is the amplitude of the quasiperiodic potential. In the two-dimensional (2D) case \(\mu = x, y\) and in the three-dimensional (3D) case \(\mu = x, y, z\) and \(r\) takes values in the set of all lattice points on a square (cubic) lattice. The Hamiltonian for the \(\pi\)-flux model has the same potential term in 2D. The hopping term is modified as follows

\[
\hat{T}_\pi = -t \sum_{r,\mu=x,y} \left[ c_r^{\dagger} e^{iA_\mu(r)} c_{r+\hat{\mu}} + h.c. \right],
\]

where we choose the gauge with \(A_\mu(r) = \pi/2\) for all sites \(r\) on the square lattice, and \(A_\mu(r) = -(−1)^x \pi/2\). For the chosen gauge, periodic boundary conditions require the lattice size in \(x\) direction to be even. The spinless honeycomb lattice model is given by a Hamiltonian of the form

\[
\hat{T}_O = -t \sum_{r,\delta_\mu} \left[ c_r^{\dagger} c_{r+\delta_\mu} + h.c. \right],
\]

\[
\hat{V}_O = W \sum_{r,\delta_\mu} \cos(Qr \cdot \delta_\mu + \phi_\mu) c_r^{\dagger} c_r.
\]

The sum over \(r_A\) is over one of the two sub-lattices, while \(r\) is over all points. The index \(i\) labels the three nearest neighbors of \(r_A\), and \(d_i\) is the vector from \(r_A\) to its nearest neighbor \(i\). The vectors \(\delta_\mu\) are a choice of each particular
model and for numerics we choose \( \delta_1 = d_1 = (2/3)\hat{x} \) and \( \delta_2 = d_2 = -(1/3)\hat{x} + (1/\sqrt{3})\hat{y} \). The kinetic part of the Hamiltonian for the one dimensional model with power law dispersion [S1] is given in momentum space

\[
\hat{T}_{1D} = -t \sum_k \text{sgn}(\cos(k)) |\cos(k)|^\sigma c_k^\dagger c_k.
\]  

We assume \( \sigma < 1 \), this expression can be readily Fourier transformed to a tight binding model with long range hopping (LRH). This yields a hopping amplitude

\[
t_{ij} \sim -2t[1 - (-1)^{i-j}] \sin[\pi((i-j) - \sigma)/2] \Gamma(1 + \sigma) |i-j|^{-(1+\sigma)}
\]

for \( |i-j| \gg 1 \) and \( \Gamma(x) \) is the Gamma function. The potential is

\[
\hat{V}_{1D} = W \sum_r \cos(Qr + \phi) c_r^\dagger c_r.
\]

II. SCALING OF THE DENSITY OF STATES

In this section we discuss the numerical method used in the analysis of the spectrum and the finite size effects of the method. We use the kernel polynomial method (KPM) to calculate the density of states \( \rho(E) \), which expands \( \rho(E) \) in terms of Chebyshev polynomials up to an order \( N_c \), and we use the Jackson kernel to filter out Gibbs oscillations due to the finite expansion order. To determine the velocity \( v \), in two-dimensions for example, we fit the low-\(|E|\) asymptote \( \rho(E) \approx \rho'(E = 0)|E| \) to extract \( \rho'(E = 0) \sim 1/v^2 \). Note that in 2D formally \( \rho'(E = 0) \) is not just a single derivate due to the \(|E|\) scaling, but we use this notation to unify 2D and 3D; the latter it is simply a second derivate. For details on the KPM technique see Ref. [S2]. We use twisted boundary conditions and we average over random twists to reduce finite size effects. Now we discuss the effect of finite lattice size \( L \) and finite cutoff \( N_c \) on \( \rho(E = 0) \) and \( \rho'(E = 0) \).

As an exemplary case we present results here for the “perfect” SOC model defined in the main text. Results on the other models are similar and we also present results on the 1D model below. Figure [S1] illustrates the dependence on \( L \) and \( N_c \). For smaller \( N_c \) such as \( N_c = 2^{12} = 4096 \), \( \rho'(0) \) for all choice of \( L \geq 55 \) almost overlap for \( W \leq 0.515 \). For \( N_c = 2^{14} = 16384 \), the \( \rho'(0) \) data converges as a function of \( L \) only for \( L \geq 144 \). Still, the \( L \) convergence is only valid for \( W \leq 0.515 \). This demonstrates that the observed convergence in \( L \) is strongly dependent on \( N_C \) and therefore requires studying the scaling in \( N_C \) for fixed \( L \).

When fixing \( L \) and varying \( N_c \), the semi-metal to metal transition becomes sharper as \( \rho(E = 0) \) rises more abruptly approaching a sharp step as shown in Fig. [S1]. This sharpening allows us to pinpoint the location of the transitions accurately, in this case we find \( W_c = 0.525 \pm 0.005 \) and \( W'_c = 0.551 \pm 0.005 \). Importantly, the peak of \( \rho(0) \) does not shrink as we vary \( L \) or \( N_c \), providing strong evidence of the presence of the intermediate metallic phase. In addition, we find that \( \rho'(0) \) does not saturate as we increase the expansion order, indicating within our numerical accuracy that at the transition \( \rho'(0) \) diverges, similar to what was found in 3D [S3]. From the above data of \( \rho'(0) \) we determine the scaling exponent \( \beta \) defined by \( \rho'(0) \sim |W_c - W|^{-\beta} \). We use \( \rho'(0) \) data obtained for \( N_c = 2^{14} \) and \( L = 144 \) and we extract \( \beta \) from a log-log fit of \( 1/\rho'(0) \) versus \( |W - W_c| \), see Fig. [S2].

A. Dispersion and velocity

In this section we demonstrate the identification of the kinetic velocity as obtained from the twist dispersion with the parameter entering the low-energy asymptote of the DOS. We also compare these numerical results with perturbation theory. We implement twisted boundary conditions by including a factor \( e^{i\theta r/L} \) for each real space field located at \( r \) and twist vector \( \theta \). Each component of \( \theta \) takes value in \((0,2\pi)\) and we compute the energy eigenstates \( E(\theta) \) using exact diagonalization for various values of the twist \( \theta \). Such a change of boundary condition has no effect on the bulk physics, but effectively moves the origin of the finite size induced momentum grid, so that plotting the spectrum as a function of the twist shows a projection of the dispersion onto 1/Lth of the Brillouin zone. Figure [S3] shows the twist dispersion for various models in one, two, and three dimensions, which clearly demonstrates the dramatic flattening of the bands at the transition. These results where obtained for system size \( L = 233 \) in 1D, \( L = 144 \) in 2D, and \( L = 21 \) in 3D. Using the twist dispersion we can estimate the velocity by fitting the lowest energy band near 0 twist to a straight line. We compare the velocity as calculated from the twist dispersion with the KPM result of the DOS and fourth order perturbation theory in Fig. [S4] which all agree well.
FIG. S1. The DOS $\rho(E = 0)$ and its derivative $\rho'(E = 0)$ for 2D perfect SOC with $Q = 2\pi F_{n-2}/F_n$ at various $L$ and $N_c$ near the semimetal-to-metal transition $W_c = 0.525 \pm 0.005$ and back to the reentrant semimetal $W'_c = 0.551 \pm 0.005$. Top and middle left: $N_c = 4096$ varying $L$. Top and middle right: $N_c = 16384$ varying $L$. The key is shared across the top four figures. Bottom: $L = 233$, varying $N_c$, with a shared key across the two. The insets are the same plots with linear scale.

B. 1D powerlaw hopping model

The parameter $\sigma$ defined in equation (S6) determines the behavior of the dispersion relation near $k = 0$. This can be seen directly from the twist dispersion in Fig. S3. We present detailed results for the 1D LRH model in Fig. S5. The DOS depends on $\sigma$ by $\rho(E) \sim |E|^{1/\sigma-1}$ (Ref. S4), which is demonstrated in Fig. S5. In the following we present detailed results for $\sigma = 1/3$ and leave the full exploration of this 1D model for future work. Focusing on $\sigma = 1/3$ is
FIG. S2. Estimate of the scaling exponent $\beta$. Left: Extracting $\beta$ from fitting (dashed lines) $1/\rho'(0)$ in 2D and $1/\rho''(0)$ in 1D for $\sigma = 1/3$ versus $|W - W_c|$ on a log-log plot displaying a clear power law. For clarity we have shifted the data of the honeycomb (HC) model so that it doesn’t overlap with the SOC model. Right: $\beta$ estimate for the models we investigated in this paper, note that the estimate of $\beta$ for the 3D Weyl model quotes the result from Ref. [S3] and for the 1D long range hopping model we find $\beta = 4 \pm 0.8$ for $\sigma = 1/3$.

numerically advantageous since as we approach the transition the scaling $\rho(E) \sim |W - W_c|^{-\beta}|E|^2$ allows us to use the second derivative of the DOS $\rho''(0)$ to estimate $\beta$ and we can compute $\rho''(0)$ accurately using the KPM. Notice that the power-law remains constant when varying $W$ in the semimetal phase, showing the 1D model is also stable to a weak quasiperiodic potential. Upon approaching the transition we find $\rho''(0)$ displays a clear divergence with no sign of saturation as we increase the expansion order (see Fig. S5), similar to the 2D model we have discussed above. We find $W_c = 2.05 \pm 0.03$ and from the power-law scaling $\rho''(0) \sim |W - W_c|^{-\beta}$ we extract $\beta = 4.0 \pm 0.8$ for $\sigma = 1/3$, see Fig. S2. Distinct from our results in 2D and 3D the transition in the 1D model is accompanied by real space localization. To demonstrate this we calculate the IPR in real space and momentum space at zero energy. The real space IPR becomes finite and momentum space IPR vanishes near the critical point $W_c$. In addition, when the momentum space IPR goes to zero the DOS becomes non-zero demonstrating that the generation of DOS is tied with momentum space delocalization, similar to the higher dimensional models.

III. WAVEPACKET DYNAMICS AS A PROBE OF THE SINGLE PARTICLE QUANTUM PHASE TRANSITION

In this section we demonstrate that wavepacket dynamics can be used as a tool to observe the single particle quantum phase transition in the models that posses a reentrant semimetal in two dimensions. Note that in three dimensions due to the diffusive states at finite energy that dominate the dynamics this probe is not useful [S3]. We initialize a wavepacket to a single site $|\psi_0\rangle$ and use the KPM to time evolve the state to obtain $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$ and from this we compute the spread of the wavepacket as a function of time from $\langle \delta r(t)^2 \rangle \equiv (\psi(t)|r^2|\psi(t)) - (\psi(t)|r|\psi(t))^2$. From the long time dynamics we extract the dynamical exponent from the scaling $\langle \delta r(t)^2 \rangle \sim t^{2z}$. We focus on the perfect SOC Hamiltonian from the main text. The KPM expands the time evolution operator in terms of Chebyshev polynomials up to an order $N_C$, which dictates the final time that can be reached in the numerical calculations. Here we focus on a large linear system size of $L = 987$ and use a KPM expansion order $N_C = 2^{12}$, which allows us to time evolve the wavepacket until it spreads out across the sample. As shown in Fig. S6 we find rather unusual wavepacket dynamics which is a signature of a sequence of semimetal-metal-semimetal transitions. As a function of increasing $W$ we find that the speed at which the wavepacket spreads out monotonically decreases until we reach the metallic phase where the dependence on $W$ is rather weak. Then, upon reentering the semimetal phase at larger $W$ the wavepacket spreading speeds back up. This is clearly demonstrated in the dynamical exponent $z$ showing non-monotonic behavior in the inset. Interestingly, our estimate of $z$ is not diffusive, consistent with the marginal nature of 2D. We expect that this wavepacket signature can be used to detect the transition in cold atom experiments.
FIG. S3. Twist dispersion for various models displaying the characteristic magic angle feature of flat bands. All results shown except for the second row (honeycomb model) are on the twist trajectory $\theta_y = 0$, and for 3D $\theta_z = 0$. Whereas for the honeycomb model, $\theta_y = -\theta_x$. First row: 3D SOC model investigated in Ref. S3 with $Q = 2\pi F_n - 2/L$, $L = 21$, $W = 0.1, 0.384, 0.5$ corresponding to before the transition, in the metallic phase and after the transition. Second row: 2D honeycomb model at $Q = 2\pi F_n - 3/L$, $L = 144$, $W = 0.4, 0.5, 0.54$ representing the states well before the transition, right before the transition, and a flattened band. Third row: 2D SOC model at $Q = 2\pi F_n - 2/L$, $L = 144$, $W = 0.35, 0.54, 0.8$ depicting states before the transition, in the metallic phase and after the transition. We have numerically checked that the twist dispersion of the $\pi$-flux model coincides with the 2D SOC, see the arguments exposed in Fig. S7 below. Fourth row: 1D power law hopping model at $Q = 2\pi F_n - 3/L$, $\sigma = 1/3$, $L = 1597$, $W = 0.5, 1.7, 2.051$ of states well before the transition, the formation of a miniband, and a flattened band.
FIG. S4. Velocity for the 2D perfect SOC model at $Q = 2\pi F_{n-2}/F_n$, as obtained from fitting the DOS near $E = 0$ (with $L = 144$, $N_c = 16384$ KPM result), fitting the twist dispersion near 0 twist (with $L = 144$ exact diagonalization), and the perturbative calculation, Eq. (4) of the main text. The dashed line is the sign-reversed perturbative result for post-transition $W$.

FIG. S5. Results for the long-range hopping model with $Q/2\pi = F_{n-3}/F_n$. Top left: Density of states $\rho(E)$ as a function of $E$ on a log-log scale calculated using KPM at $L = 1597$, with an $N_c = 4096$ with $W = 0$. By varying $\sigma$ the power-law decreases following $\rho(E) \sim |E|^{1/\sigma - 1}$. Top middle: Fixed $\sigma = 1/3$ and varying $W$, when $W$ is small, the power law is well preserved. As the model approaches the transition the power law regime is pushed to lower and lower energy due to the formation of minibands. The solid line represent actual data, and dashed lines are fits to the expected form $\rho(E) \sim |E|^{1/\sigma - 1}$. To accurately extract the scaling of the prefactor of the DOS, i.e. $\rho(E) \sim |W - W_c|^{-\beta} |E|^{1/\sigma - 1}$, we turn to the second derivative of $\rho(E)$. Top right: The second derivative $\rho''(0)$ as a function of $W$ for various $N_C$ with $L = 28657$ displaying a clear divergence as the transition is approached, signifying the DOS is becoming non-analytic. As shown in Fig. S2, we find $\rho''(0)$ diverges with $|W - W_c|$ in a power law fashion. To avoid the issues involved with fitting, that we find are most severe in this 1D model we use $\rho''(0)$ computed directly with the KPM. Bottom left and middle: Real space and momentum space inverse participation ratio (IPR) of energy eigenstate closest to $E = 0$, denoted as $I_R(q = 2)$ and $I_M(q = 2)$ respectively, calculated for various $L$ and averaged over 200 realizations. The $L$ dependence clearly shows that when the real space IPR is delocalized $I_R(q = 2) \sim 1/L$ the momentum space IPR is localized and vice-versa. This demonstrates the transition in 1D goes from a semimetal to an Anderson insulator. Bottom right: The momentum space IPR $I_M(q = 2)$ (left vertical axis) and the zero energy DOS $\rho(0)$ (right vertical axis) for $L = 987$ as a function of $W$, which demonstrates that the zero energy DOS becomes non-zero when the wavefunctions delocalize in momentum space.
and are interested in diagonal components $G$ reentrant semimetal at $W$ and passing into the metallic phase at $W$.

FIG. S6. Wave packet dynamics displaying the spread of the wavepacket $\langle \delta r(t)^2 \rangle$ as a function of time $t$ computed from the KPM on a system size of $L = 987$ with a KPM expansion order $N_C = 2^{12}$. (Left) Wavepacket spreading for $W$ in the semimetal and passing into the metallic phase at $W \approx 0.54$. (Right) Similar results but for $W$ passing from the metallic phase to the reentrant semimetal at $W \approx 0.57$. The data clearly shows a non-monotonic wavepacket spreading for increasing quasiperiodic potential strength which gives rise to a non-monotonic behavior in the dynamic exponent $z$ shown in the inset, which we extract via fits to the long time dynamics (the dashed lines mark the entry into the metallic phase).

IV. ANALYTIC RESULTS

This part of the supplement is devoted to the summary of details on analytical arguments presented in the main text.

A. Perturbative calculation of velocity renormalization

In this section we present the perturbative calculation of velocity renormalization using the language of retarded Green’s functions,

$$\hat{G}_0(E) = [E + i\eta - \hat{T}]^{-1}, \quad \hat{G}(E) = [E + i\eta - \hat{T} - \hat{\Sigma}]^{-1},$$

(S9a)

and are interested in diagonal components $G_{k,k'}$ with $k = k'$, only (e.g. for the DOS we only need $\rho(E) = -(1/\pi)\text{Im}\sum_k \text{Tr}G_{k,k}(E)$). We define the self energy at momentum $k$ by all diagrams which are $G_0(k,E)$ irreducible and write

$$G_{k,k}(E) = [G_0(k,E)^{-1} - \Sigma(k,E)]^{-1}. \quad \text{(S9b)}$$

We expand about a given node $K_0$ of the dispersion $T(K_0 + p) \approx T(K_0) + h(K_0)(p)$ to leading order in $p \ll 1/a$.

For models which satisfy the symmetry constraints exposed in the main text (see also Sec. IV D) $\Sigma(K_0 + p, E) = E\Sigma_E + h(p)\Sigma_p$ to leading order in $E, p$. Henceforth, we choose the energy offset such that $T(K) = 0$. Then,

$$G_{k,k}(E) = Z[E - (v/u_0)h(p)]^{-1} \quad \text{with } Z = 1 - \Sigma_E, v/u_0 = (1 + \Sigma_p)/Z. \quad \text{(S10)}$$

In this section we evaluate the self energy to leading and, for some models, next to leading order in powers of $W$ and summarize them in Tab. IV A discussion of infinite order perturbation theory can be found in Sec. IV D.

To illustrate the procedure we analyze the model of 2D perfect SOC for which the states at small $k$ with Hamiltonian $H(k) = t(\sin(k_x)\sigma_x + \sin(k_y)\sigma_y) \approx t\mathbf{k} \cdot \mathbf{\sigma}$ are connected to the states at $k \pm Q\hat{e}_{x,y}$ and therefore to leading order perturbation theory

$$\Sigma^{(2)}(k) = (W/2)^2 \sum_{\pm} \frac{1}{E - H(k \pm Q\hat{e}_x)} + x \leftrightarrow y \approx -E4\alpha^2 - t\mathbf{k} \cdot \mathbf{\sigma}(2\alpha^2(1 - \cos(Q))) \quad \text{(S11)}$$

For the next to leading order, all states at Manhatten distance $2Q$ from the origin are integrated out and we obtain

$$\Sigma^{(4)}(k) \approx -\frac{E}{16} \left(\frac{W}{t}\right)^4 \left(4 \cos(Q) + 10 \cos(2Q) + 11\right) \csc^4(Q) \sec^2(Q)$$

$$+ \left(\frac{W}{t}\right)^4 \frac{t\mathbf{k} \cdot \mathbf{\sigma}}{16} \left(4 - 5 \cos(Q) + 6 \cos(2Q)\right) \csc^4(Q) \sec(Q). \quad \text{(S12)}$$
FIG. S7. Graphic demonstration that the model of perfect SOC in 2D is a direct sum of two decoupled $\pi$ flux models. The model of perfect SOC, on the left of the equality sign, is characterized by direction dependent hopping matrices. Using blue squares and red circles to depict the bipartition, hopping only connects $\square, \uparrow$ with $|\sigma, \downarrow\rangle$, and separately $\square, \downarrow$ with $|\sigma, \uparrow\rangle$. The hopping in $y$-direction is imaginary and directed (this results from the asymmetry of $\sigma_y$) and, in conclusion, leads to the inclusion of a flux $\pi$ plaquette. The onsite potential does not note violate the described block-diagonalization.

| $Z-1$ | 2D SOC | 3D SOC | 1D LRH | $\delta_{\mu} = d_{1,2,3}$ | $\delta_{\mu} = O_{d/2}d_{1,2,3}$ | $\delta_{\mu} = d_{1,2}$ |
|-------|--------|--------|--------|-------------------|-------------------|-------------------|
| $Z - 1$ | $1/\sin(Q)^2$ | $3/2\sin(Q)^2$ | $1/2\sin(Q)^2$ | $8\sin(3Q/4)^2$ | $8\sin(5Q/4)^2$ | $1/4\sin(3Q/4)^2$ |
| $Z - 1$ | $\cos(Q) - 1$ | $\cos(Q) - 1$ | $0$ | $1/4$ | $5/4$ | $5/4$ |

TABLE I. Perturbative corrections for a variety of magic angle models in units of $W^2/t^2$. Note that for the honeycomb model (marked by $\square$) and $\delta_{\mu} = d_{1,2,3}$, the symmetry protection of nodes is lost. It implies a relocation of $K$-point node $\delta K = W^2(1, -\sqrt{3})/(12t^2(1 + 2\cos(Q/2))$ and a distorted velocity matrix.

This is the origin of Eq. (4) of the main text. It turns out that the results obtained for the 2D model of perfect SOC directly apply to the $\pi$ flux model. This is best graphically shown, see Fig. S7, the model of 2D perfect SOC is a direct sum of two $\pi$-flux models which in the absence of interactions completely decouple. By consequence, all single particle results obtained for model of 2D perfect SOC also hold for the $\pi$-flux model.

### B. Renormalization of interactions

In this section we present an analytical estimate of the renormalization of the interaction upon projection onto certain minibands and approaching the transition, we concentrate on $d > 1$. Let the bare ($W = 0$) model in the continuum be written as ($K_i$ are various Dirac/Weyl nodes, with linear $k \cdot p$ Hamiltonian $h^{(K_i)}(p)$)

$$S = \sum_{K_i} \int^{1/a} (dp) \int d\tau \bar{c}^{(K_i)}(p) [\partial_\tau + h^{(K_i)}(p)] c^{(K_i)}(p) + \sum_{K_{1,2,3,4}} \int^{1/a} (dp_j) \int d\tau (2\pi)^d g^{(K_{1,2})} \delta_{K_1 + K_2 - K_3 - K_4} \delta(p_1 + p_3 - p_2 - p_4) \left[ \bar{c}^{(K_1)}(p_1) c^{(K_2)}(p_2) \right] \left[ \bar{c}^{(K_3)}(p_3) c^{(K_4)}(p_4) \right] / |p_1 - p_2|^{2\sigma}.$$ (S13)

The spectrum of $h^{(K_i)}(p)$ has the form $v_0|p|$ with bare value $v_0 \sim ta$ and, for contact interaction ($\sigma = 0$), $g^{(K_i)} \sim U a^d$, while for Coulomb interaction ($\sigma = d - 1$) $g^{(K_i)} \propto \delta_{K_1, K_2}$. Perturbation theory indicates a dimensionless parameter

$$\frac{g^{(K_i)}}{v_0/a^{d-1}} \sim \frac{U}{t} \text{ for } \sigma = 0 \text{ (contact interaction)},$$ \hspace{1cm} (S14)

$$\alpha = \frac{g^{(K_i)}}{v_0} \text{ for } \sigma = d - 1 \text{ (Coulomb interaction)}.$$ \hspace{1cm} (S15)
We now consider the effect of integrating out high energy states and projecting onto a miniband with effective Brillouin zone size $1/a'$. This leads to

$$S = \sum_{K_i} \int_{1/a'}^{1/a'} dp' \int d\tau \bar{c}_{<}^{(K_i)}(p')Z^{-1}[\partial_\tau + \frac{v}{v_0} h^{(K_i)}(p')]c_{<}^{(K_i)}(p')$$

$$+ \sum_{K_{1,2,3,4}} \prod_{j=1}^{4} \int_{1/a'} dp'_j \int d\tau (2\pi)^d g(K_i) \delta_{K_1+K_3-K_2-K_4} \delta<p'_1+p'_3-p'_2-p'_4> [\bar{c}_{<}^{(K_i)}(p'_1)c_{<}^{(K_3)}(p'_2)] [\bar{c}_{<}^{(K_i)}(p'_3)c_{<}^{(K)}(p'_4)] \frac{1}{|p'_1-p'_2|^{\sigma}}. \tag{S16}$$

The renormalizations $Z$ and $v/v_0$ originate from scalar and matrix components of the self-energy and were calculated perturbatively above. We now first rescale $p_\perp = \frac{\pi}{2} p$ with $p \in (0, 1/a)$ and then define $c_{<}^{(K)}(a'p/a')Z^{-1/2}(a'/a')^{d/2} = \bar{c}_{<}^{(K)}(p)$. Under this rescaling, we restore the form of Eq. \eqref{S13}, including its UV cut-off $1/a$, but obtain the rescaling $v_0 \rightarrow va/a'$, $g \rightarrow g(a'/a')^{d-\sigma} Z^2$. From this we obtain the final formula for renormalization of the dimensionless coupling constant

$$\frac{U_{\text{eff}}/t_{\text{eff}}}{U/t} = \gamma \left( \frac{a}{a'} \right)^{d-1} \frac{Z^2}{v/v_0} \quad \text{(contact interaction)}, \tag{S17}$$

$$\frac{\alpha_{\text{ren}}}{\alpha_{\text{bare}}} = \frac{Z^2}{v/v_0} \quad \text{(Coulomb)}. \tag{S18}$$

Here, $\gamma$ is an unknown constant of order unity which depends on details of the cut-off of the linearized theory. Importantly, the integration reduces the bare contact interaction by a factor $(a/a')^{d-1}$, except in the closest vicinity where the vanishing velocity overtakes the reduction, see Fig. S8.

C. Relationship to number theory

In this section we show the relationship of the sequence of relevant perturbative processes with certain well known sequences from number theory. Starting from the scattering process of order $l_1 = 1$ we want to determine the sequence \{l_n\}_{n=1}^\infty, for which the $l_n$th order momentum transfer carves out smaller minibands than the $l_{n-1}$th order. In formulae, this implies for the 2D model of perfect SOC of the main text and arbitrary incommensuration wavevector $Q$ the condition $\sin^2(l_n Q) < \sin^2(l_{n-1} Q)$. We now concentrate on the specific case $Q = 2\pi/\phi^2 = \pi(3 - \sqrt{5})$. For this situation, the defining condition on the sequence of $l_n$ is $\sin^2(\pi l_n \sqrt{5}) < \sin^2(\pi l_{n-1} \sqrt{5})$. The sequence \{l_n\}_{n=1}^\infty for which $l_n \sqrt{5}$ successively approaches integers is the sequence of denominators of the leading rational approximants, i.e. the sequence of denominators of continued fraction convergents of $\sqrt{5}$ (OEIS ID A000176). This sequence is also half the value of the even fibonacci $l_n = F_{3n}/2$.

This sequence also connects to the formation of minibands as found with the finite size $Q_n = 2\pi F_{n-2}/F_n$. Intuitively, when $F_n$ is even ($n$ is a multiple of 3), then at order $F_n/2$, the Dirac nodes gap out, but then for $F_{n+1}$ and $F_{n+2}$ this perturbative gap must have moved to small but finite energy, forming the miniband. This motivates using $Q_{3n+1}$ and $Q_{3n+2}$ to study the effective model of successive minibands, as we do in Sec. IV.

Therefore, we offer a proof that connects this sequence to the perturbative minibands which requires the following facts about Fibonacci:

- $F_{3n}$ is even while $F_{3n+1}$ and $F_{3n+2}$ is odd.
- Catalan’s Identity: $(-1)^{n-r} F_r^2 = F_n^2 - F_{n+r} F_{n-r}$. 

FIG. S8. Divergence of contact interaction according to Eq. \eqref{S18} for the model of 2D SOC. Here, the fourth order perturbative self energy was employed and we used $\gamma = 1/5$. 

\begin{align*}
\text{FIG. S8. Divergence of contact interaction according to Eq. \eqref{S18} for the model of 2D SOC. Here, the fourth order perturbative self energy was employed and we used $\gamma = 1/5$.} \\
\end{align*}
To determine the order of perturbation theory where a gap is opened, we need to find an integer \( g_n \) such that \( g_nQ_n = 2\pi q \times F_n \) such that \( q \) is an integer closest to \( F_n/2 \) modulo \( F_n \). This is accomplished by the following theorem.

**Theorem.** Let \( n = 3m + r \) for \( r = 0, 1, 2 \), then the integer \( g_n = F_{3m}/2 \) is the smallest integer such that \( g_nF_{n-2} \equiv \frac{F_n + \delta_n}{2} \mod F_n \) with integer \( |\delta_n| \leq 1 \). In particular, \( \delta_{3m} = 0 \), \( \delta_{3m+1} = (-1)^m \), and \( \delta_{3m+2} = (-1)^{m+1} \).

**Proof.** We break this up into cases. Since \( F_{n-2} \) does not divide \( F_n \), we merely need to find a \( g_n \) that satisfies the relevant cases in order to find the unique \( g_n \), as long as \( g_n < F_n \).

**Case 1:** \( r = 0 \). For this case we can prove the above by noting that if \( g_{3m} = F_{3m}/2 \), and \( F_{n-2} \) is necessarily odd, then (We use \( N \) to represent an arbitrary, unimportant, integer.)

\[
g_nF_{n-2} = \frac{1}{2}F_{3m}(2N + 1) \equiv \frac{1}{2}F_{3m} \mod F_n,
\]

with \( \delta_n = 0 \).

The value \( g_n \) is smallest since \( \delta_n \) must vary by \( 2 \) in order for the equation \( \frac{F_n + \delta_n}{2} \) to remain integer valued, and the condition \( |\delta_n| < 1 \) prevents that.

**Case 2:** \( r = 1 \). For this case we observe using the previous fact about Fibonacci's that

\[
F_{3m}F_{3m-1} = F_{3m+1}F_{3m-2} + (-1)^{3m},
\]

and therefore since \( F_{3m-2} \) is odd

\[
\frac{1}{2}F_{3m}F_{3m-1} = (N + \frac{1}{2})F_{3m+1} + \frac{1}{2}(-1)^{3m} \equiv \frac{F_{3m+1} + (-1)^{3m}}{2} \mod F_n,
\]

and therefore \( g_{3m+1} = F_{3m}/2 \) with \( \delta_{3m+1} = (-1)^m \).

In order to show that \( g_n \) is smallest, only \( \delta_{3m+1} = -(-1)^m \) could be a problem, but we notice that \( \delta_{3m+1} = -(-1)^m \) is satisfied (uniquely) for \( g_n = F_{3m+1} - F_{3m}/2 > F_{3m}/2 \).

**Case 3:** \( r = 2 \). For this case we take Catalan’s identity with \( r = 2 \) to get

\[
F_{3m}^2 = F_{3m+2}F_{3m-2} - (-1)^{3m},
\]

and therefore since \( F_{3m-2} \) is odd

\[
\frac{1}{2}F_{3m}F_{3m} = (N + \frac{1}{2})F_{3m+2} - \frac{1}{2}(-1)^{3m} \equiv \frac{F_{3m+2} - (-1)^{3m}}{2} \mod F_n,
\]

so again \( g_{3m+2} = F_{3m}/2 \) with \( \delta_{3m+2} = (-1)^{m+1} \).

In order to show that \( g_n \) is smallest, only \( \delta_{3m+1} = (-1)^m \) could be a problem, but we notice that \( \delta_{3m+1} = (-1)^m \) is satisfied (uniquely) for \( g_n = F_{3m+2} - F_{3m}/2 > F_{3m}/2 \).

Therefore, the order of perturbation theory that opens up a gap nearest to \( E = 0 \) for \( Q = 2\pi F_{3m+r-2}/F_{3m+r} \) for \( r = 0, 1, 2 \) is \( F_{3m}/2 \).

**D. Generality of the magic-angle phenomenon - symmetry protection**

In this part of the supplement we discuss the generality of our findings by highlighting the general condition for the appearance of the magic angle phenomenon, namely the stability of the semimetal at weak coupling.

We concentrate on nodes in the kinetic term \( T \) which are protected by a symmetry group \( G_T \). For example, this analysis applies to each model we have considered in 2D as well as Dirac semimetals in 3D. Note that in general \( G_T \) is a subgroup of all symmetry operations of the kinetic term. Let \( U_{S_T} \) be the representation of \( S_T \in G_T \) in the (e.g. spinorial) Hilbert space, then the symmetry of the Hamiltonian implies \( T(k) = U_{S_T}^\dagger T(S_T k) U_{S_T} \). We concentrate on high symmetry points where \( S_T K = K, \forall S_T \in G_T \). Then, a non-trivial representation implies degeneracy in view of \( [T(K), U_{S_T}] = 0 \forall S_T \in G_T \) (formally, two non-commuting \( U_{S_T} \) are needed). We further assume a group \( G_V \) of spatial (point group) symmetries of the quasiperiodic background \( V \), such that

\[
V(x) = \sum_{S_V \in G_V} \tilde{U}_{S_V} W \tilde{U}_{S_V}^\dagger e^{iQ \cdot x} S_V \tilde{\epsilon}_0 + h.c.
\]

(S24)
Here now, $\tilde{U}_{S_V}$ is the representation of $S_V \in G_V$ and $\tilde{e}_0$ is an arbitrary vector in $\mathbb{R}^d$.

In this section, we consider Eq. (S9) formally to all orders in perturbation theory. The semimetallic behavior persists if a) $\Sigma(k)$ is hermitian and b) $T(k) + \Sigma(k)$ has the same symmetry protected touching point as $T(k)$, i.e. if $\Sigma(k)$ respects the symmetries ensuring the semimetal. In view of the incommensuration, perfect resonance is formally absent to any order in perturbation theory and therefore, the decay rate $1/\tau \sim \sum_{k'}|T_{kk'}|^2\delta(E_k - E_{k'})$ (more generally: the anti-hermitian part of the self-energy) vanishes ($T_{kk'}$ denotes the T-matrix). Thus a) is fulfilled and $1/\tau \neq 0$ signals the breakdown of perturbation theory (spontaneous unitarity breaking). We can then show to all orders in perturbation theory that the semimetal is stable provided $G_T$ is a subgroup of $G_V$.

We proceed to the proof of $\Sigma(k) = U_{S_T}^\dagger \Sigma(S_T k) U_{S_T}$ under the outlined assumptions. To get a feeling, we first consider second order perturbation theory,

$$\Sigma^{(2)}(k) = \sum_{S_V \in G_V} \tilde{U}_{S_V} W \tilde{U}_{S_V}^\dagger [E^+ - T(k + QS_V \tilde{e}_0)]^{-1} \tilde{U}_{S_V} W^\dagger \tilde{U}_{S_V}^\dagger.$$  \hspace{1cm} (S25)

We compare to

$$U_{S_T}^\dagger \Sigma^{(2)}(S_T k) U_{S_T} = \sum_{S_V \in G_V} U_{S_T}^\dagger \tilde{U}_{S_V} W \tilde{U}_{S_V}^\dagger U_{S_T} [E^+ - U_{S_T}^\dagger T(S_T k + QS_V \tilde{e}_0) U_{S_T}]^{-1} U_{S_T}^\dagger \tilde{U}_{S_V} W^\dagger \tilde{U}_{S_V}^\dagger U_{S_T}$$

$$= \sum_{S_V \in G_V} U_{S_T}^\dagger \tilde{U}_{S_V} W \tilde{U}_{S_V}^\dagger U_{S_T} [E^+ - T(k + QS_T^{-1} S_V \tilde{e}_0)]^{-1} U_{S_T}^\dagger \tilde{U}_{S_V} W^\dagger \tilde{U}_{S_V}^\dagger U_{S_T}.$$  \hspace{1cm} (S26)

This expression is invariant provided the action of $S_T$ onto $G_V$ is a bijection of $G_V$ onto itself $\forall S_T \in G_T$, i.e. $S_T S_V \in G_V \forall S_V \in G_V$ and $S_T G_V = G_V$ as this allows to uniquely relable the summation index. Taking $S_V = 1$ implies that $S_T \in G_V$ and hence $G_T$ is a subgroup of $G_V$. By consequence, the representation in the Hilbert space fulfills $\tilde{U}_{S_T^{-1} S_V} = U_{S_T}^\dagger \tilde{U}_{S_V}$ and $\Sigma^{(2)}(k)$ is invariant under the symmetries protecting the semimetal. We now continue with the next order $\Sigma^{(4)}$, from there the generality of the statement becomes apparent,

$$\Sigma^{(4)}(k) = \sum_{S_V \in G_V} \sum_{S_V' \in G_V} \tilde{U}_{S_V} W \tilde{U}_{S_V}^\dagger [E^+ - T(k + QS_V \tilde{e}_0)]^{-1} \tilde{U}_{S_V'} W \tilde{U}_{S_V'}^\dagger [E^+ - T(k + QS_V' \tilde{e}_0 + QS_V' \tilde{e}_0)]^{-1} \tilde{U}_{S_V'} W^\dagger \tilde{U}_{S_V'}^\dagger.$$  \hspace{1cm} (S27)

The exclusion $S_V' \tilde{e}_0 + S_V \tilde{e}_0 \neq 0$ ensures the irreducibility with respect to $G_k$. Again we can apply an $S_T$ transformation and exploit the two conditions exposed above to relabel both $S_T$ and $S_V'$. This implies the invariance of $\Sigma^{(4)}$. This procedure can be used to arbitrary order in perturbation theory.

V. MULTIFRACTAL ANALYSIS

In this section, we explain the procedure of extracting the multifractal exponents and the underlying physical interpretations.

A. Scaling exponent $\tau_M$

We now discuss how we extract $\tau_M(q)$ from inverse participation ratio (IPR). For a given wavefunction in momentum space, the finest grid is $2\pi/L \times 2\pi/L$. We introduce an integer binning factor $B$ which controls the resolution of the momentum space wavefunction. The IPR constructed in this way has been dubbed the momentum space IPR \cite{S3} and given by

$$I_M(q, L; B) = \sum_{k'} \phi_E(k'; B) 2^q \sim \left(\frac{Ba}{L}\right)^{\tau_M(q)},$$  \hspace{1cm} (S28)

where $k'$ denotes the wavevector of the binned wavefunction grid and $\phi_E(k'; B)$ is the binned wavefunction. The scaling behavior only holds when $1 \ll B \ll L/a$. To extract $\tau_M(q)$, we choose two consecutive values of binning
FIG. S9. $\tau_R(q)$ with different values of $W$ with $L = 144$ and 100 realizations. For $W = 0.35$ and $W = 0.7$, the multifractal spectra approach to plane wave, $\tau_R(q) = 2(q - 1)$, as increasing $b$. For $W = 0.53$, the spectrum is multifractal described by a nonlinear function. For $W = 1.75$, $\tau_R$ approaches to a localized spectrum, $\tau_R(q) = 0$ for $q > 0$, as increasing $b$. The existing data still suffer from a strong finite size effect and do not clearly show a localized spectrum. We therefore turn to the finite size dependence of the real space wavefunction with $W = 1.75$, which indeed shows localization as the real space IPR is $L$ independent in this regime.

As a complementary analysis, we study the multifractal spectrum of the real space wavefunctions at zero energy. We construct the corresponding real space scaling exponent spectrum $\tau_R(q)$ which encodes plane wave, multifractal, and localized wavefunctions.

For $W/t < 0.525$, the real space wavefunction is a plane wave, characterized by the Fourier modes at Dirac points $(k_x, k_y) = (0, 0), (0, \pi), (\pi, 0), \text{and } (\pi, \pi)$. The multifractal spectrum $\tau_R(q)$ is characterized by a straight line $\tau_R(q) = 2(q - 1)$. Plane wave states can also be found for $0.55 < W < 1.5$, the inverted semimetallic regime. For $0.525 < W/t < 0.55$, the real space wavefunctions show multifractal behavior characterized by a nonlinear $\tau_R(q)$ spectrum. For $W/t \gg 1.5$, the real space wavefunctions become localized, $\tau_R(q) = 0$ for $q > 0$.

We numerically compute the $\tau_R(q)$ spectrum for various values of $W$ in different phases. In Fig. S9 we compute $W/t = 0.35, 0.53, 0.7, 1.75$ for $L = 144$ and average over 100 realizations. $W/t = 0.35$ and $W/t = 0.7$ show plane wave spectrum as increasing the real space binning factor $b$. $W/t = 0.53$ demonstrate a weakly nonlinear multifractal spectrum with a fitting function $\tau_R(q) \approx 2(q - 1) - 0.16(q - 1)$ for $|q| < 1$. A much larger system size is needed for quantitatively determining the spectrum which is beyond the scope of this work. For $W/t = 1.75$, the spectrum gradually approaches to localized like behavior as increasing $b$. In our $L = 144$ data, we do not find a clear localized spectrum, due to finite size effects. We therefore turn to the real space IPR data as a function of system size in Fig. S10. This indeed shows strong evidence for localization as the IPR is $L$ independent for $W/t \geq 1.75$.

FIG. S10. The inverse participation ratio of real space wavefunctions with different system sizes. Blue circles represent the data of $L = 89$ with 100 realization; red squares represent data of $L = 144$ with 100 realization; black diamonds represent data of $L = 233$ with 50 realization. The collapse of data with different sizes ($W/t \geq 1.75$) indicate localized regime.

At last, we average $\tau_M(q;B_1,B_2)$ over phases in the quasiperiodic potential. For $L = 144$, we construct $\tau_M$ with 100 realization. We only use 10 realization for $L = 610$. For real space scaling exponents ($\tau_R$), we adopt similar procedures to extract their values.

B. Real space multifractality

As a complementary analysis, we study the multifractal spectrum of the real space wavefunctions at zero energy. We construct the corresponding real space scaling exponent spectrum $\tau_R(q)$ which encodes plane wave, multifractal, and localized wavefunctions.
C. Interpretation of unfreezing transition

As we have demonstrated in the main text, the momentum space wavefunctions serve as a proxy for the semimetal-metal transition. The multifractal analysis in momentum space here is distinct from the conventional notion of wavefunctions in real space. We discuss the interpretation of the multifractal spectrum in depth here.

For $W = 0$, the zero energy wavefunction is composed of the Fourier modes at the Dirac points. The zero energy states are linear combinations of these four plane waves. The probability distributions (integrating over the spin degrees of freedom) of the momentum space wavefunction generically contains four peaks, which we call “ballistic peaks”. In the multifractal $\tau_M(q)$ spectrum, these ballistic peaks correspond to a frozen spectrum, $\tau_M(q) = 0$ for $q > 1$.

The frozen feature in the momentum space wavefunction suggests that the ballistic peaks are sharply defined, with the finest localization length $\pi/L$. The $\tau_M(q)$ extracted from the numerics weakly depend on the choice of binning factors $B_1$ and $B_2$. As $W$ increases, satellite peaks with weaker amplitude arise. When $W \approx W_c$, the $\tau_M(q)$ still show freezing behavior for $B = 1, 2$ but become generically non-zero for larger binning factors. Such features suggest that the distance between a ballistic peak and the nearest satellite peaks is around $2 \pi/L$ to $4 \pi/L$. The ballistic peaks start to hybridize with the satellite peaks when $W > W_c$. This corresponds to an unfreezing transition in momentum space, which describes a zero-measure set to an extensive set of Fourier modes. The $W_c$ determined here coincides well with the semimetal-metal transition extracted from the density of states calculations.

For larger values of $W$, an inverse semimetal transition, metal-to-semimetal, takes place. The same multifractal analysis in momentum space also applies.

VI. WANNIER STATES AND BUILDING HUBBARD MODELS

In order to analytically build the Hubbard models analyzed in the main text, we use the Hamiltonian as perviously defined

\begin{equation}
\hat{H} = \hat{T} + \hat{V} + \hat{U},
\end{equation}

\begin{equation}
\hat{T} = \sum_{\mathbf{r}, \mu} \left[ \frac{it}{2} \sigma_{\uparrow} c_{\mathbf{r} \mu}^\dagger \sigma_{\uparrow} c_{\mathbf{r}+\hat{\mu}} + \text{h.c.} \right],
\end{equation}

\begin{equation}
\hat{V} = W \sum_{\mathbf{r}, \mu} \cos(Q_n r_\mu + \phi_\mu) c_{\mathbf{r} \mu}^\dagger c_{\mathbf{r} \mu},
\end{equation}

\begin{equation}
\hat{U} = U \sum_{\mathbf{r}} c_{\mathbf{r} \uparrow}^\dagger c_{\mathbf{r} \uparrow} c_{\mathbf{r} \downarrow}^\dagger c_{\mathbf{r} \downarrow}.
\end{equation}

We take $Q_n = 2\pi F_{n-2}/F_n$ and the system size to be $L = m F_n$ such that $F_n$ defines a supercell of size $\ell = F_n$. The model has a particle-hole symmetry when $\phi_\mu = \pi/2$, which we will concentrate on in order to isolate bands near $E = 0$.

The first task is to isolate bands. With $L = m \ell$, our Brillouin Zone will have $m^2$ sampled points. Due to the imposed discrete translational symmetry, one can write the single particle Hamiltonian $\hat{H}_{\text{sp}} = \hat{T} + \hat{V}$ as

\begin{equation}
\hat{H}_{\text{sp}} = \bigoplus_{n_x, n_y = 0}^{m-1} \hat{H}_n,
\end{equation}

for $\mathbf{n} = (n_x, n_y)$ and, using Bloch’s theorem, the individual Hamiltonians are (in first quantized notation)

\begin{equation}
\hat{H}_n = \sum_{\mathbf{r}, \mu} \left[ \frac{it}{2} e^{-i2\pi n_\mu/L} |\mathbf{n}, \mathbf{r}\rangle \langle \mathbf{n}, \mathbf{r} + \hat{\mu}| \otimes \sigma_{\mu} + \text{h.c.} \right] + W \sum_{\mathbf{r}, \mu} \cos(Q_n r_\mu + \phi_\mu) |\mathbf{n}, \mathbf{r}\rangle \langle \mathbf{n}, \mathbf{r}|,
\end{equation}

on a system size of size $\ell$. In the thermodynamic limit $m \to \infty$, and we can plot dispersions to see if a gap has opened. Once diagonalized, we have a set of states $\{E_{n,j}\}$, and looking near $E = 0$, we can form projectors onto energy states within a miniband

\begin{equation}
\hat{P} = \sum_{E_{n,j} \in \text{Miniband}} |\mathbf{n}, j\rangle \langle \mathbf{n}, j|.
\end{equation}

This projector should have an integer multiple of $m^2$ states within it, and each $(n_x, n_y)$ pair should contribute the same number of states. This is a check to determine if we have a “good band.”
Further, we can get an idea of where the Wannier centers should be by looking at the integrated local density of states

\[ \rho_{\text{Band}}(r) = \langle r | \hat{P} | r \rangle. \]  

(S34)

Considering systems with periodic boundary conditions, we consider the position operators \{cos(2π\hat{x}/L), sin(2π\hat{x}/L), cos(2π\hat{y}/L), sin(2π\hat{y}/L)\}, and we construct the projected operators

\[ \{ \hat{P} \cos(2\pi \hat{x}/L) \hat{P}, \hat{P} \sin(2\pi \hat{x}/L) \hat{P}, \hat{P} \cos(2\pi \hat{y}/L) \hat{P}, \hat{P} \sin(2\pi \hat{y}/L) \hat{P} \}. \]  

(S35)

These operators no longer commute with one another and cannot be simultaneously diagonalized. The solution is approximate joint diagonalization (AJD) achieved by minimizing a cost function: for a set of operators \( \mathcal{O} \), we need to find a unitary matrix \( U \) such that

\[ \sigma(U) = \sum_{\mathcal{O}} \sum_{i \neq j} |(U^\dagger A U)_{ij}|^2 \]  

(S36)

is minimized. An efficient algorithm for this was developed for signal processing \[ [S6] \] and enumerated for maximally localized Wannier states in Ref. \[ [S7] \]. Our algorithm to achieve this, written in Julia, can be found in Ref. \[ [S8] \].

The columns of the resulting unitary matrix \( U \) are the maximally localized Wannier states. The resulting single particle part of tight-binding Hamiltonian is found numerically to be given approximately by

\[ \hat{H}_{\text{Wannier}} = U^\dagger \hat{H}_{\text{sp}} \hat{P} U \approx \sum_{\text{R,}\tau} \left[ \frac{i \epsilon_{\text{eff}}}{2} |W_{\text{R,}\tau}| \langle W_{\text{R+\hat{\mu},\tau'}} | |\sigma_{\mu}\rangle_{\tau,\tau'} + \text{h.c.} \right], \]  

(S37)

for Wannier states \( |W_{\text{R,}\tau}\rangle \) labeled by the emergent lattice positions \( \text{R} \) and internal index \( \tau = 1, 2 \). The interaction term also gets renormalized (again, returning to second quantized notation)

\[ \hat{H}_{\text{Wannier-int}} = U_{\text{eff}} \sum_{\text{R}} d_{\text{R,1}}^d d_{\text{R,2}}^d d_{\text{R,1}} d_{\text{R,2}} \]  

(S38)

where \( d_{\text{R,}\tau} \) annihilates the states \( |W_{\text{R,}\tau}\rangle \), and

\[ U_{\text{eff}} = U \sum_{\text{R}} \{ |W_{\text{R,1}}^\dagger (r)|^2 |W_{\text{R,2}}^\dagger (r)|^2 + |W_{\text{R,2}}^\dagger (r)|^2 |W_{\text{R,1}}^\dagger (r)|^2 - 2 |W_{\text{R,1}}^\dagger (r) W_{\text{R,2}}^\dagger (r) W_{\text{R,1}} (r) W_{\text{R,2}} (r)| \}, \]  

(S39)

where \( \langle \text{r}, \sigma | W_{\text{R,}\tau} \rangle = W_{\text{R,}\tau}^\dagger (\text{r}) \) and \( U_{\text{eff}} \) is found to be (numerically) independent of \( \text{R} \).

To perform the calculations, we look close to the transition \( W_c \) calculated previously and find where the smallest gap opens in the dispersion. In the range where that gap opens and closes, we perform Lanczos to find the Bloch states and then we perform AJD to find the Wannier states. After making sure the states are “good” states (exponentially localized and make the appropriate emergent lattice), we can find the Hamiltonian as described above.

### A. Computed Wannier functions

As described in Sec. \[ [IV.C] \] we can probe minibands by using successive pairs of odd Fibonaccis (even Fibonaccis gap out the Dirac nodes, not allowing us to make the effective Hubbard model described above). We perform the calculation for \( \ell = F_n = 13, 21 \) (second miniband), \( \ell = F_n = 55, 89 \) (third miniband), and \( \ell = 233, 377 \) (fourth miniband). In the main text, we present data for \( \ell = 13 \), and here we show data for the point of highest \( U_{\text{eff}}/t_{\text{eff}} \approx 4115U/t \).

After tracking the gap opening and closing when \( \ell = 377 \), we construct the Wannier states (at \( W = 0.52445t \) and \( m = 8 \)), and the results are in Fig. \[ [S1] \]. We see Wannier centers on top of the \( \rho_{\text{Band}}(r) \) in Fig. \[ [S1] \] upper-left, along with a visual representation of the resulting \( H_{\text{Wannier}} \) on the upper-right (clearly showing a banded Hamiltonian). The Wannier state is visually seen in Fig. \[ [S1] \] lower-left and after we bin the data, we find the states are exponentially localized in Fig. \[ [S1] \] lower-right.

Doing this multiple times leads to an estimate of the effective interactions on either side of the metal transition in Fig. \[ [S12] \]. We should note that for \( \ell = 13, 21 \), part of the data is pulled from a multi-band Hubbard model by tracking \( U_{\text{eff}}/t_{\text{eff}} \) on the Wannier functions with maximal overlap prior to the multi-band Hubbard model. Also, the Wannier states for \( \ell = 89 \) could not fully be fully converged, so the data for \( U_{\text{eff}}/t_{\text{eff}} \) is appropriately noisy (and an underestimate).
FIG. S11. (Upper left) The integrated density of states $\rho_{\text{band}}(x,y)$ along with Wannier centers (red dots) for $\ell = 377$ and $m = 8$ and $W = 0.52445t$. (Upper right) The magnitude of the elements of the Wannier Hamiltonian $H_{\text{Wannier}}$. (Lower left) 3D representation of a single Wannier function $|W(r)|^2$ and (Lower right) The exponential localization of the Wannier function $|W(r)|^2 \sim e^{-r/\xi}$.

FIG. S12. The interaction of the center band approaching the transition. Each successive pair of odd $\ell$ represent the opening of a new miniband. The data labeled “3 bands” comes from the multiorbital models, following the Wannier states continuously connected to the single-orbital model. Note that $Q = 2\pi/\varphi^2$ for golden ratio $\varphi$ and $Q_\ell = 2\pi F_n - 2/\ell$ with $\ell = F_n$.

B. Finite energy bands and multi-orbital Hubbard model

It is interesting to note that at finite energy, flat bands develop and in some cases intersect the band near $E = 0$ which is the focus of this text. As a clear example, note for $\ell = 13$, see that a flat, Dirac bands appear around the region labeled 1 in Fig. S13 (upper left) and intersect the band in the region labeled 3. These flat bands have greatly increased $U_{\text{eff}}/t_{\text{eff}}$ away from the transition. When the multiorbital Hubbard model appears, the dispersion changes
FIG. S13. (Upper left) For $\ell = 13$, we see a region (labeled 1) where one Dirac band exists around $E = 0$ (the figures in the main text are constructed here). There is also an extremely flat band at finite energy that intersects the band in the region labeled 3. (This data is taken for $m \to \infty$ by random sampling the Brillouin zone and $\phi_\mu = \pi/2$.) (Upper right) The dispersion in region 3 at $W = 0.52t$, the second red line in the upper left figure. (Middle left) The integrated density of states $\rho_{\text{band}}(x, y)$ for the three band model. We can see a line of three states tiled in an $8 \times 8$ grid. (Middle right) A visual representation of the single-particle part of the multi-orbital Hubbard model. The Wannier states are separated by their average energy $-\mu$, 0, $+\mu$, and they have hopping matrix elements to neighbors and next-to-nearest neighbors on the diagonal. Each Wannier site is double degenerate and the hopping matrix elements are Pauli matrices as color coded. (Bottom left) The Wannier Hamiltonian separated into the 3 orbits (the red lines); we see that it is banded and dominated by the hoppings shown in the middle-right figure. (Bottom right) The Hubbard $U$ matrix for the multi-orbital model. The highest values of the Hubbard $U$ matrix comes from states continuously connected to flat bands in the upper-left figure that intersect the middle band in region 3.
left). Lastly, the multiorbital Hubbard $U$ is a matrix in this case and is visually represented in Fig. S13 lower right).

[S1] M. Gärtnner, S. V. Syzranov, A. M. Rey, V. Gurarie, and L. Radzihovsky, Phys. Rev. B 92, 041406 (2015).
[S2] A. Weiße, G. Wellein, A. Alvermann, and H. Fehske, Rev. Mod. Phys. 78, 275 (2006).
[S3] J. H. Pixley, J. H. Wilson, D. A. Huse, and S. Gopalakrishnan, Phys. Rev. Lett. 120, 207604 (2018).
[S4] S. V. Syzranov and L. Radzihovsky, Annual Review of Condensed Matter Physics 9, 35 (2018).
[S5] F. Evers and A. D. Mirlin, Reviews of Modern Physics 80, 1355 (2008).
[S6] J. Cardoso and A. Souloumiac, SIAM Journal on Matrix Analysis and Applications 17, 161 (1996).
[S7] F. Gygi, J.-L. Fattebert, and E. Schwegler, Computer Physics Communications 155, 1 (2003).
[S8] “Approximate joint diagonalization,” https://github.com/jhwilson/AJD.jl [Online; accessed 12-Sept-2018].