Supplementary information for: Flat bands and perfect metal in trilayer moiré graphene

Christophe Mora,[1] Nicolas Regnault,[1] and B. Andrei Bernevig[2]

[1] *Laboratoire de Physique de l'Ecole normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris-Diderot, Sorbonne Paris Cité, Paris, France*

[2] *Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

(Dated: May 23, 2019)

S-I. BREAKING PARTICLE-HOLE SYMMETRY

The particle-hole (p-h) symmetry is important in proving that all bands in the spectrum of trilayer twisted graphene are connected. It gives a band landscape symmetric with respect to zero energy and implies that features, such as Dirac points and other gapless crossings, or symmetries occurring at finite energy always come in pairs. It maintains globally the gapless structure of the spectrum. The other essential symmetry is the combined spatial-time symmetry $\mathcal{C}_{2z}\mathcal{T}$ - this symmetry locally maintains the gapless structure of the band spectrum. Breaking $\mathcal{C}_{2z}\mathcal{T}$ directly open gaps at Dirac points locally and hence isolates finite sets of bands. In contrast to that, we expect the gapless band structure to keep its integrity if the terms breaking p-h symmetry are not too strong.

In a real trilayer graphene system, the rotation angles between the planes are finite and there are corrections to the emergent Eq. (1) of the main text. There are two main effects that break p-h symmetry: (i) k^2 corrections to the Dirac cones approximation $\sim \mathbf{k}\cdot\boldsymbol{\sigma}$ close to the K points in each layer, (ii) the three K points are not aligned at finite rotation angle. We note that (i) is the first step towards the complete band structure of each graphene layer with both the K and K' points. The vicinities of K and K' are indeed fully decoupled in Eq. (1) of the main text. (ii) can be simply taken into account by choosing a different basis in each layer such that the vectors $\mathbf{q}_1^{ab}$ are parallel. This results into the Hamiltonian

$$H^{(ab)}(\delta\mathbf{p}_a,\delta\mathbf{p}_b) = v_F\left(M_{\theta_{1a}}^{-1}\delta\mathbf{p}\right)\cdot\boldsymbol{\sigma}\ \delta_{a,b} + w^{ab}\sum_{j=1}^{3}\delta_{\delta\mathbf{p}_a,\delta\mathbf{p}_b+\mathbf{q}_j^{a,b}}T^j \tag{S-1}$$

where $M_{\theta_{1a}}$ is the in-plane rotation of angle θ_{1a}, reducing to Eq. (1) of the main text for vanishingly small twist angles. Eq. (S-1) explicitely breaks p-h symmetry. The numerical resolution of Eq. (S-1) is displayed in Fig. S-1 for the representative case $p = q = 1$ and for several values of α. Inspecting the 20 states close to the Fermi energy along symmetry lines, we find band crossings between all states despite the breaking of p-h symmetry.

S-II. SYMMETRIES FOR ARBITRARY p AND q

We first review the particular case $p = q = 1$. The effective single-valley model of Eq. (1) (see main text) is obtained by keeping only the states close to the K point in each layer. It is decoupled from its time-reversed counterpart built with the states around the K' points. Hence, Eq. (1) does not respect time-reversal symmetry. For $p = q = 1$, the symmetry group of this one-valley model is the magnetic space group $P6'2'2$, the same as for twisted bilayer graphene, characterized by the generators

$$\mathcal{C}_{3z} = \exp(i2\pi\sigma_z/3)\delta_{Q_m,C_{3z}Q_n}, \qquad \mathcal{C}_{2x} = \sigma_x\delta_{Q_m,C_{2x}Q_n}, \qquad \mathcal{C}_{2z}\mathcal{T} = \sigma_x\delta_{Q_m,Q_n}K. \tag{S-2}$$

The band spectrum is invariant with respect to these three symmetries. The antiunitary $C_{2z}T$ symmetry is a combination of time-reversal and C_{2z} symmetry acting locally on the moiré lattice. It commutes with the spatial symmetries $\mathcal{C}_{3z}$ and $\mathcal{C}_{2x}$. Whereas $\mathcal{C}_{3z}$ maps each layer into itself, $\mathcal{C}_{2x}$ exchanges the layers 1 and 3 and leaves the layer 2 invariant.

Besides the magnetic space group $P6'2'2$, the model also exhibits a particle-hole (p-h) symmetry inherited from the original p-h symmetry in each graphene layer. The corresponding operator - see Eq. (7) and (8) in the main text -

$$\mathcal{P} = \delta_{Q_m,-Q_n}\zeta_{Q_n}, \qquad \mathcal{P}\tilde{H}(k)\mathcal{P}^\dagger = -\tilde{H}(-k), \tag{S-3}$$

commutes with the generators (S-2) of the magnetic space group, and squares to 1 in contrast with the p-h operator in the bilayer case which squares to -1.

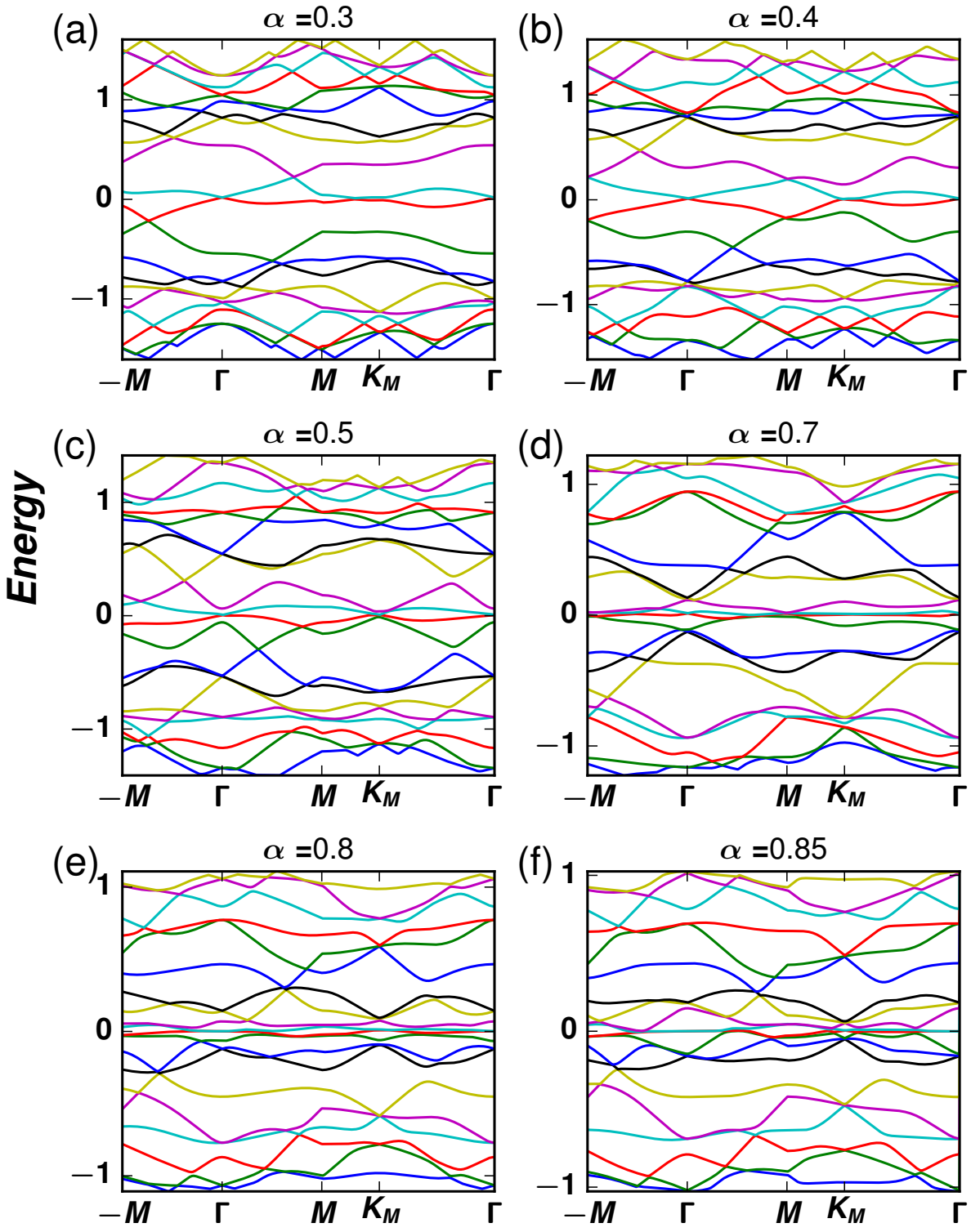

FIG. S-1: Moiré bands computed from Eq. (S-1) for $p = q = 1$ and $\theta_{1,2} = \theta_{23}$. 20 bands around zero energy are represented along the moiré Brillouin zone trajectory $-M \to \Gamma \to M \to K_M \to \Gamma$ for $\alpha = 0.3, 0.4, 0.5, 0.7, 0.8, 0.85$ (a-f). In principle, Eq. (S-1) has two independent parameters, α and θ_{12}, and the ratio between them is not universal. For this plot, we have nevertheless chosen the conversion rule $\theta_{12} = 1.05^\circ$ for $\alpha = 0.606$ compatible with experiment results on graphene structures.

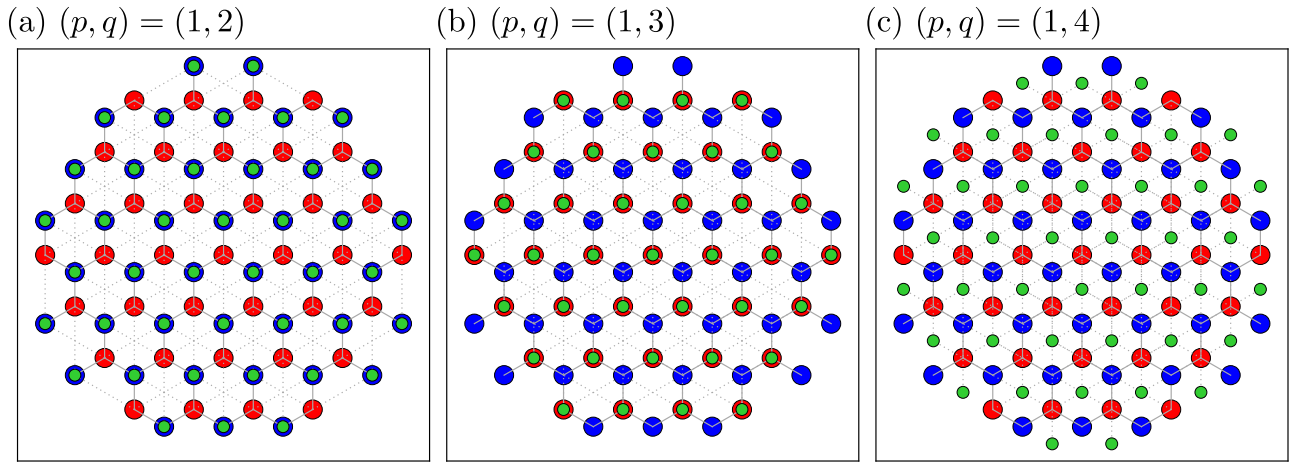

FIG. S-2: Three lattices of Dirac cones for $\alpha = 0$ corresponding to different $(p,q) = (1,2)$ (a), $(1,3)$ (b), and $(1,4)$ (c). Red (resp. blue, green) points correspond to the middle (resp. bottom, top) layer. The right lattice (c) has separate Dirac cones, corresponding to the case (i) (see supplementary main text), whereas the left (a) and middle (b) lattices have pairs of overlapping Dirac cones and 1 isolated Dirac cone, corresponding to the case (ii) of the supplementary main text.

The rotation symmetry $\mathcal{C}_{3z}$ and the antiunitary symmetry $C_{2z}T$ are valid also for arbitrary p and q, *i.e.* when the rotation angles are different but still commensurate. Interestingly, if p or q is different from 1, the symmetries $\mathcal{C}_{2x}$ and $\mathcal{P}$ are individually broken but their product $\mathcal{C}_{2x}\mathcal{P}$ remains a symmetry of the one-valley Hamiltonian (4) (see main text). We thus introduce the mirror p-h symmetry operator

$$\mathbf{\Pi}_{\pi/6} = \mathcal{P}\mathcal{C}_{2x}\mathcal{C}_{3z} = \begin{pmatrix} 0 & e^{-2i\pi/3} \\ e^{2i\pi/3} & 0 \end{pmatrix} \delta_{Q_m,\Pi_{\pi/6}Q_n}\zeta_{Q_n}; \quad \zeta_{Q_1} = \zeta_{Q_3} = 1; \quad \zeta_{Q_2} = -1, \tag{S-4}$$

obtained by combining the product $\mathcal{C}_{2x}\mathcal{P}$ with the rotation symmetry $\mathcal{C}_{3z}$. ζ_{Q_n} is $+1$ for Q_n belonging to the bottom and top layers and -1 for the middle layer. The invariant plane of the mirror symmetry $\Pi_{\pi/6}$ crosses orthogonally the graphene layers along lines. These lines make an angle of $\pi/6$ with respect to the x axis and go through the Γ and K_M points. By construction, each layer is thus invariant upon the mirror symmetry $\Pi_{\pi/6}$. The action on the Hamiltonian (4) is

$$\mathbf{\Pi}_{\pi/6}\tilde{H}(k)\mathbf{\Pi}^{\dagger}_{\pi/6} = -\tilde{H}(\Pi_{\pi/6}k), \tag{S-5}$$

corresponding to a p-h symmetry. Eq. (S-5) implies a symmetric band spectrum around zero energy where each state k has a mirror-symmetric partner $\Pi_{\pi/6}k$ with opposite energy.

S-III. POSITIONS OF THE DIRAC CONES FOR $\alpha = 0$

As discussed in the main text, the full connectivity of the moiré band model requires essentially the $C_{2z}T$ symmetry to protect Dirac cones, or at least to have them gapped by pairs, the mirror p-h symmetry $\mathbf{\Pi}_{\pi/6}$ to reduce the parity of Dirac points to their parity in the zero energy manifold, and the continuity with respect to the case $\alpha = 0$ where the positions of Dirac points are easily determined. As illustrated in Fig. S-2, we find two configurations at $\alpha = 0$: either (i) the model has three Dirac points at distinct positions Γ, K_M, K'_M in the Brillouin zone, or (ii) two Dirac points are on top of each other and separated from the third one. The case (i) occurs for $q - p = 1 \mod 3$ whereas (ii) occurs for $q - p = 0, 2 \mod 3$.

S-IV. DENSITIES OF ELECTRONS CLOSE TO THE FERMI ENERGY

Twisted bilayer graphene, with a small angle, exhibits a local density of states for the (almost) flat bands that is well-localized to the AA regions of the Moiré pattern [1–3], forming a triangular lattice. This spatial localization is understood at zero energy from the absence of tunneling between AA and AB, BA regions [4]. In the trilayer geometry, it is not possible to isolate a finite set of bands as we prove in the main text. However, we can integrate

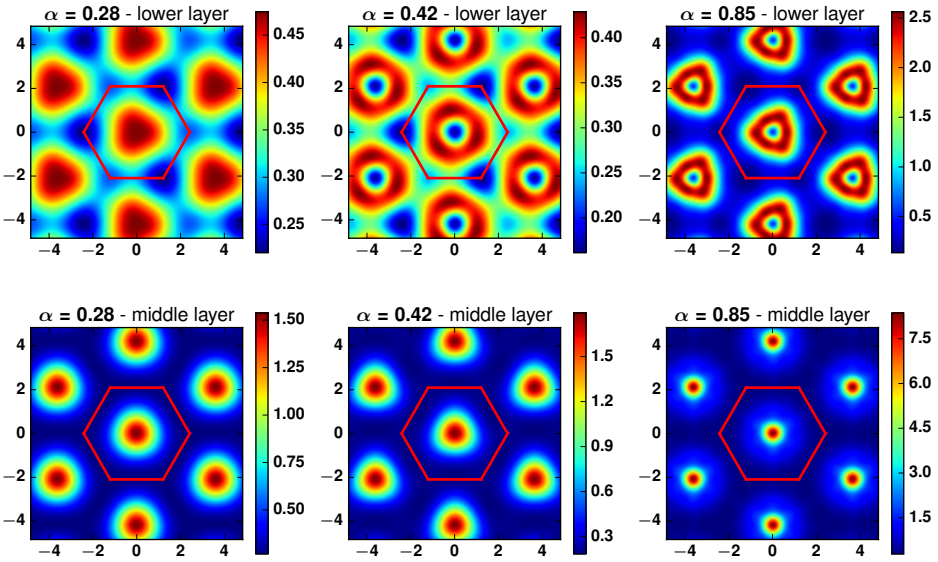

FIG. S-3: Local density of states for the A sublattice, and $p = q = 1$, integrated for $|\varepsilon| < \varepsilon_{\max}$. Its counterpart for the B sublattice is infered by C_6 symmetry, and the upper layer one is obtained from the lower layer by particle-hole symmetry. We choose $\varepsilon_{\max} = 0.02$ and $\alpha = 0.28, 0.42, 0.85$.

the local density of states (LDOS) over a narrow energy range close to zero energy similarily to what has been done in the bilayer case [4]. The result is shown in Fig. S-3 for $\alpha = 0.28, 0.42, 0.85$. In the middle layer, localization around the AA region occurs more dramatically when bands are nearly dispersionless close, see $\alpha = 0.85$. Although the whole pattern forms a triangular lattice, the localization around the AA region is never really strong for the lower and top layers.

S-V. BAND SPECTRA FOUR AND FIVE LAYERS

We conjecture in the main text that the property of full connectivity for the band spectrum with $C_{2z}T$ symmetry depends crucially on the number of Dirac cones, *i.e.* on the parity of the number of graphene layers. We check this prediction by numerically solving the case of four and five layers in the simplest case of evenly rotated planes. The corresponding band spectra, displayed in Fig. S-4 and Fig. S-5, confirm the conjecture.

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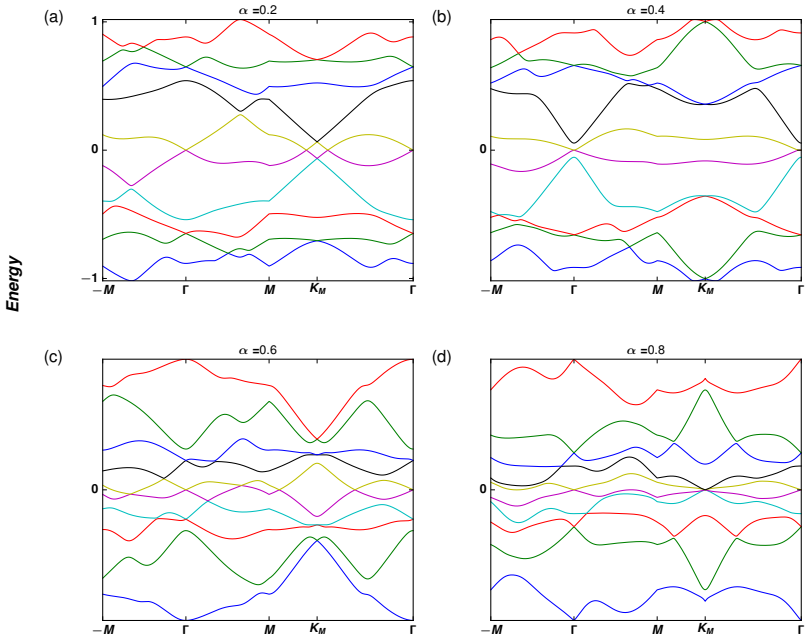

FIG. S-4: Moiré bands computed for four twisted layers and $C_{2z}T$ symmetry. The angle of rotation is chosen to be the same between consecutive planes and we represent ten bands around zero energy. As explicitely visible for $\alpha = 0.4$ and 0.8, it is clearly possible to isolate finite connected sets of bands in the spectrum.

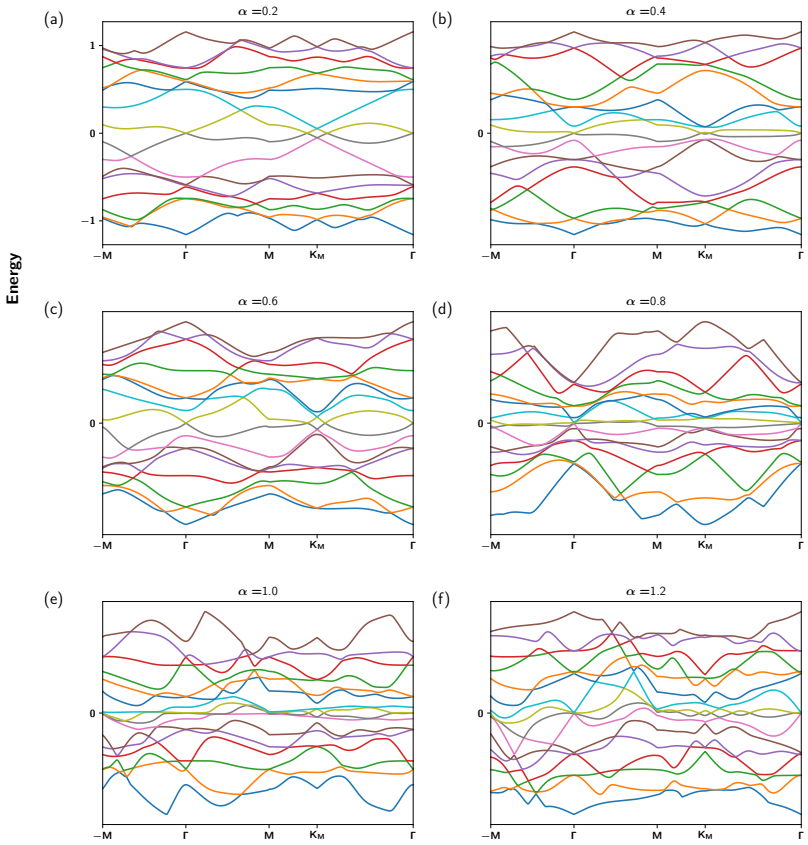

FIG. S-5: Moiré bands computed for five twisted layers and $C_{2z}T$ symmetry with equally spaced angles and ten bands around zero energy. All spectra are fully connected in agreement with our conjecture presented in the main text.