Topology and interactions within the magic angle twisted bilayer graphene narrow bands

Oskar Vafek

National High Magnetic Field Laboratory

and

Department of Physics, Florida State University, Tallahassee, FL

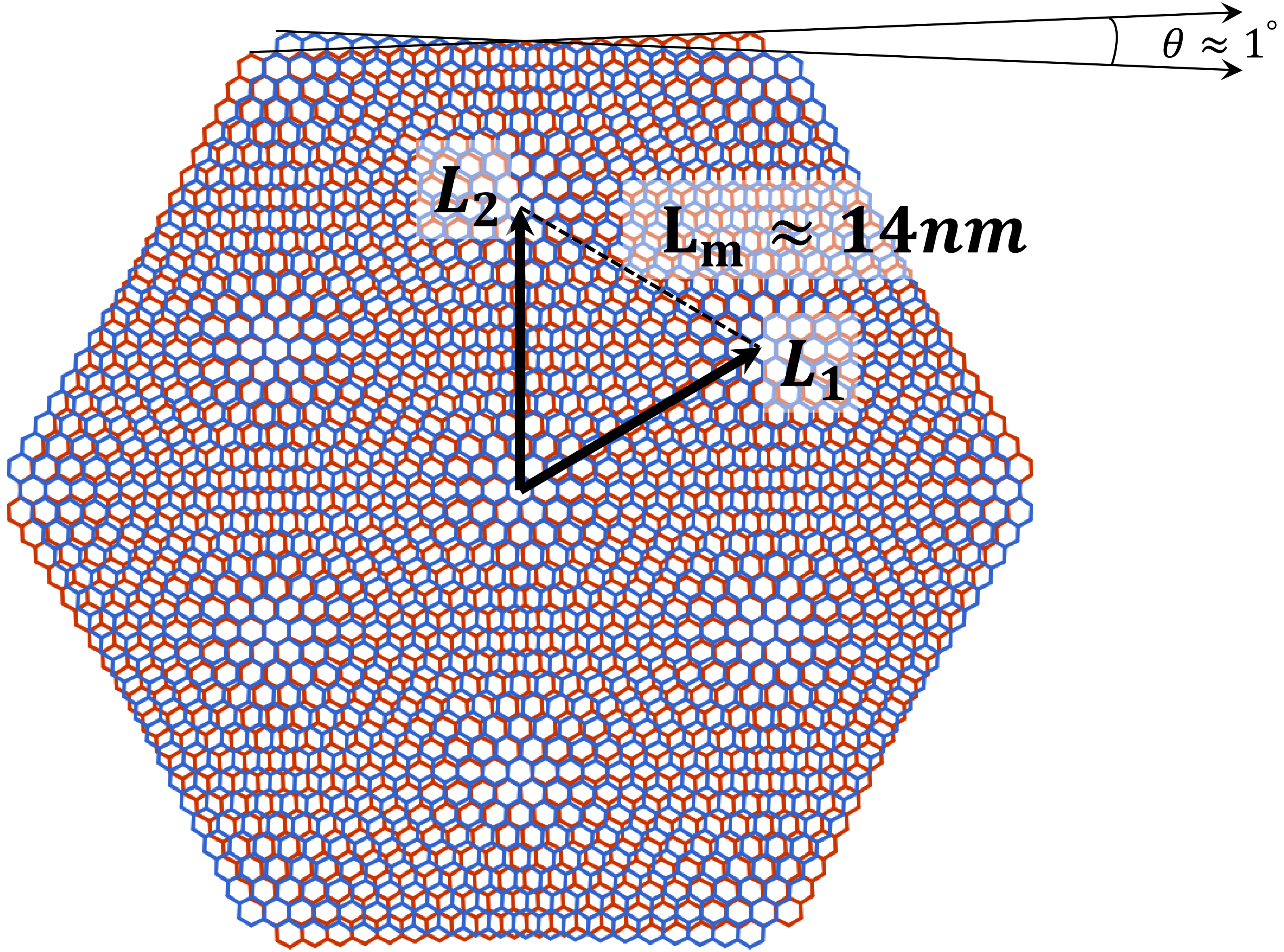
Lecture 1:

- Physical origin of the narrow bands: structure and back-of-the-envelope of the argument
  minimal continuum model

- Band topology and the role of the emergent symmetries
  The tool which we will use to detect the narrow band topology is the non-Abelian Berry phase
  or the ``Wilson loops''
  explain how to think about it physically, show the results of the calculation and show its eigenstates

- Turn on the interactions: Generalized ferromagnetism and Chern states
  itineracy at strong coupling and cascades between heavy and light fermions

- *Surprises
  period 2-stripe state, insulator despite $C_{2z}T$ and valley U(1) symmetry AND Wilson loops of all sub-bands become trivial. Candidate for the Chern 0 insulator at odd filling (ν=3)

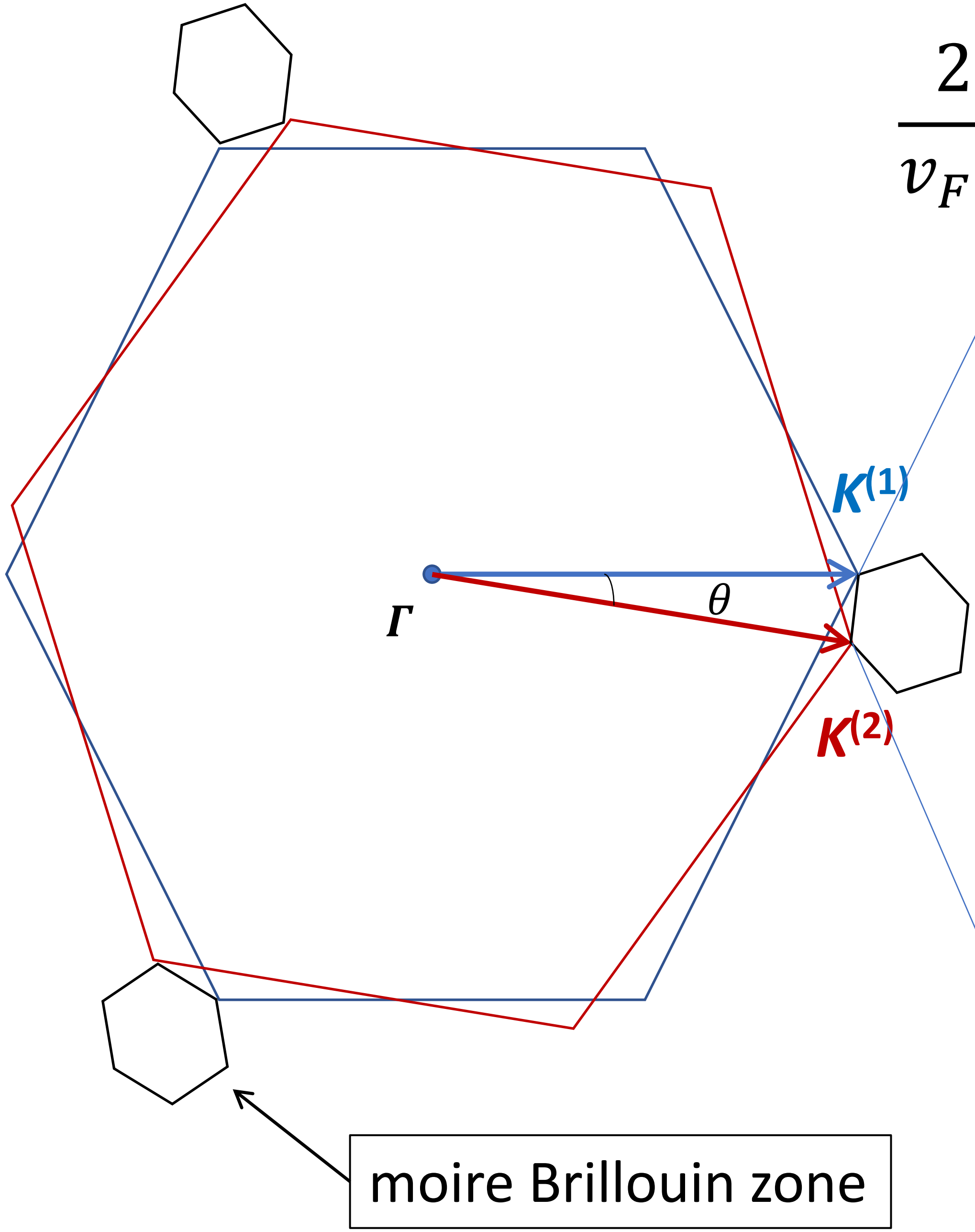


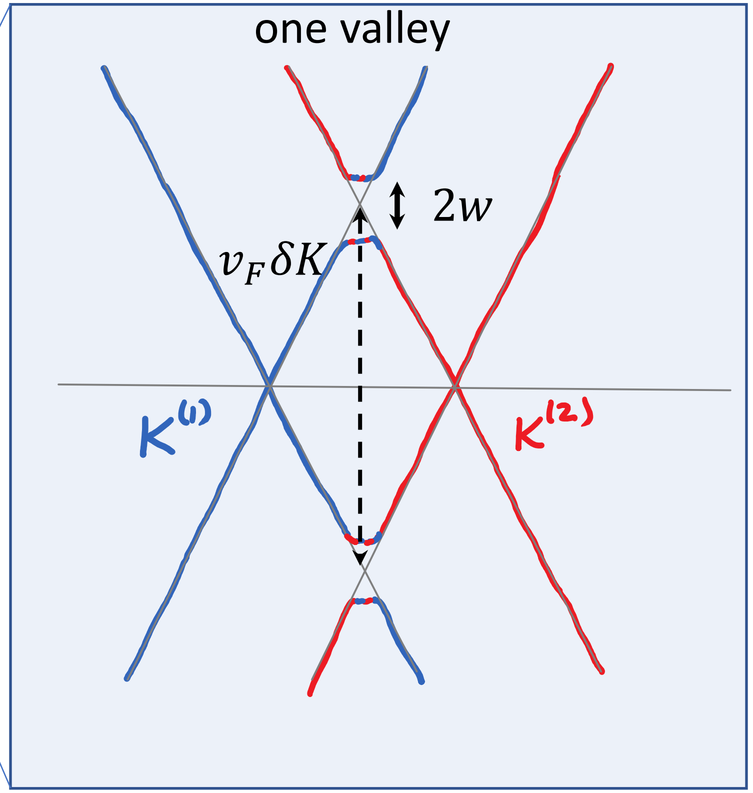
$\theta \approx 1^{\circ}$
L_2
$\mathbf{L_m} \approx \mathbf{14}nm$
L_1

$$\frac{2w}{v_F\,\delta K}$$

$2w$ ← controlled by pressure

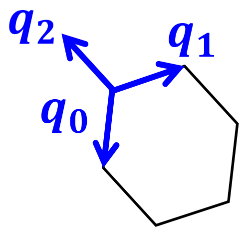
$v_F\,\delta K$ ← controlled by angle





Lopes dos Santos et al PRL (2007)
Li et al Nature Phys (2010)
Shallcross et al PRB (2010)
Mele PRB (2010), (2011)
Bistritzer&MacDonald PNAS (2011)

Minimal continuum low energy model



$$H_{BM} = \begin{pmatrix} \hbar v_F \boldsymbol{p} \cdot \sigma_{\theta} & T(\boldsymbol{r}) \\ T^{\dagger}(\boldsymbol{r}) & \hbar v_F \boldsymbol{p} \cdot \sigma \end{pmatrix}$$

Perfect particle-hole symmetry if ignored
Z.Song et.al. PRL2019; Hejazi et.al. PRB2019

AA region interlayer tunneling

$$T(\boldsymbol{r}) = \begin{pmatrix} w_0 \sum_{j=0}^{2} e^{-i\boldsymbol{q}_j \cdot \boldsymbol{r}} & w_1\left(e^{-i\boldsymbol{q}_0 \cdot \boldsymbol{r}} + e^{-i\phi} e^{-i\boldsymbol{q}_1 \cdot \boldsymbol{r}} + e^{i\phi} e^{-i\boldsymbol{q}_2 \cdot \boldsymbol{r}}\right) \\ \phi \rightarrow -\phi & w_0 \sum_{j=0}^{2} e^{-i\boldsymbol{q}_j \cdot \boldsymbol{r}} \end{pmatrix}$$

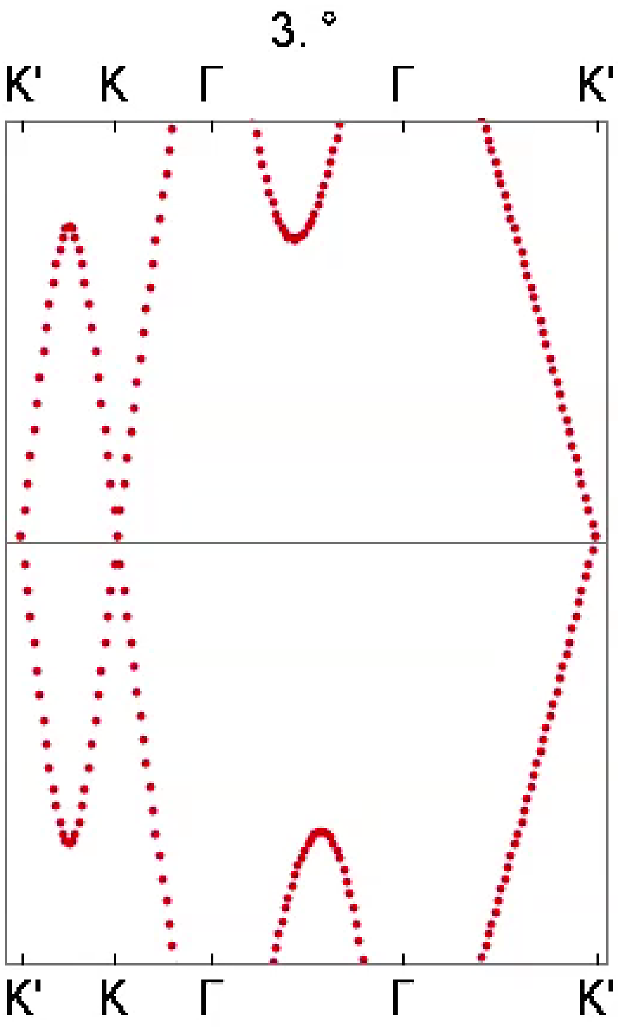
$\phi = 2\pi/3$

AB region interlayer tunneling

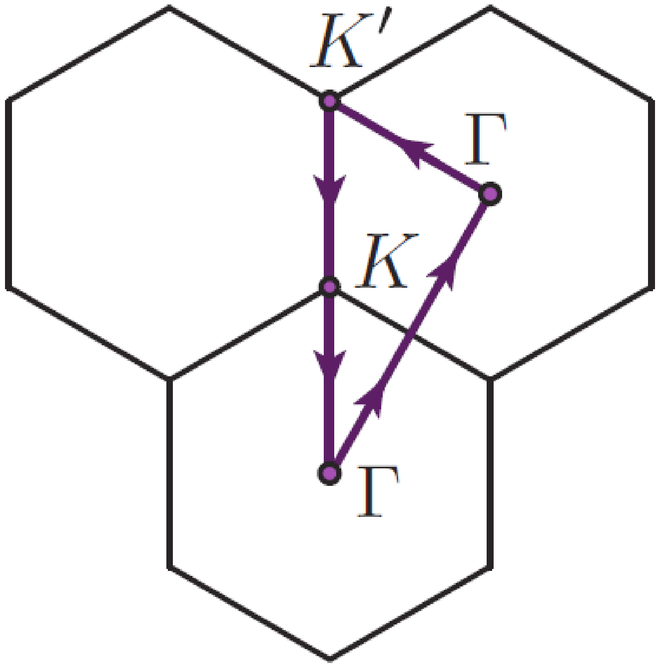
Lopes dos Santos et al PRL (2007)
Bistritzer&MacDonald PNAS (2011)

Effective field theory perspective: L. Balents SciPost Phys. 7, 048 (2019)
Systematic improvement on BM + treatment of arbitrary smooth lattice deformation: OV and Jian Kang 2208.05933, 2208.05953

Energy



moire Brillouin zone



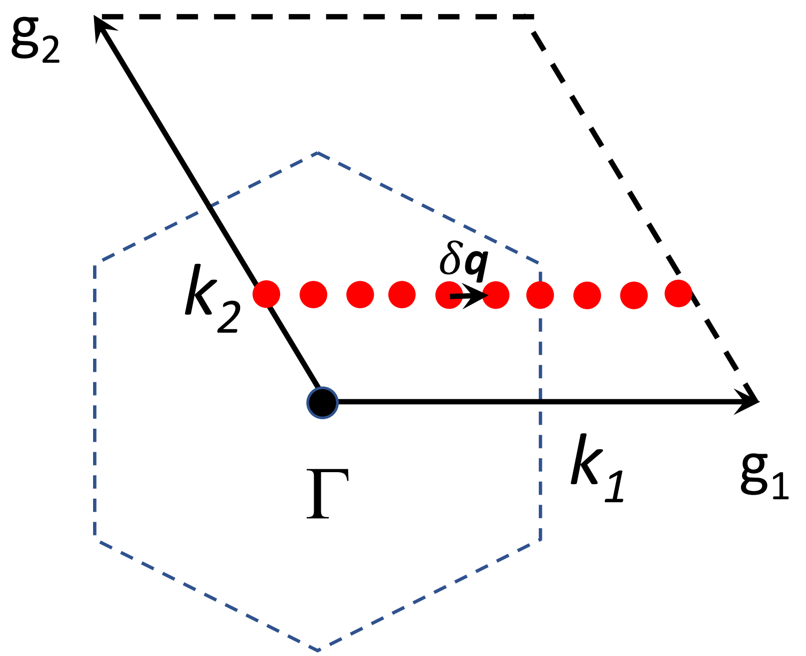
Bistritzer&MacDonald PNAS (2011)

Position operator within the narrow bands:

probing the band topology via the non-Abelian Berry phase

Projected position operator along g_1: $\boxed{\hat{\mathcal{P}} e^{-i\delta\boldsymbol{q}\cdot\boldsymbol{r}} \hat{\mathcal{P}}}$ In the thermodynamic limit: $\delta\boldsymbol{q} \rightarrow 0$

seek eigenstates of the form: $\sum_{b} \sum_{j=0}^{N-1} \alpha_{j,b} \left| k_2 \boldsymbol{g_2} + j\, \delta\boldsymbol{q}, b \right\rangle$



Then, $\Lambda_{bb'}(k_2, j)\, \alpha_{j+1,b'} = \epsilon_{\boldsymbol{k}} \alpha_{j,b}$

where $\Lambda_{bb'}(k_2, j) = \left\langle u_{k_2\boldsymbol{g_2}+j\,\delta\boldsymbol{q},b} \middle| u_{k_2\boldsymbol{g_2}+(j+1)\,\delta\boldsymbol{q},b'} \right\rangle$

and $u_{\boldsymbol{k}\,a}$ is the periodic part of the Bloch function

$$\Lambda(k_2, 0)\Lambda(k_2, 1)\ldots\Lambda(k_2, N-1)\alpha_0 = \epsilon_{\boldsymbol{k}}^N \alpha_0$$

$$\lim_{N\rightarrow\infty} \Lambda(k_2, 0)\Lambda(k_2, 1)\ldots\Lambda(k_2, N-1) = W(k_2)$$

unitary

R. Yu, X. L. Qi, B. A. Bernevig, Z. Fang, and X. Dai, PRB 84, 075119 (2011)

Position operator within the narrow bands:

probing the band topology via the non-Abelian Berry phase

For smooth $|u_{\boldsymbol{k}\,a}\rangle$

anti-Hermitian

$$\lim_{\delta\boldsymbol{q}\to 0}\langle u_{\boldsymbol{k}\,a}|u_{\boldsymbol{k}+\delta\boldsymbol{q},b}\rangle = \delta_{ab} + \langle u_{\boldsymbol{k}\,a}|\nabla_{\boldsymbol{k}}|u_{\boldsymbol{k}\,b}\rangle\cdot\delta\boldsymbol{q}$$

$$= \delta_{ab} - \langle \nabla_{\boldsymbol{k}} u_{\boldsymbol{k}\,a}|u_{\boldsymbol{k}\,b}\rangle\cdot\delta\boldsymbol{q}$$

$$= \delta_{ab} - \langle u_{\boldsymbol{k}\,b}|\nabla_{\boldsymbol{k}}|u_{\boldsymbol{k}\,a}\rangle^{*}\cdot\delta\boldsymbol{q}$$

Hermitian

$$= e^{-i\boldsymbol{A}_{ab}(\boldsymbol{k})\cdot\delta\boldsymbol{q}}$$

unitary

$$W(k_2) = \left[e^{-i\oint \boldsymbol{A}_{ab}(\boldsymbol{k})\cdot d\boldsymbol{k}}\right]_{path\ ordered} \Rightarrow$$

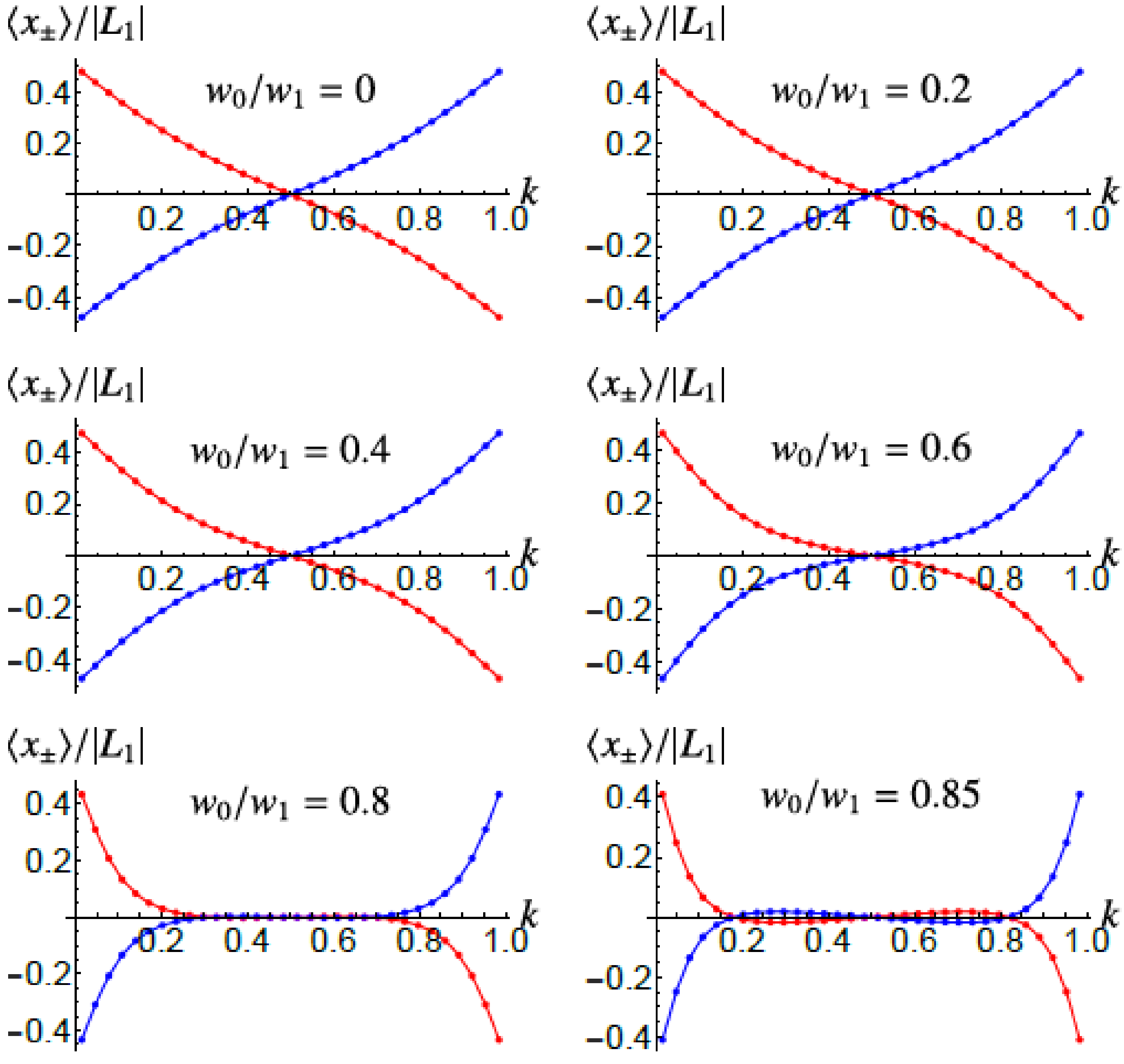
W's eigenvalues can be expressed as $e^{-2\pi i<x_{\pm}/L_m>}$

In practice N is finite and $\Lambda(k_2,\mathrm{j})=\mathrm{U}\Sigma V^{\dagger} \to \mathrm{U}V^{\dagger}$

$$W(k_2) \to \mathrm{U}V^{\dagger}(k_2,0)\mathrm{U}V^{\dagger}(k_2,1)\ldots\mathrm{U}V^{\dagger}(k_2,N-1)$$

A numerical advantage of this method is that W does not depend on the choice of the phase $|u_{\boldsymbol{k}\,a}\rangle$

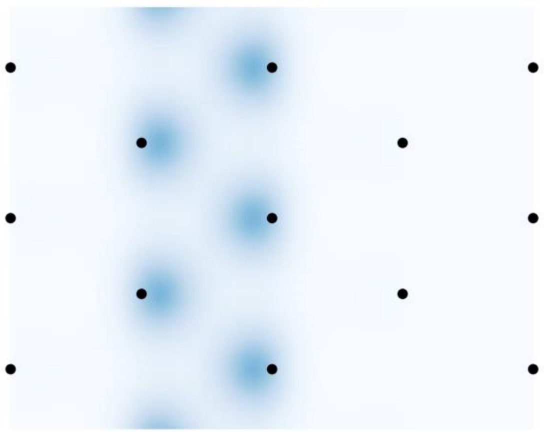
Narrow band ``Wilson loops''

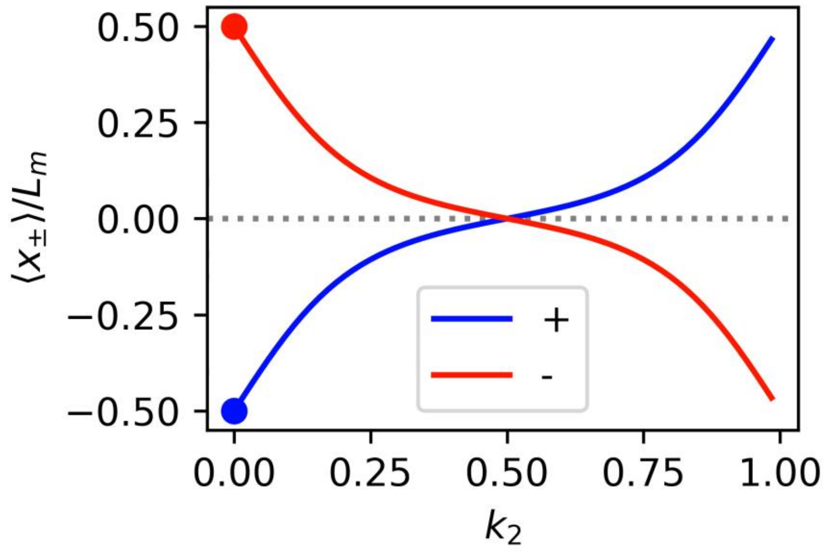


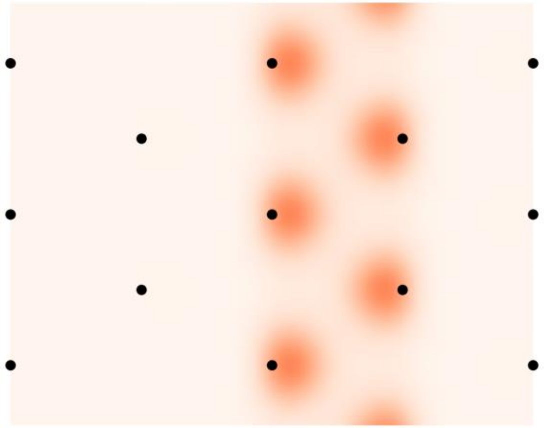
Within each valley the narrow bands are topologically non-trivial (similar to Z_2 TI)

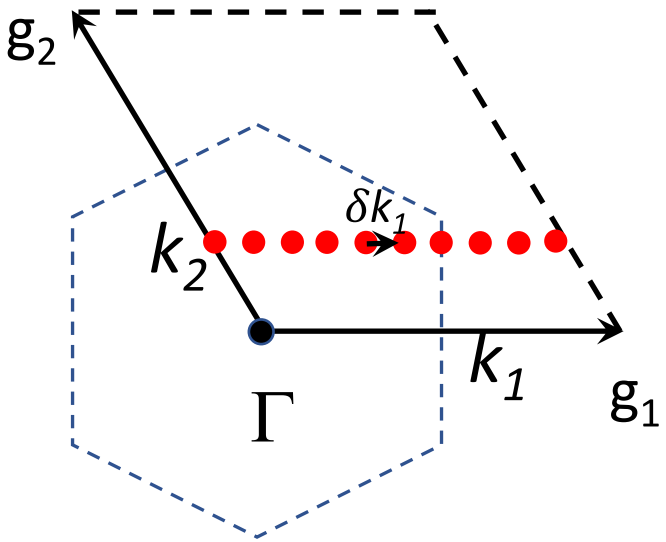
Z. Song et al, PRL 123, 036401 (2019); J. Kang and OV, PRB 102, 035161 (2020)

Band topology and hybrid Wannier states







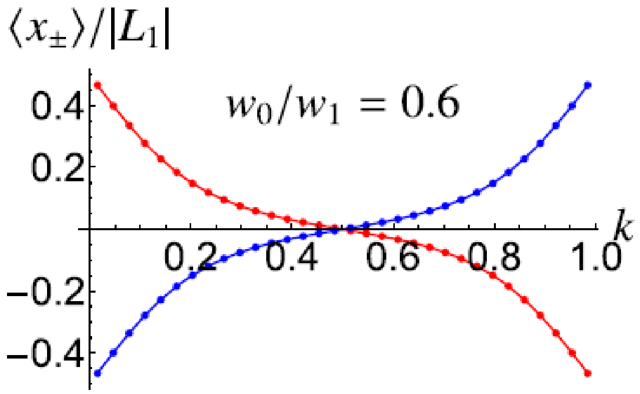


video courtesy Xiaoyu Wang (NHMFL)

Z. Song et al, PRL 123, 036401 (2019); J. Kang and OV PRB 2020

The role of symmetry in TBG band topology

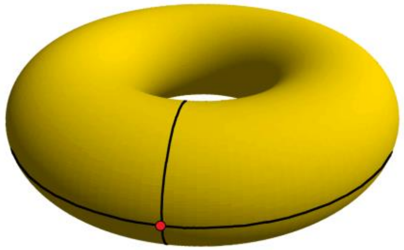
- The reason why the ``Wilson loop'' eigenvalues $\langle x_{\pm} \rangle$ are opposites is the $C_{2z}T$ symmetry of the continuum model. This is because



$$W^*(k_2) = \mathcal{U}\, W(k_2)\, \mathcal{U}^\dagger$$

So, because our eigenvalue of $W(k_2)$ has a non-zero imaginary part, its complex conjugate is also an eigenvalue of $W(k_2)$.

- The reason why the ``Wilson loop'' winds is because the winding number around the two Dirac nodes is the same **and** because the sum of the Berry phases of the two bands along any non-contractable cycle is trivial

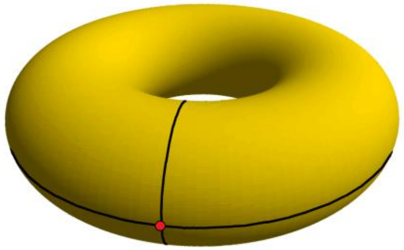


H. C. Po, L. Zou, A. Vishwanath, and T. Senthil, PRX (2018)
J. Ahn, S. Park, and B.-J. Yang, PRX 9, 021013 (2019)
Fang Xie, Zhida Song, Biao Lian, and B. Andrei Bernevig PRL 124, 167002 (2020)

The role of symmetry in TBG band topology

- In general, the $C_{2z}T$ symmetry requires $\det W(k_2) = \pm 1$

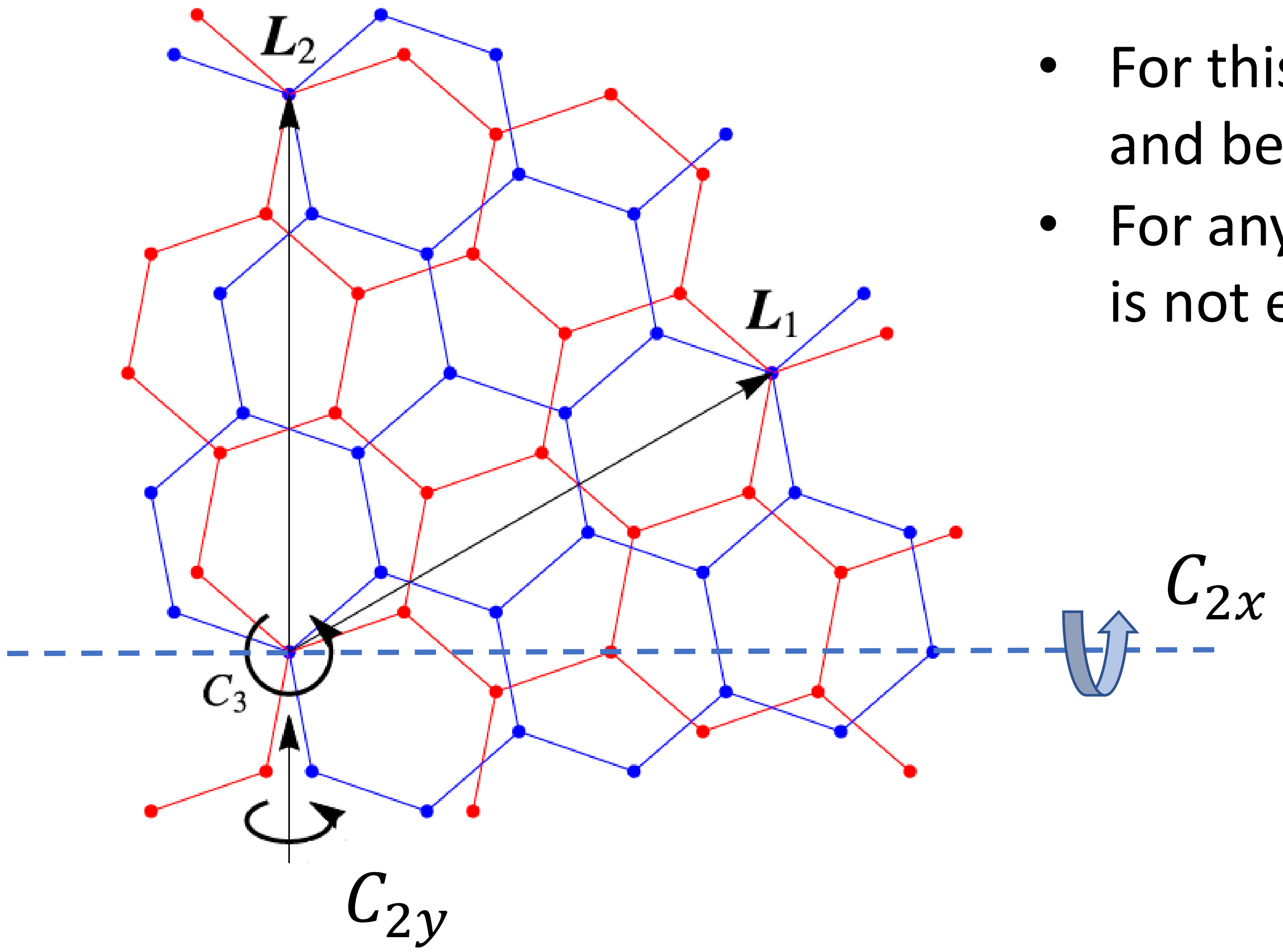
$\det W(k_2) = +1$	$\det W(k_2) = -1$
• the two eigenvalues are complex conjugates of each other	• the two eigenvalues are real and (1,-1) independent of k_2 (i.e. trivial winding) (we find this in the $C_{2z}T$ symmetric period-2 stripe state)



Fang Xie, Zhida Song, Biao Lian, and B. Andrei Bernevig PRL 124, 167002 (2020)
Fang Xie, Jian Kang, B Andrei Bernevig, OV, Nicolas Regnault arXiv:2209.14322

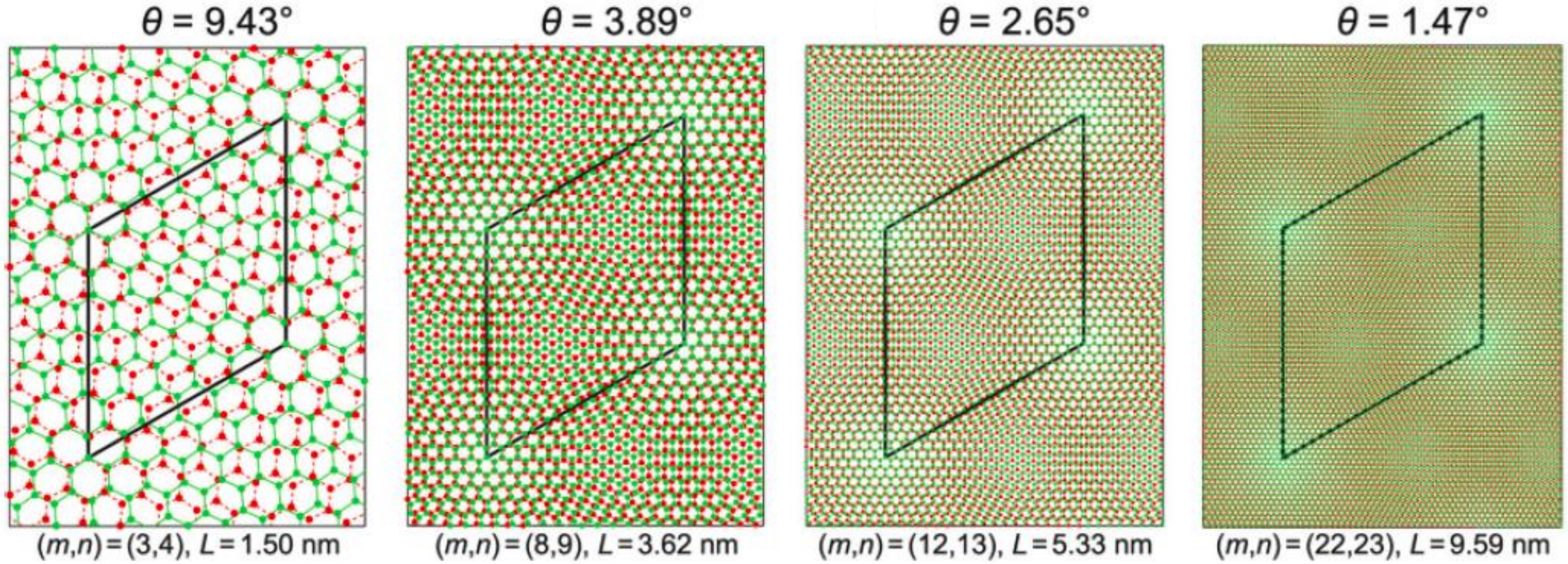
Emergence of symmetries at low twist angle

Example of the so called D_3 structure (graphene layers are twisted about the site)



- For this structure, C_{2x} is not an exact symmetry and because C_{2y} is, neither is $C_{2z}T$
- For any tight-binding model, valley conservation is not exact

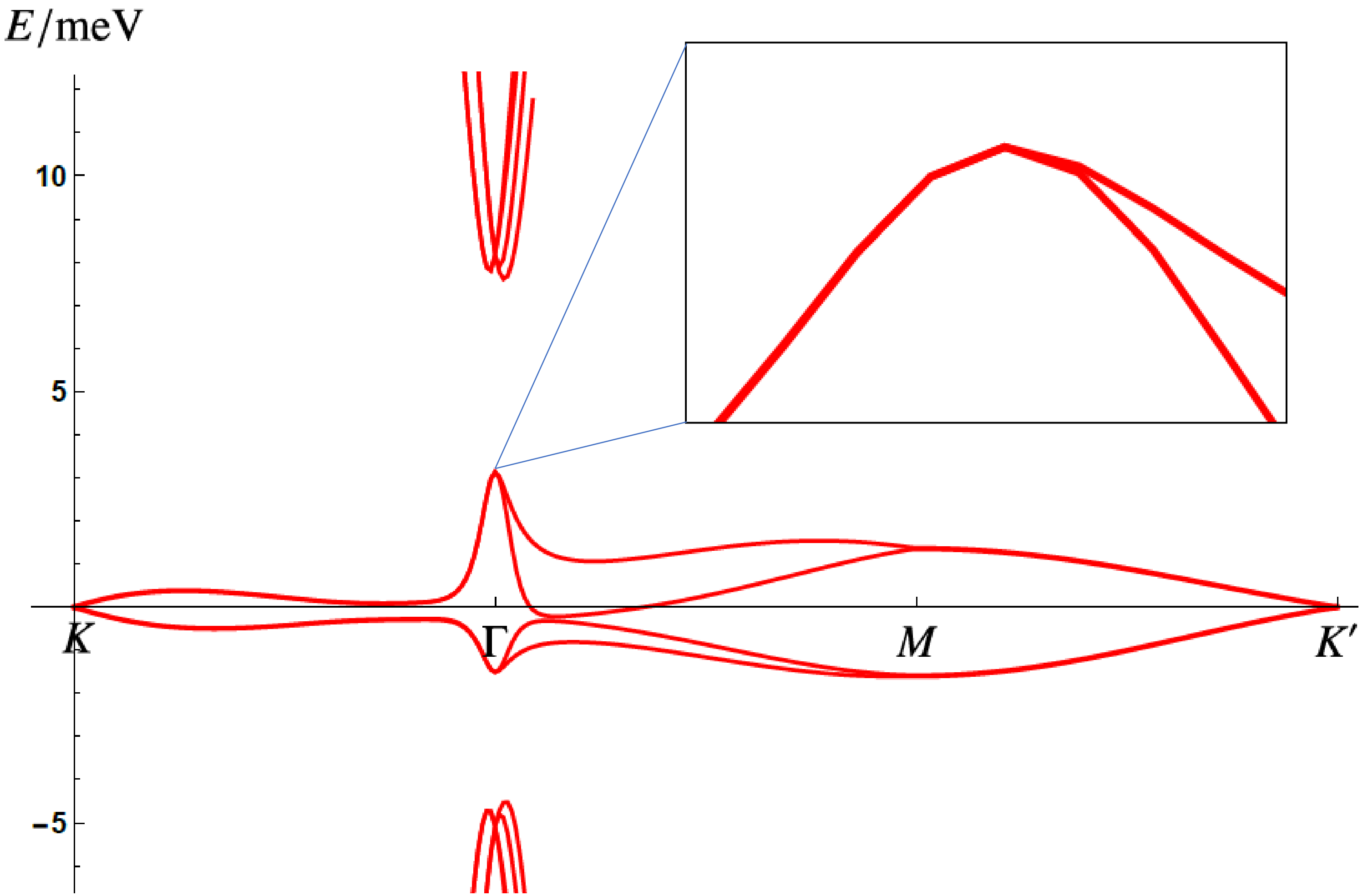
Emergence of symmetries at low twist angle



from Moon and Koshino PRB 85, 195458 (2012)

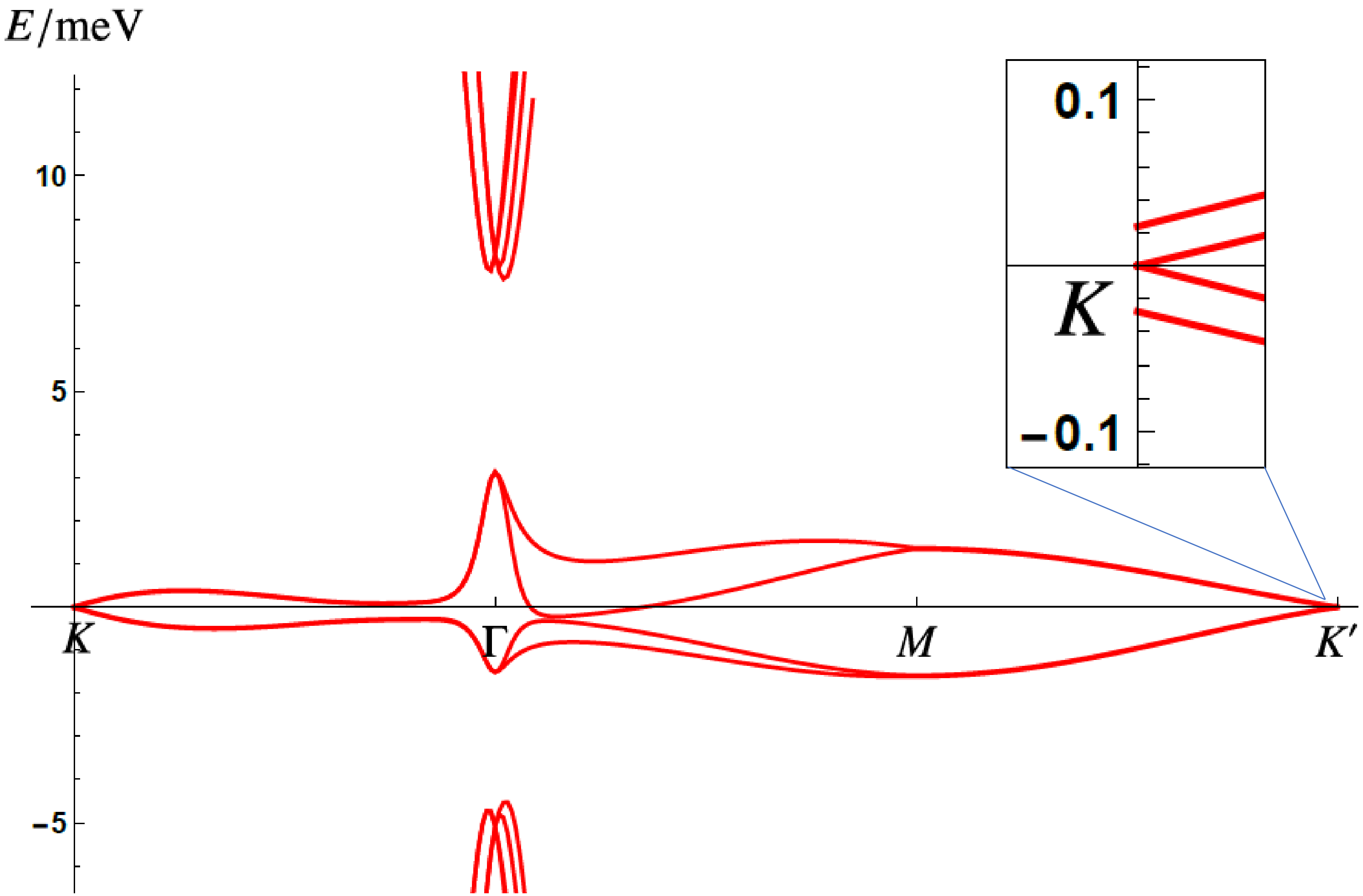
L. Zou, H.C. Po, A. Vishwanath, and T. Senthil PRB **98**, 085435 (2018)

$$(m, n) = (25,26) \qquad (\theta = 1.3^o)$$



Jian Kang and OV PRX 8, 031088 (2018)

$$(m,n) = (25,26) \qquad (\theta = 1.3^o)$$



Jian Kang and OV PRX 8, 031088 (2018)

Electron correlations

$$H_{kin} = \int d\boldsymbol{r}\ \chi_\sigma^\dagger \begin{pmatrix} H_{BM} & 0 \\ 0 & H_{BM}^* \end{pmatrix} \chi_\sigma$$

$$\chi_\sigma(\boldsymbol{r}) = \sum_{n\boldsymbol{k}} \begin{pmatrix} \Psi_{n\boldsymbol{k}}(\boldsymbol{r}) d_{\sigma,\boldsymbol{K},n,\boldsymbol{k}} \\ \Psi_{n\boldsymbol{k}}^*(\boldsymbol{r}) d_{\sigma,\boldsymbol{K}',n,-\boldsymbol{k}-\boldsymbol{q}_1} \end{pmatrix}$$

$$V_{int} = \frac{1}{2}\int d\boldsymbol{r} d\boldsymbol{r}'\, V(\boldsymbol{r}-\boldsymbol{r}')\delta\rho(\boldsymbol{r})\delta\rho(\boldsymbol{r}')$$

$$\delta\rho(\boldsymbol{r}) = \chi_\sigma^\dagger(\boldsymbol{r})\chi_\sigma(\boldsymbol{r}) - \frac{1}{2}\{\chi_\sigma^\dagger(\boldsymbol{r}), \chi_\sigma(\boldsymbol{r})\}$$

$$\frac{1}{2}\{\chi_\sigma^\dagger(\boldsymbol{r}), \chi_\sigma(\boldsymbol{r})\} = \bar{\rho}_{E_c}(\boldsymbol{r}) = 2 \sum_{|\epsilon_{nk}|\leq E_c} \Psi_{n\boldsymbol{k}}^*(\boldsymbol{r})\Psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

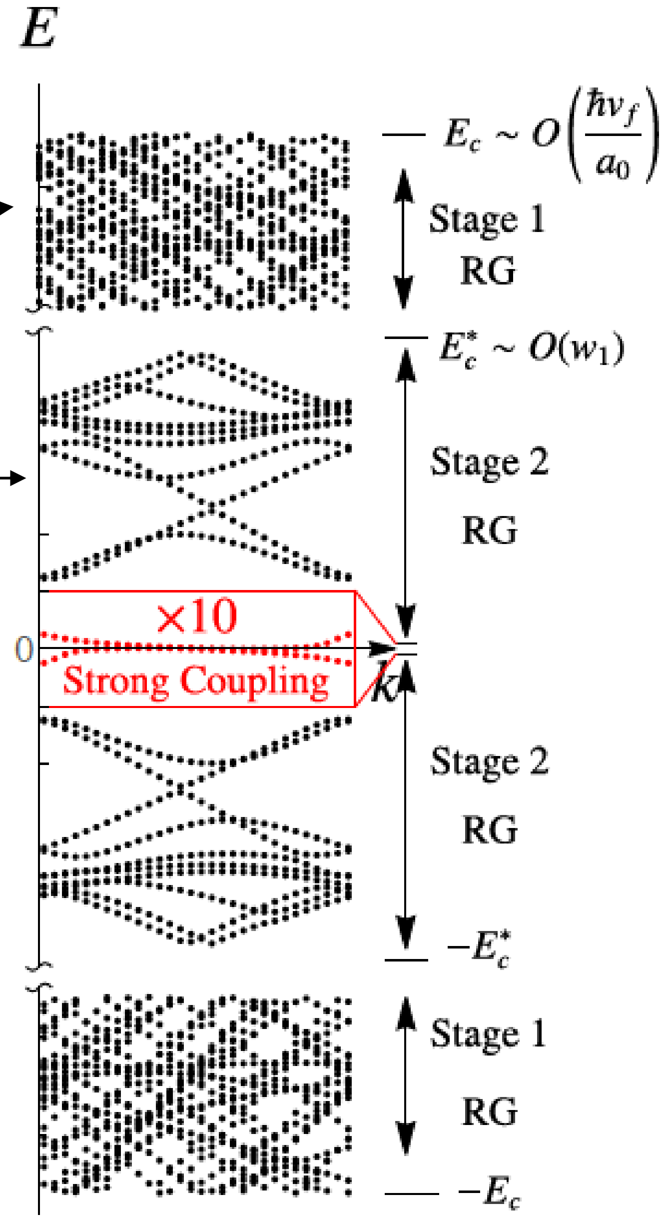
OV and J. Kang PRL2020

Correlated electron physics in the narrow bands: RG perspective

Stage 1:
Coulomb interaction and interlayer tunneling are **perturbative**

Stage 2:
Coulomb interaction **perturbative**, interlayer tunneling **non-perturbative**

Final step:
Coulomb interaction **non-perturbative**: strong coupling



OV and Jian Kang, PRL 125, 257602 (2020)

Coulomb interaction is non-perturbative within the narrow bands: strong coupling

(renormalized) H_{kin} $\ll$ $V_{int} = \frac{1}{2}\int d\boldsymbol{r}d\boldsymbol{r}'\,V(\boldsymbol{r}-\boldsymbol{r}')\delta\rho(\boldsymbol{r})\delta\rho(\boldsymbol{r}')$

Charge neutrality point: any many-body state that is annihilated by $\delta\rho(\boldsymbol{r})$ is a ground state

Even integer filling: ground states are many-body eigenstates of $\delta\rho(\boldsymbol{r})$

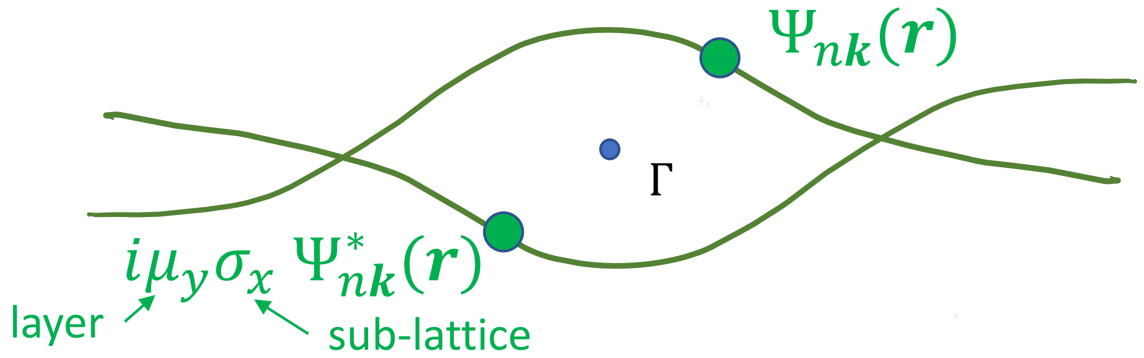
Odd integer filling: if sublattice is perfectly polarized (i.e. chiral limit) Chern states are ground states

Generalized ferromagnets are favored by the projected Coulomb interactions

OV and J. Kang PRL2019,2020; Bultinck et al PRX2020, Bernevig et al 2020TBG series

Spin-valley U(4) symmetry in the strong coupling limit

Particle-hole symmetry:
(Z.Song et.al. PRL2019; Hejazi et.al. PRB2019)



$$\rho(\boldsymbol{r}) = \sum_{\sigma,\boldsymbol{k}\boldsymbol{k}'} \left(d^\dagger_{\sigma,\boldsymbol{K},+,\boldsymbol{k}}\ , d^\dagger_{\sigma,\boldsymbol{K},-,\boldsymbol{k}}\ , d^\dagger_{\sigma,\boldsymbol{K}',+,\boldsymbol{k}}\ , d^\dagger_{\sigma,\boldsymbol{K}',-,\boldsymbol{k}}\right) \begin{pmatrix} A_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) & B_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) & 0 & 0 \\ C_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) & D_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) & 0 & 0 \\ 0 & 0 & D_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) & -C_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) \\ 0 & 0 & -B_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) & A_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{r}) \end{pmatrix} \begin{pmatrix} d_{\sigma,\boldsymbol{K},+,\boldsymbol{k}'} \\ d_{\sigma,\boldsymbol{K},-,\boldsymbol{k}'} \\ d_{\sigma,\boldsymbol{K}',+,\boldsymbol{k}'} \\ d_{\sigma,\boldsymbol{K}',-,\boldsymbol{k}'} \end{pmatrix}$$

commutes with $1,\ \tau_z 1,\ \tau_y\tilde{\sigma}_y,\ \tau_x\tilde{\sigma}_y$

independent spin rotations within each valley

rotations between the valleys!

In the chiral limit B and C vanish and $U(4) \to U(4) \times U(4)$

Bultinck et al PRX 2020, Bernevig et al 2020 TBG series
J. Kang and OV, PRL2019 and OV and J.Kang PRL2020

Coulomb interaction is non-perturbative within the narrow bands: strong coupling

(renormalized) $H_{kin} \ll V_{int} = \frac{1}{2}\int d\boldsymbol{r}d\boldsymbol{r}'\, V(\boldsymbol{r}-\boldsymbol{r}')\delta\rho(\boldsymbol{r})\delta\rho(\boldsymbol{r}')$

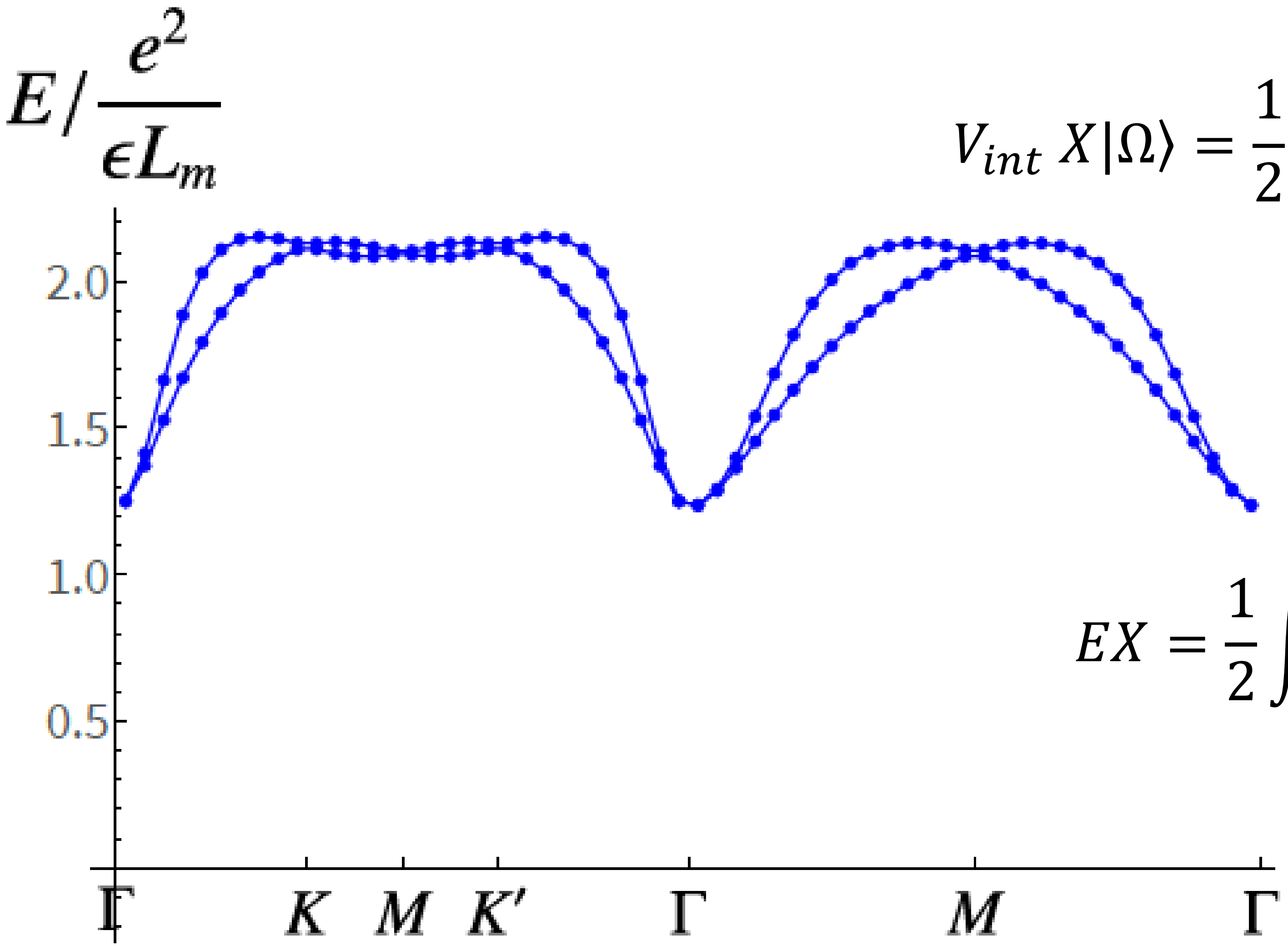
Charge neutrality point: any many-body state that is annihilated by $\delta\rho(\boldsymbol{r})$ is a ground state

Valley polarized state is annihilated by $\delta\rho(\boldsymbol{r}) \Rightarrow$ it is a ground state

Any state that can be obtained from the valley polarized state by the spin-valley $U(4)$ rotation is also a ground state

OV and J. Kang PRL2019,2020; Bultinck et al PRX2020, Bernevig et al 2020TBG series

Exact single particle excitation spectrum at CNP in the strong coupling limit: Bloch basis after RG

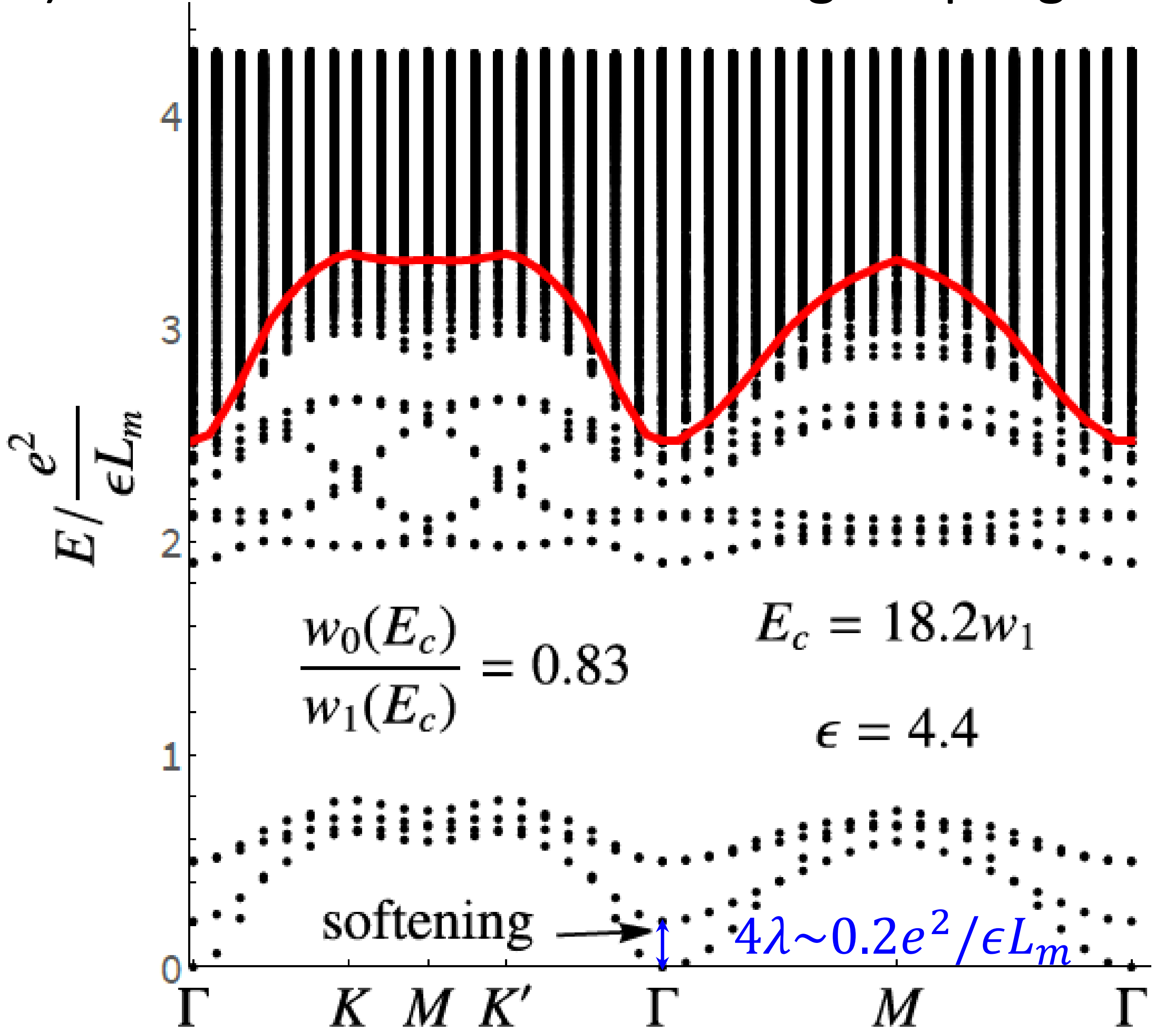


$$V_{int}\, X|\Omega\rangle = \frac{1}{2}\int dr\, dr' V(r-r')\big[\delta\varrho(r),[\delta\varrho(r'),X]\big]|\Omega\rangle$$

$$EX = \frac{1}{2}\int dr\, dr' V(r-r')\big[\delta\varrho(r),[\delta\varrho(r'),X]\big]$$

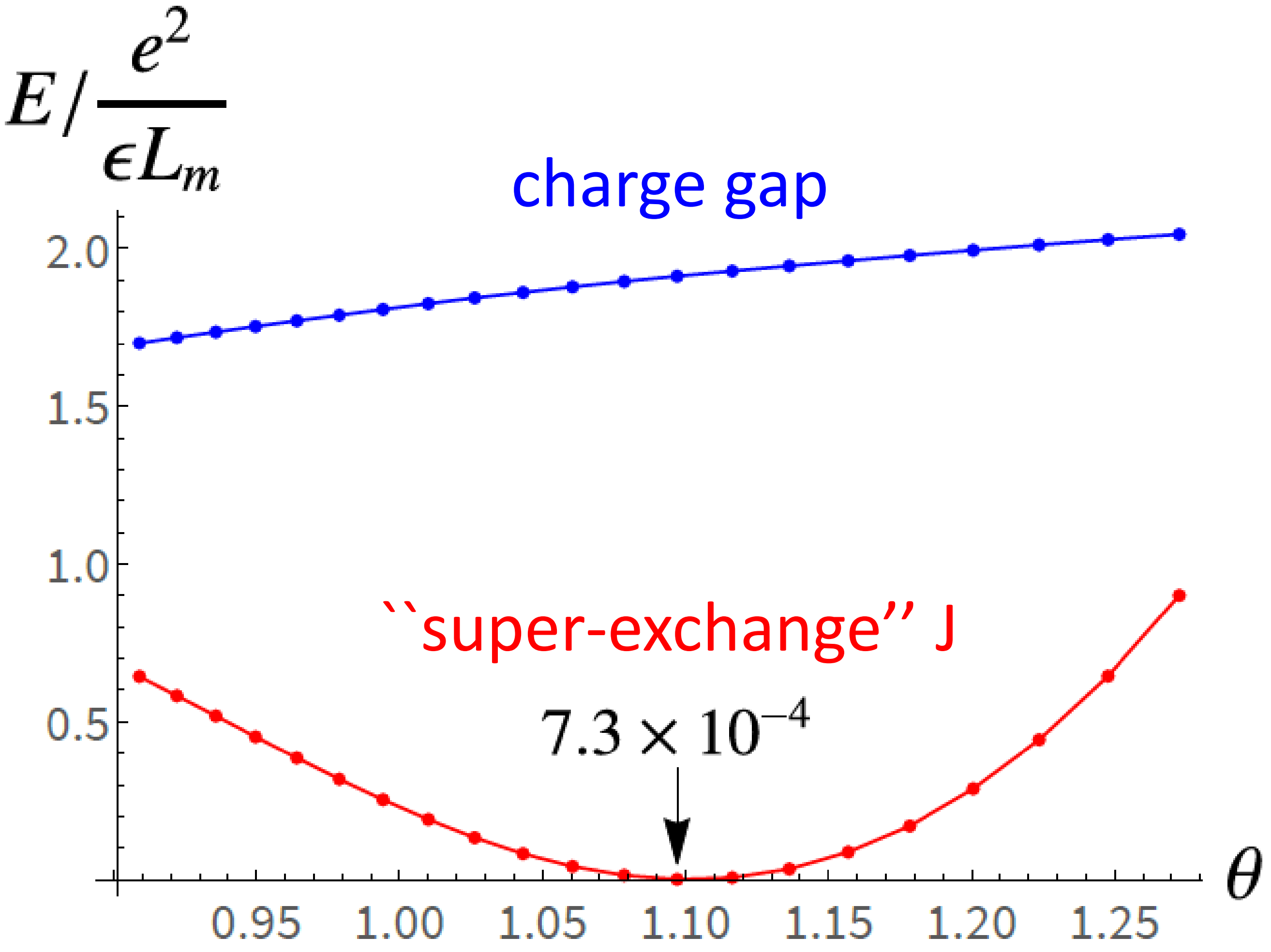
OV and Jian Kang, PRL 2020 (see also Andrei Bernevig et al TBG series)

Exact (neutral) collective modes in the strong coupling limit: Bloch basis after RG



OV and Jian Kang, PRL 2020

Justification for the strong coupling approach



Jian Kang and OV (unpublished)

Exact single particle excitation spectrum at integer filling in the strong coupling: chiral limit ${}^{w_0}/_{w_1} = 0$

$$\left(E - E_v^{(0)}\right) X|\Omega_v\rangle$$

$$= \frac{1}{2}\int d\boldsymbol{r}\, d\boldsymbol{r}' V(\boldsymbol{r}-\boldsymbol{r}')\big[\delta\varrho(\boldsymbol{r}), [\delta\varrho(\boldsymbol{r}'), X]\big]|\Omega_v\rangle + \int d\boldsymbol{r}\, d\boldsymbol{r}' V(\boldsymbol{r}-\boldsymbol{r}')[\delta\varrho(\boldsymbol{r}), X\,]\delta\bar{\varrho}_v(\boldsymbol{r}')|\Omega_v\rangle$$

In the chiral limit this matrix is diagonal in n,m due to CC_2T

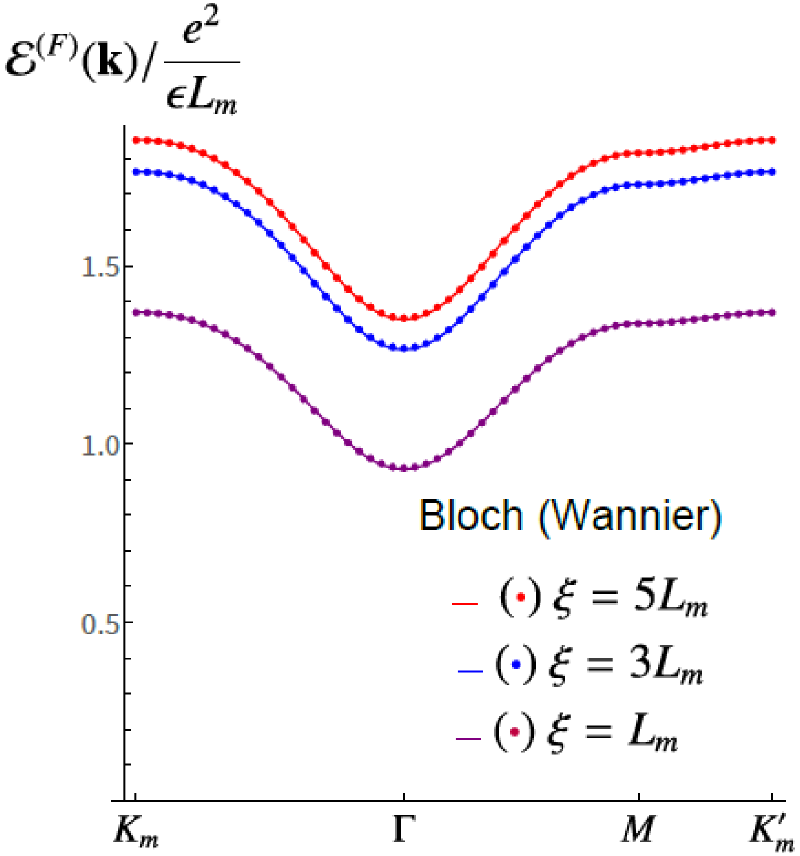
$$\delta\bar{\varrho}_v(\boldsymbol{r}) = \frac{v}{2}\sum_{k}\sum_{n=\pm}\Psi^{\dagger}_{n\boldsymbol{k}}(\boldsymbol{r})\Psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

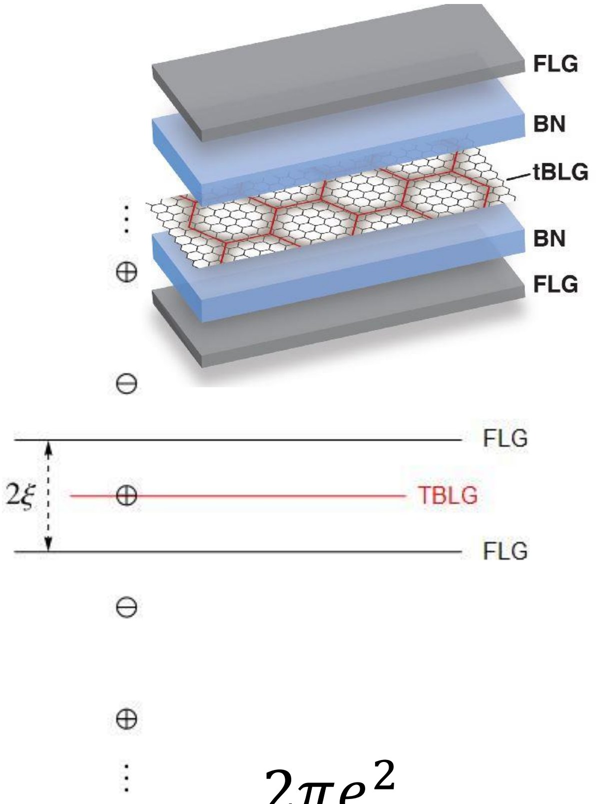
$$\boxed{\begin{aligned}&\frac{1}{2}\int d\boldsymbol{r}\, d\boldsymbol{r}' V(\boldsymbol{r}-\boldsymbol{r}')\sum_{m'\boldsymbol{p}'}\Psi^{\dagger}_{n\boldsymbol{k}}(\boldsymbol{r})\Psi_{m'\boldsymbol{p}'}(\boldsymbol{r})\Psi^{\dagger}_{m'\boldsymbol{p}'}(\boldsymbol{r}')\Psi_{m\boldsymbol{k}}(\boldsymbol{r}')\\ &\mp\frac{v}{2}\int d\boldsymbol{r}\, d\boldsymbol{r}' V(\boldsymbol{r}-\boldsymbol{r}')\sum_{m'\boldsymbol{p}'}\Psi^{\dagger}_{m'\boldsymbol{p}'}(\boldsymbol{r})\Psi_{m'\boldsymbol{p}'}(\boldsymbol{r})\Psi^{\dagger}_{n\boldsymbol{k}}(\boldsymbol{r}')\Psi_{m\boldsymbol{k}}(\boldsymbol{r}')\end{aligned}}$$

OV and Jian Kang 104, 075143 (2021)

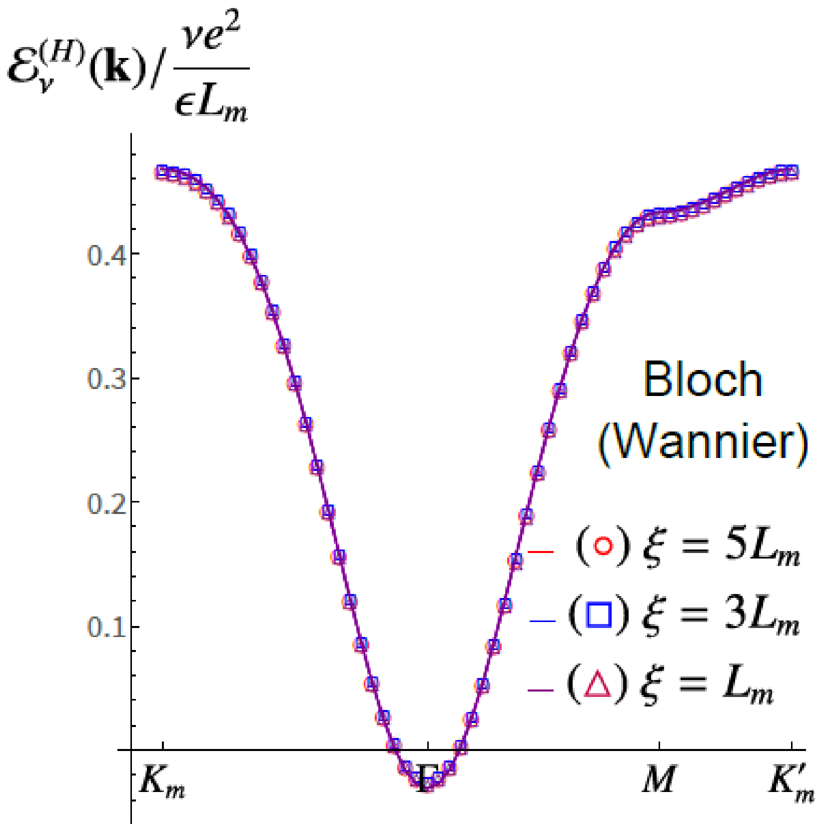
Exact single particle excitation spectrum at integer filling in the strong coupling: chiral limit ${}^{w_0}/_{w_1} = 0$

$$\mathcal{E}^{hole}(\boldsymbol{k}) = \mathcal{E}^{(F)}(\boldsymbol{k}) - \mathcal{E}_\nu^{(H)}(\boldsymbol{k}) \qquad \mathcal{E}^{particle}(\boldsymbol{k}) = \mathcal{E}^{(F)}(\boldsymbol{k}) + \mathcal{E}_\nu^{(H)}(\boldsymbol{k})$$





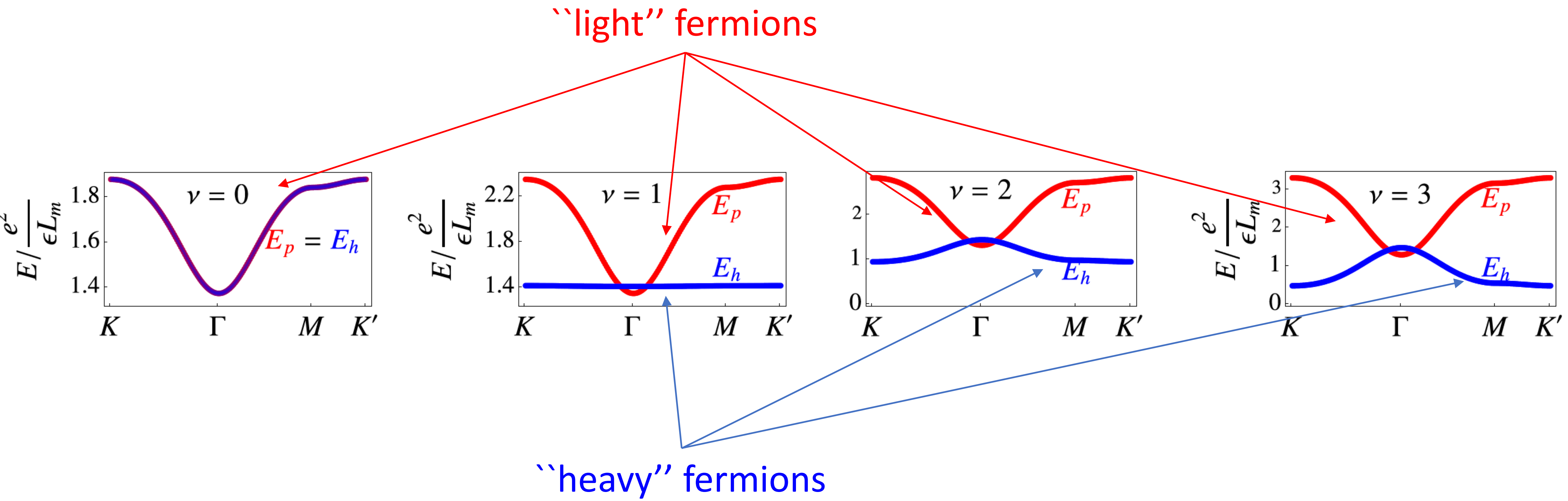
$$V_q = \frac{2\pi e^2}{\epsilon q} tanh(q\xi)$$



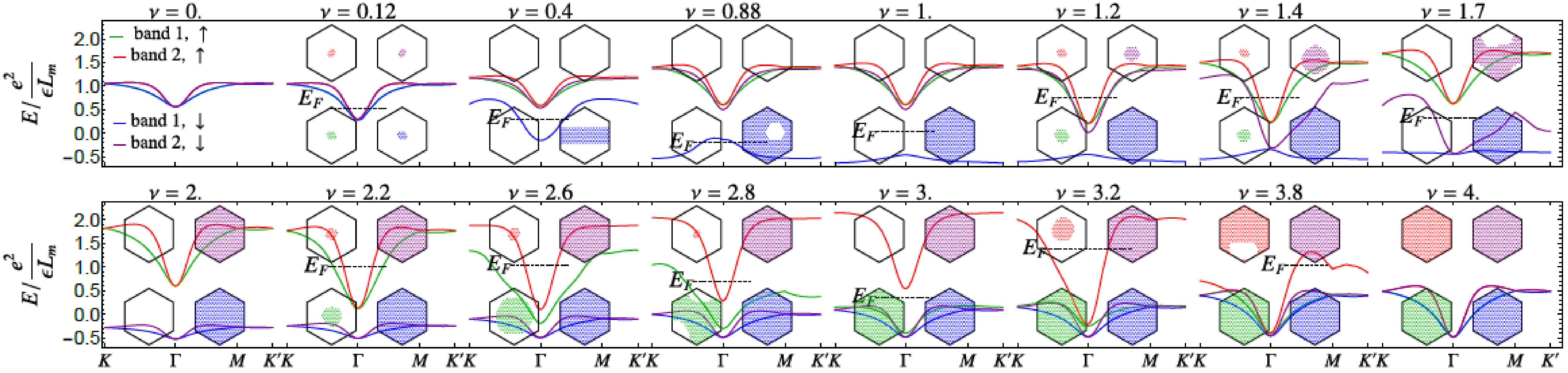
OV and Jian Kang 104, 075143 (2021)

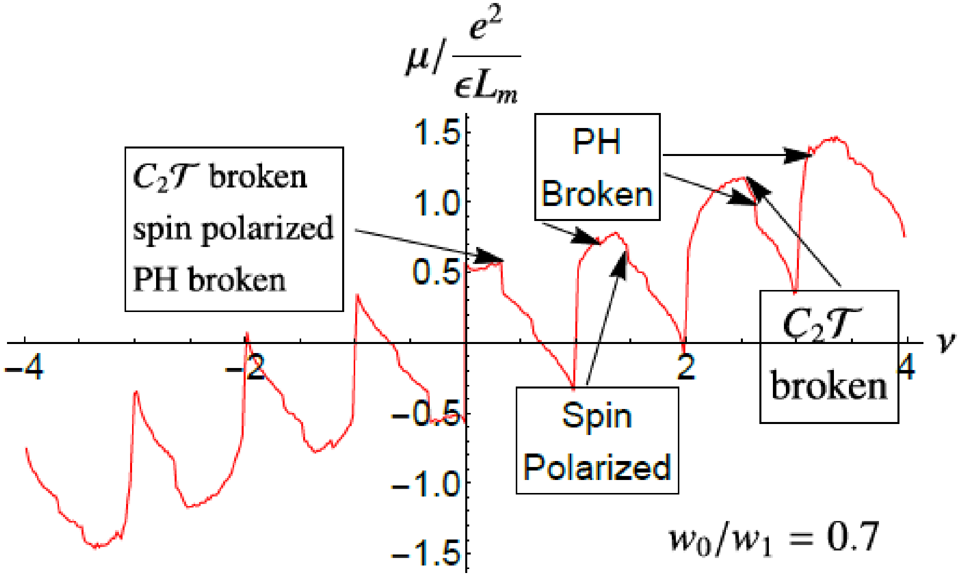
Exact single particle excitation spectrum at integer filling in the strong coupling: chiral limit $w_0/w_1 = 0$

$$\mathcal{E}^{hole}(\boldsymbol{k}) = \mathcal{E}^{(F)}(\boldsymbol{k}) - \mathcal{E}_\nu^{(H)}(\boldsymbol{k}) \qquad \mathcal{E}^{particle}(\boldsymbol{k}) = \mathcal{E}^{(F)}(\boldsymbol{k}) + \mathcal{E}_\nu^{(H)}(\boldsymbol{k})$$



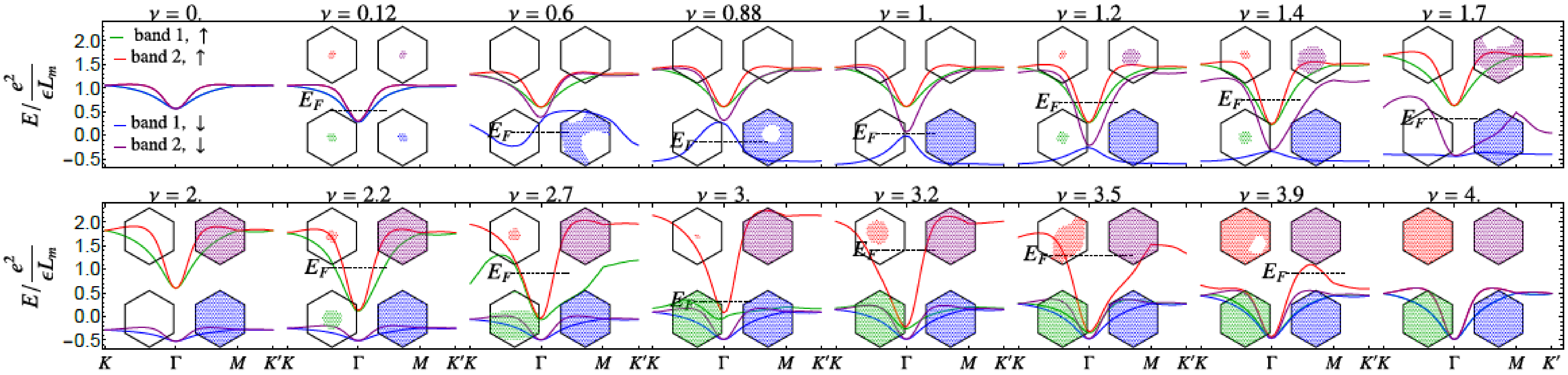
Interpolating between the integer filling using (uniform) Hartree-Fock

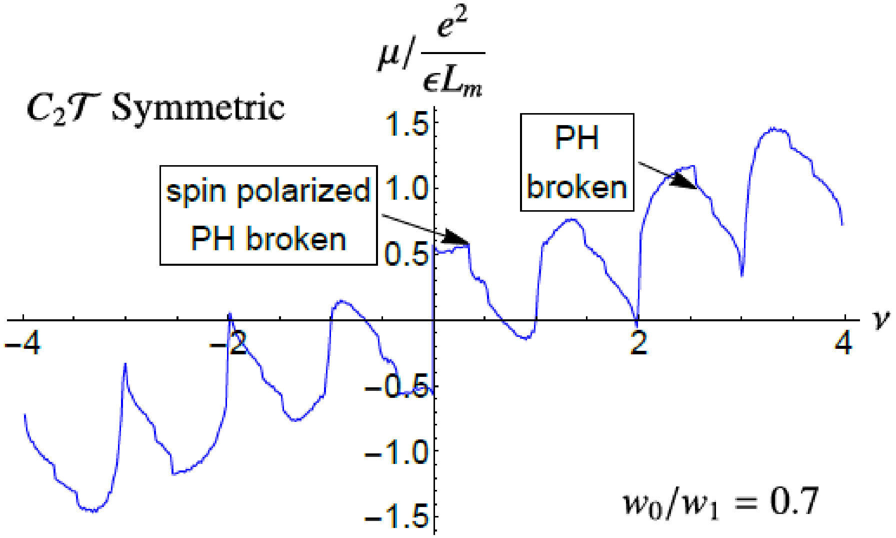




J.Kang, B.A. Bernevig and OV PRL 127, 266402 (2021)

Interpolating between the integer filling using (uniform) Hartree-Fock





J.Kang, B.A. Bernevig and OV PRL 127, 266402 (2021)