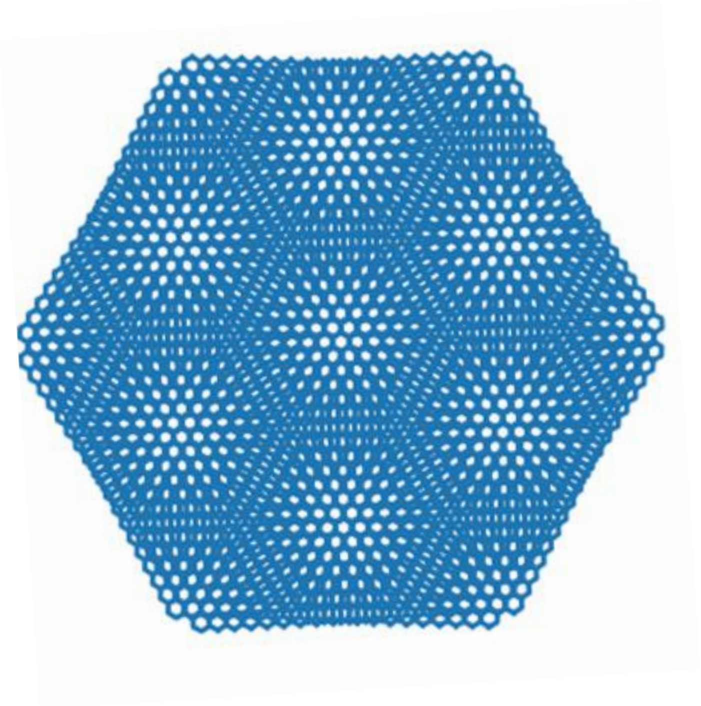
Lecture 2.2: Topological Moire Bands

吴冯成
武汉大学

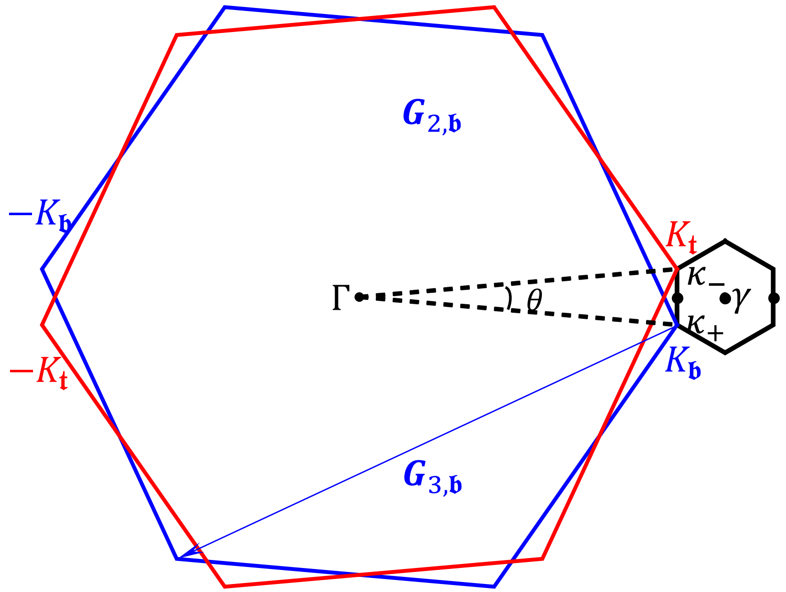
wufcheng@whu.edu.cn

2026.7.6

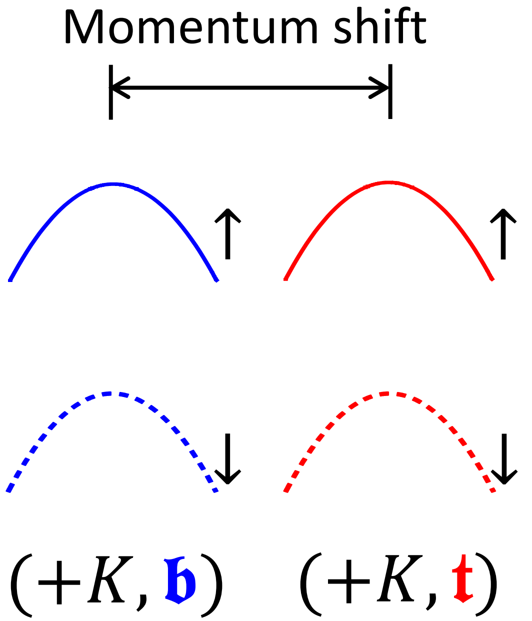
Moiré Hamiltonian



Twisted homobilayer in *AA* stacking



Momentum space

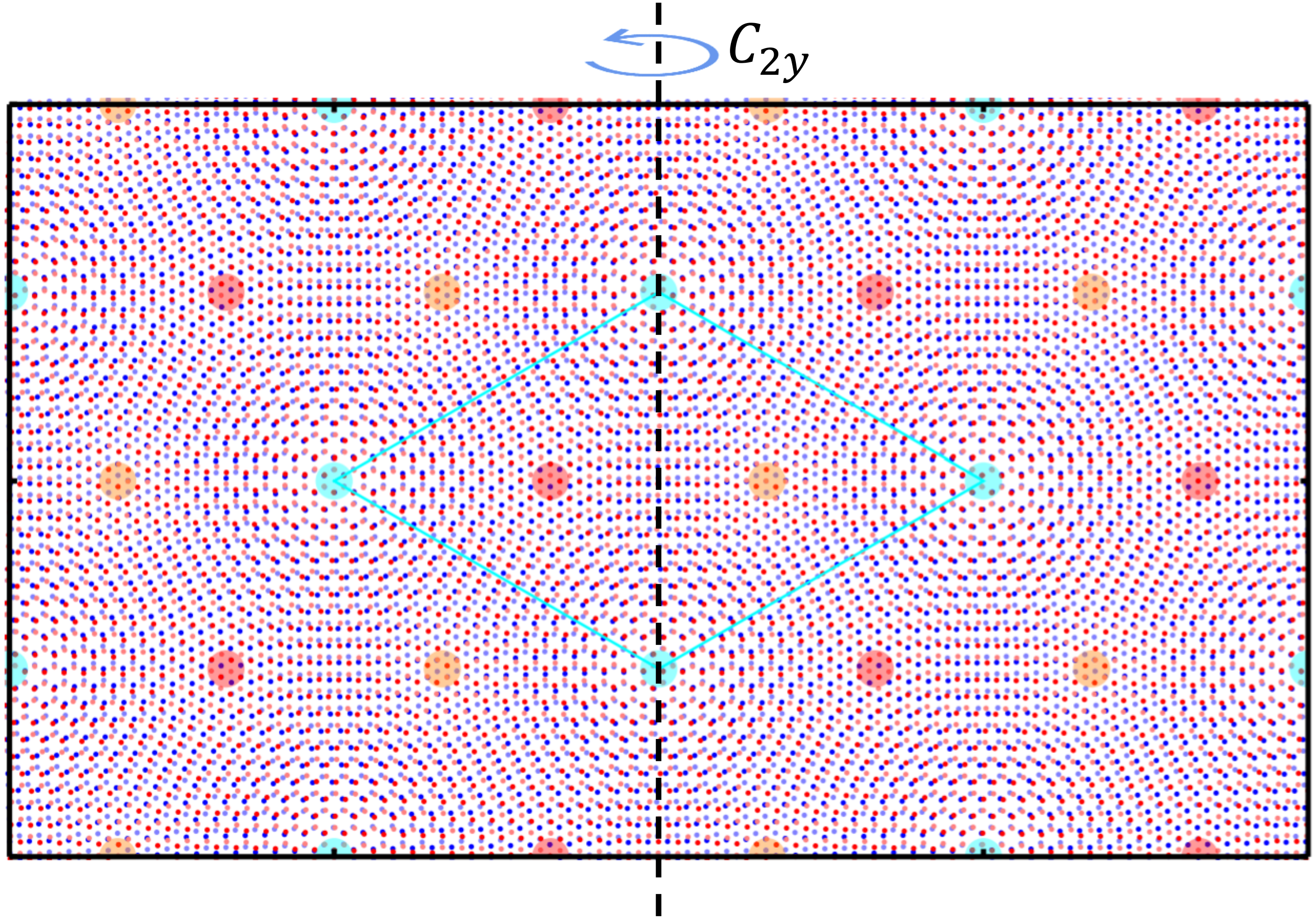


Schematic band structure

$$\mathcal{H}_\uparrow = \begin{pmatrix} -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_+(\boldsymbol{r}) & \Delta_{\mathrm{T}}(\boldsymbol{r}) \\ \Delta_{\mathrm{T}}^\dagger(\boldsymbol{r}) & -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_-(\boldsymbol{r}) \end{pmatrix}$$

F. Wu, T. Lovorn, E. Tutuc, I. Martin, A. H. MacDonald, PRL **122**, 086402 (2019)

Moiré Hamiltonian



D_3 point group: C_{3z}, C_{2y}

- Moiré Hamiltonian:

$$\mathcal{H}_\uparrow = \begin{pmatrix} -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_+(\boldsymbol{r}) & \Delta_{\mathrm{T}}(\boldsymbol{r}) \\ \Delta_{\mathrm{T}}^\dagger(\boldsymbol{r}) & -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_-(\boldsymbol{r}) \end{pmatrix}$$

$$\Delta_{\mathrm{T}}(\boldsymbol{r}) = w(1 + e^{-i\boldsymbol{b}_2\cdot\boldsymbol{r}} + e^{-i\boldsymbol{b}_3\cdot\boldsymbol{r}})$$

$$\Delta_\pm(\boldsymbol{r}) = 2V \sum_{j=1,3,5} \cos(\boldsymbol{b}_j \cdot \boldsymbol{r} \pm \psi)$$

$$\Delta_+(x,y) = \Delta_-(-x,y)$$

- Model Parameters:

a_M, m^*, V, ψ, w

Layer Pseudospin Skyrmions

Moiré Hamiltonian:

$$\mathcal{H}_\uparrow = \begin{pmatrix} -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_+(\boldsymbol{r}) & \Delta_\mathrm{T}(\boldsymbol{r}) \\ \Delta_\mathrm{T}^\dagger(\boldsymbol{r}) & -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_-(\boldsymbol{r}) \end{pmatrix}$$

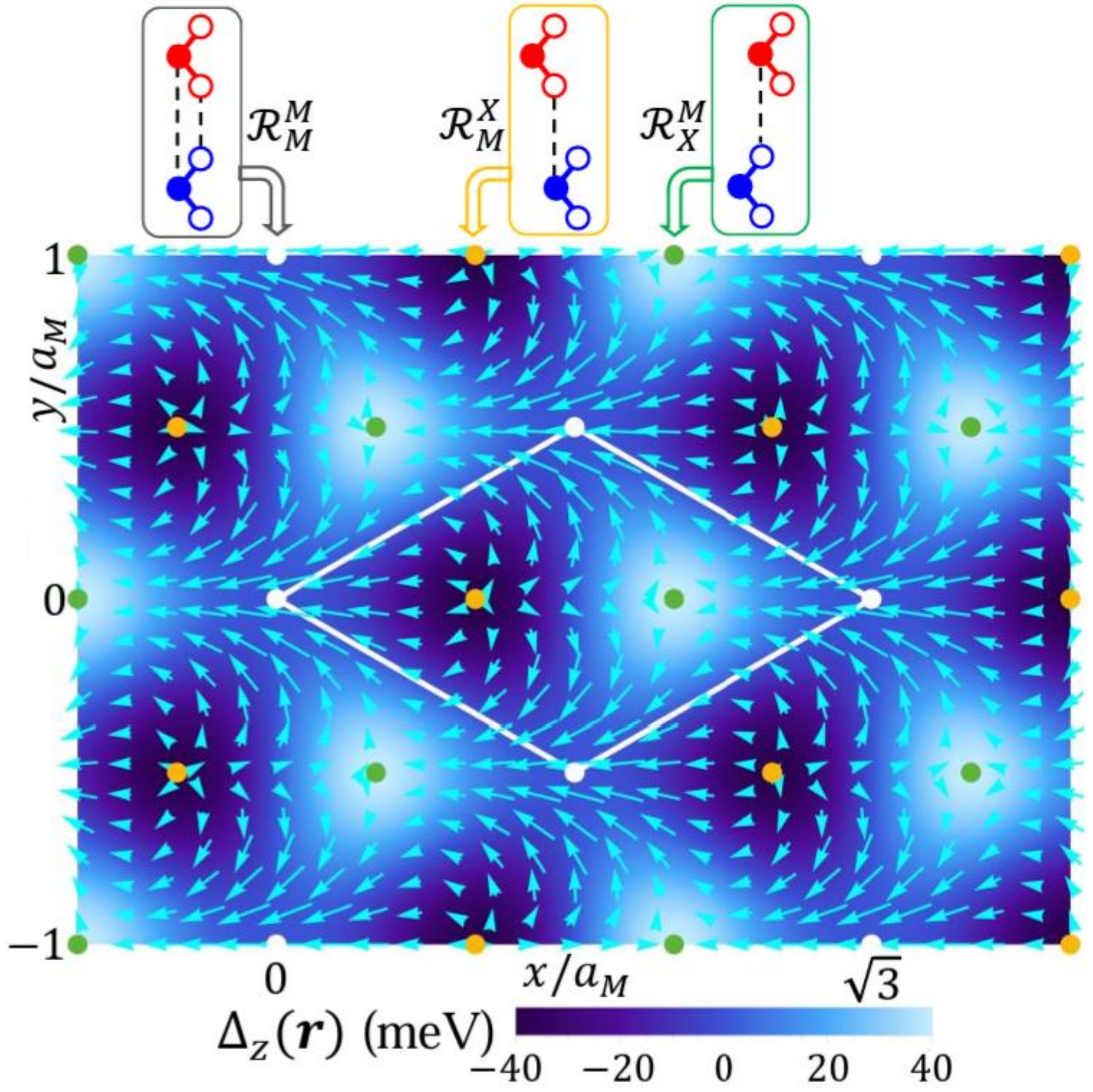
- **Layer pseudospin magnetic field:**

$$\boldsymbol{\Delta}(\boldsymbol{r}) = \left(\mathrm{Re}\Delta_\mathrm{T}^\dagger, \mathrm{Im}\Delta_\mathrm{T}^\dagger, \frac{\Delta_+ - \Delta_-}{2}\right)$$

- **Layer pseudospin skyrmions:**

$$N_w \equiv \frac{1}{4\pi}\int_\mathrm{MUC} d\boldsymbol{r}\frac{\boldsymbol{\Delta}\cdot(\partial_x\boldsymbol{\Delta}\times\partial_y\boldsymbol{\Delta})}{|\boldsymbol{\Delta}|^3}$$

$$= \begin{cases} +1, & V\sin\psi > 0 \\ -1, & V\sin\psi < 0. \end{cases}$$



Bloch Theorem & Plane-Wave Expansion

- Bloch Theorem

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{n\mathbf{k}}(\mathbf{r})$$

$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

- Plane Wave Expansion

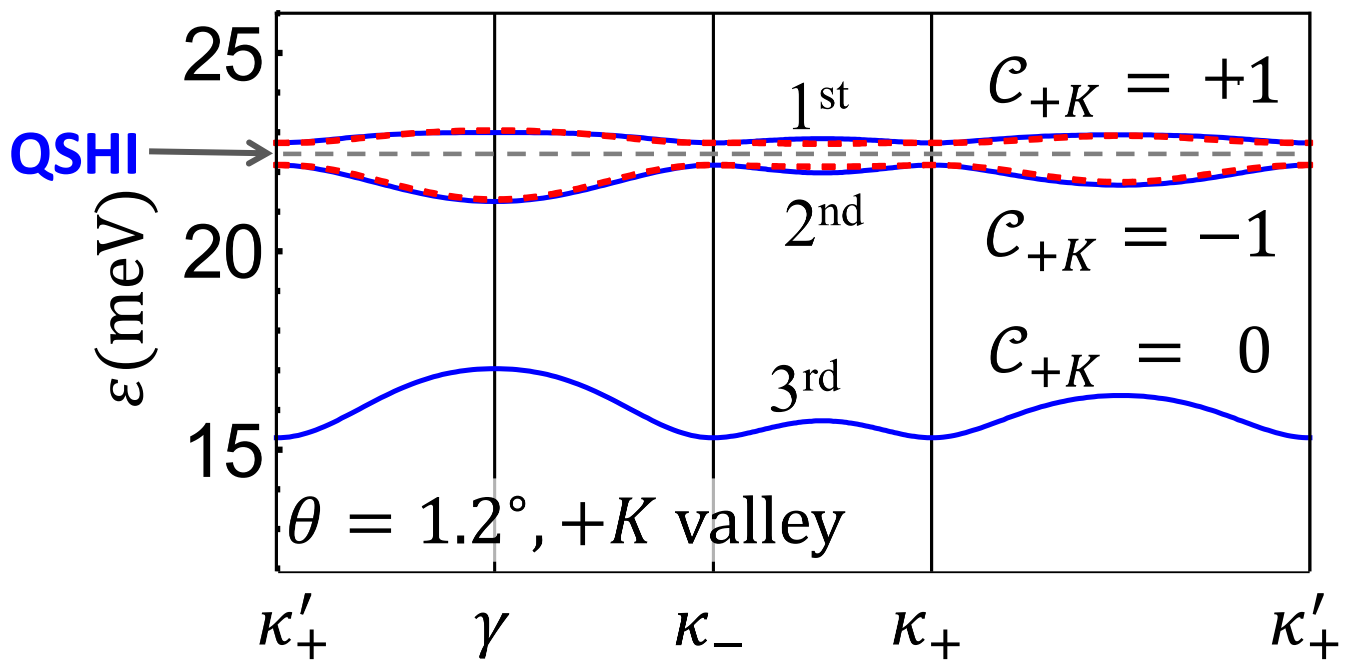
$$u_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{A}}\sum_{\mathbf{G}} c^{n}_{\mathbf{k}+\mathbf{G}}\, e^{i\mathbf{G}\cdot\mathbf{r}}$$

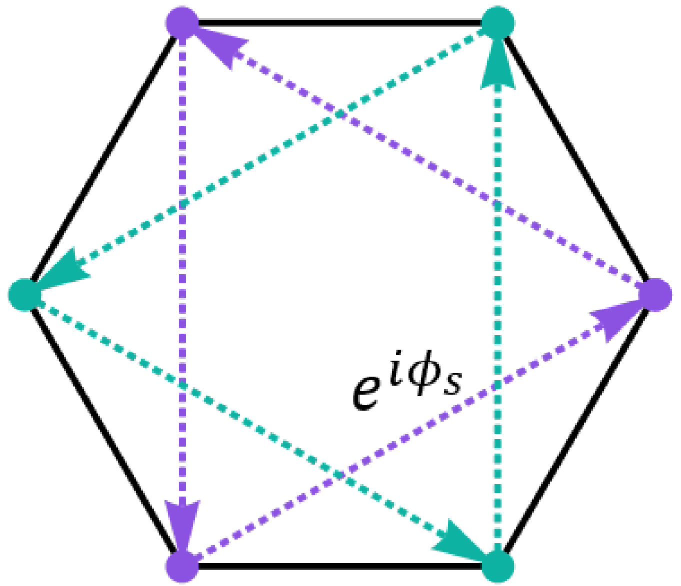
- Matrix Eigenvalue Problem

$$\sum_{\mathbf{G}'} H_{\mathbf{G},\mathbf{G}'}(\mathbf{k})\, c^{n}_{\mathbf{k}+\mathbf{G}'} = E_n(\mathbf{k})\, c^{n}_{\mathbf{k}+\mathbf{G}}$$

In $tMoTe_2$, the wave function is a 2-component spinor at each k.

Kane-Mele Model





- In "local stacking" approximation, $V \approx 8$ meV, $\psi \approx -89.6°$, $w \approx -8.5$ meV for *t*MoTe2.
- Kane-Mele model (Haldane Model in one valley; valley ⬄ spin)

$$H_{\rm TB} = \sum_{\ell,s} \sum_{\boldsymbol{R}\boldsymbol{R}'}^{\prime} t_0\, c^\dagger_{\boldsymbol{R}\ell s} c_{\boldsymbol{R}'(-\ell)s} + \sum_{\ell,s} \sum_{\boldsymbol{R}} \sum_{\boldsymbol{a}_M}^{\prime} t_1 \mathrm{Exp}[i\ s\ \boldsymbol{\kappa}_\ell \cdot \boldsymbol{a}_M]\ c^\dagger_{(\boldsymbol{R}+\boldsymbol{a}_M)\ell s} c_{\boldsymbol{R}\ell s}$$

F. Wu, T. Lovorn, E. Tutuc, I. Martin, A. H. MacDonald, PRL **122**, 086402 (2019)

Quantum Geometry

- Overlap expansion:

$$\begin{aligned}&\langle u_{\boldsymbol{k}-\boldsymbol{p}/2}|u_{\boldsymbol{k}+\boldsymbol{p}/2}\rangle\\ \approx&1+ip_\alpha\mathcal{A}_\alpha(\boldsymbol{k})-\frac{1}{2}p_\alpha p_\beta\mathrm{Re}[\langle\partial_{k_\alpha}u_{\boldsymbol{k}}|\partial_{k_\beta}u_{\boldsymbol{k}}\rangle]\\ \approx&\exp[ip_\alpha\mathcal{A}_\alpha(\boldsymbol{k})-\frac{1}{2}\hat{g}_{\alpha\beta}(\boldsymbol{k})p_\alpha p_\beta],\end{aligned}$$

- Berry Connection $\mathcal{A}_\alpha(\boldsymbol{k})=-i\langle u_{\boldsymbol{k}}|\partial_{k_\alpha}|u_{\boldsymbol{k}}\rangle$

- Berry Curvature $\Omega_{\boldsymbol{k}}=\partial_{k_x}\mathcal{A}_y(\boldsymbol{k})-\partial_{k_y}\mathcal{A}_x(\boldsymbol{k})$

- Quantum Metric $\hat{g}_{\alpha\beta}(\boldsymbol{k})=\mathrm{Re}[\langle\partial_{k_\alpha}u_{\boldsymbol{k}}|\partial_{k_\beta}u_{\boldsymbol{k}}\rangle]-\mathcal{A}_\alpha(\boldsymbol{k})\mathcal{A}_\beta(\boldsymbol{k})$

- Quantum Geometry Tensor:

$$\begin{aligned}\hat{\Lambda}_{\alpha\beta}(\boldsymbol{k})&=\langle\partial_{k_\alpha}u_{\boldsymbol{k}}|\partial_{k_\beta}u_{\boldsymbol{k}}\rangle-\mathcal{A}_\alpha(\boldsymbol{k})\mathcal{A}_\beta(\boldsymbol{k})\\&=\langle\partial_{k_\alpha}u_{\boldsymbol{k}}|(\hat{I}-\hat{P}_{\boldsymbol{k}})|\partial_{k_\beta}u_{\boldsymbol{k}}\rangle\\&=\hat{g}_{\alpha\beta}(\boldsymbol{k})+\frac{i}{2}\epsilon_{\alpha\beta}\Omega_{\boldsymbol{k}}\end{aligned}$$

Quantum Geometry

$$\hat{\Lambda}_{\alpha\beta}(\boldsymbol{k}) = \langle \partial_{k_\alpha} u_{\boldsymbol{k}} | \partial_{k_\beta} u_{\boldsymbol{k}} \rangle - \mathcal{A}_\alpha(\boldsymbol{k}) \mathcal{A}_\beta(\boldsymbol{k})$$
$$= \langle \partial_{k_\alpha} u_{\boldsymbol{k}} | (\hat{I} - \hat{P}_{\boldsymbol{k}}) | \partial_{k_\beta} u_{\boldsymbol{k}} \rangle$$
$$= \hat{g}_{\alpha\beta}(\boldsymbol{k}) + \frac{i}{2} \epsilon_{\alpha\beta} \Omega_{\boldsymbol{k}}$$

- $\hat{I}$ is the identity matrix and $\hat{P}_{\boldsymbol{k}}$ is the projector $| u_{\boldsymbol{k}} \rangle \langle u_{\boldsymbol{k}} |$.
- The tensor $\widehat{\Lambda}$ is the projection of $\hat{I} - \hat{P}_{\boldsymbol{k}}$ onto the subspace spanned by $\{| \partial_{k_x} u_k \rangle, | \partial_{k_y} u_k \rangle\}$
- The projector $\hat{I} - \hat{P}_{\boldsymbol{k}}$ is semipositive definite, so is the tensor $\widehat{\Lambda}$
- $\mathrm{Tr}\widehat{\Lambda} \geq 0$ and $\det\widehat{\Lambda} \geq 0$
- $\mathrm{Tr}\widehat{\Lambda} = \mathrm{Tr}\hat{g}$ and $\det\widehat{\Lambda} = -\frac{\Omega^2}{4} + \det g$ ➔ $\mathrm{Tr}\hat{g}_{\boldsymbol{k}} \geq 0, \det\hat{g}_{\boldsymbol{k}} \geq \frac{\Omega_k^2}{4}$
- Because $\hat{g}_{\boldsymbol{k}}$ is a 2×2 matrix, $(\mathrm{Tr}\hat{g}_{\boldsymbol{k}})^2 \geq 4\det\hat{g}_{\boldsymbol{k}}$ ➔ $\mathrm{Tr}\hat{g}_{\boldsymbol{k}} \geq | \Omega_k |$ [Trace Inequality]

Wilson Loop

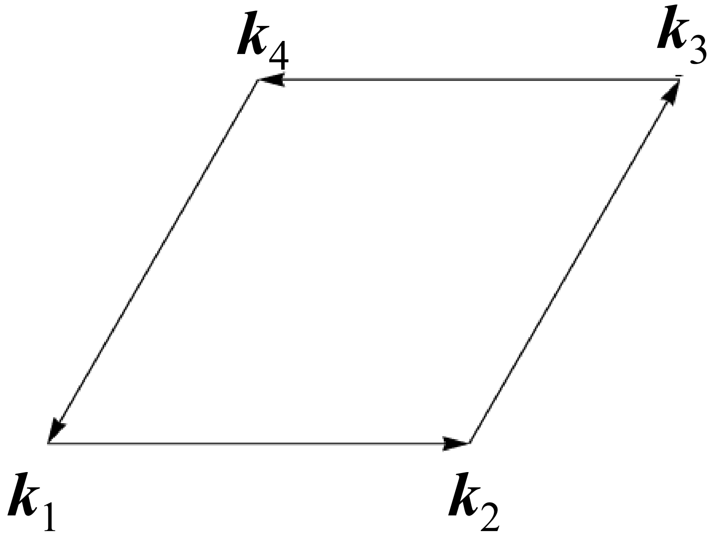
- Wilson loop:

$$\mathcal{W}(\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_N, \boldsymbol{k}_{N+1} = \boldsymbol{k}_1) = \prod_{j=1}^{N} M_{\boldsymbol{k}_j, \boldsymbol{k}_{j+1}}$$

$$\approx \exp[i \sum_{\boldsymbol{k}_j} \mathcal{A}_\alpha(\boldsymbol{k}_j)\delta k_\alpha - \frac{1}{2}\sum_{\boldsymbol{k}_j} \hat{g}_{\alpha\beta}(\boldsymbol{k}_j)\delta k_\alpha \delta k_\beta]$$

$$\approx \exp[i \int_{\Gamma_L} \Omega_{\boldsymbol{k}} d^2\boldsymbol{k} - \frac{1}{2}\sum_{\boldsymbol{k}_j} \hat{g}_{\alpha\beta}(\boldsymbol{k}_j)\delta k_\alpha \delta k_\beta]$$

$$M_{\boldsymbol{k}_j,\boldsymbol{k}_{j+1}} = \langle u_{\boldsymbol{k}_j} | u_{\boldsymbol{k}_{j+1}} \rangle$$



Γ_L is the interior enclosed by the loop L formed by $\boldsymbol{k}_j$ for $j = 1,\ldots,N + 1$, and $\delta\boldsymbol{k} = \boldsymbol{k}_{j+1} - \boldsymbol{k}_j$.

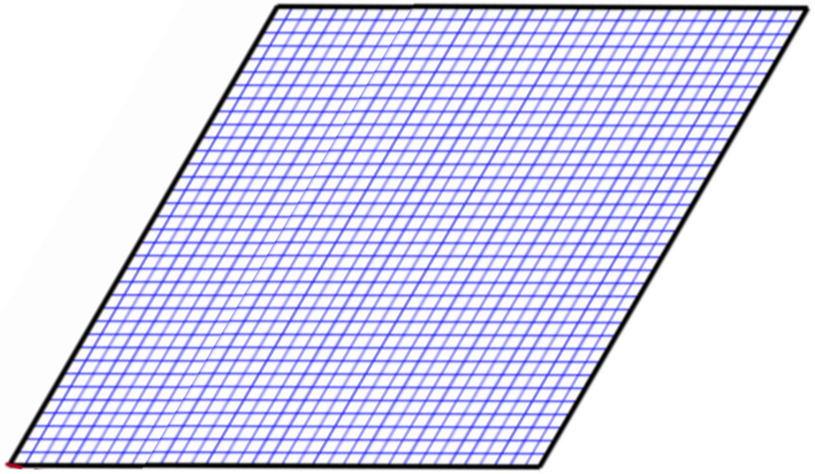
Berry Curvature

$$\mathcal{W}(\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_N, \boldsymbol{k}_{N+1} = \boldsymbol{k}_1) = \prod_{j=1}^{N} M_{\boldsymbol{k}_j, \boldsymbol{k}_{j+1}}$$

$$\approx \exp[i \int_{\Gamma_L} \Omega_{\boldsymbol{k}} d^2\boldsymbol{k} - \frac{1}{2} \sum_{\boldsymbol{k}_j} \hat{g}_{\alpha\beta}(\boldsymbol{k}_j) \delta k_\alpha \delta k_\beta]$$

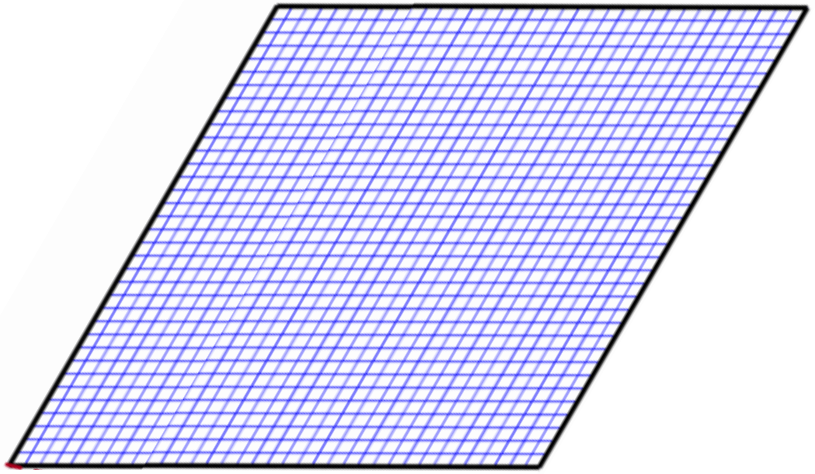
$$\Downarrow$$

$$\Omega_{\boldsymbol{k}} \approx \frac{\arg[\mathcal{W}]}{\mathcal{A}_{\Gamma_L}}$$



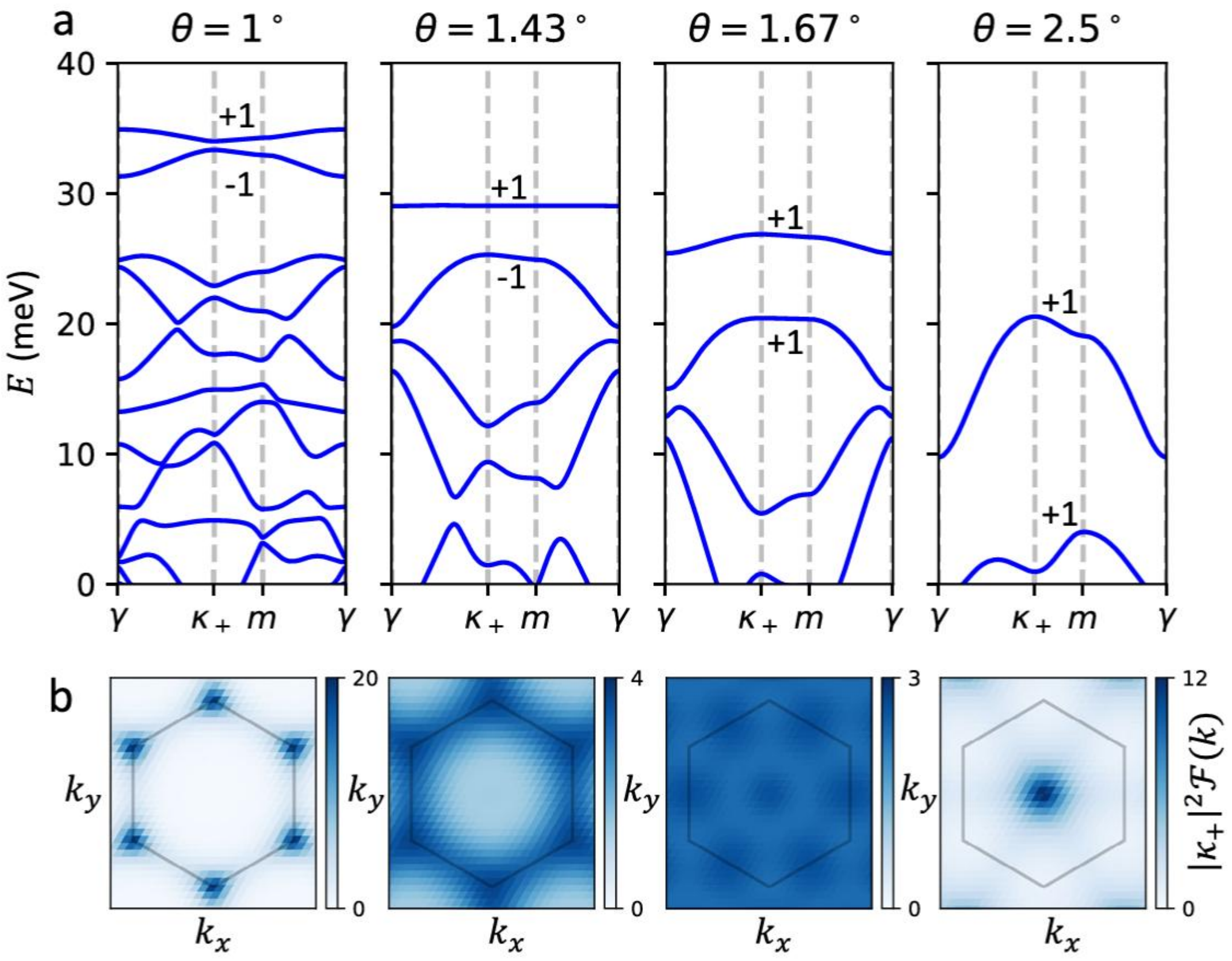
Quantum Metric

$$
\begin{aligned}
&\langle u_{\boldsymbol{k}-\boldsymbol{p}/2} | u_{\boldsymbol{k}+\boldsymbol{p}/2} \rangle \\
\approx & 1 + i p_\alpha \mathcal{A}_\alpha(\boldsymbol{k}) - \frac{1}{2} p_\alpha p_\beta \mathrm{Re}[\langle \partial_{k_\alpha} u_{\boldsymbol{k}} | \partial_{k_\beta} u_{\boldsymbol{k}} \rangle] \\
\approx & \exp[i p_\alpha \mathcal{A}_\alpha(\boldsymbol{k}) - \frac{1}{2} \hat{g}_{\alpha\beta}(\boldsymbol{k}) p_\alpha p_\beta],
\end{aligned}
$$



$$
\hat{g}_{\alpha\beta} p_\alpha p_\beta \approx 1 - \left| \langle u_{\boldsymbol{k}-\frac{\boldsymbol{p}}{2}} | u_{\boldsymbol{k}+\frac{\boldsymbol{p}}{2}} \rangle \right|^2
$$

Topological Moire Bands and Magic Angle



T. Devakul et al., Nat. Comm. 12, 6730 (2021)

Wannier States

- Wannier states:

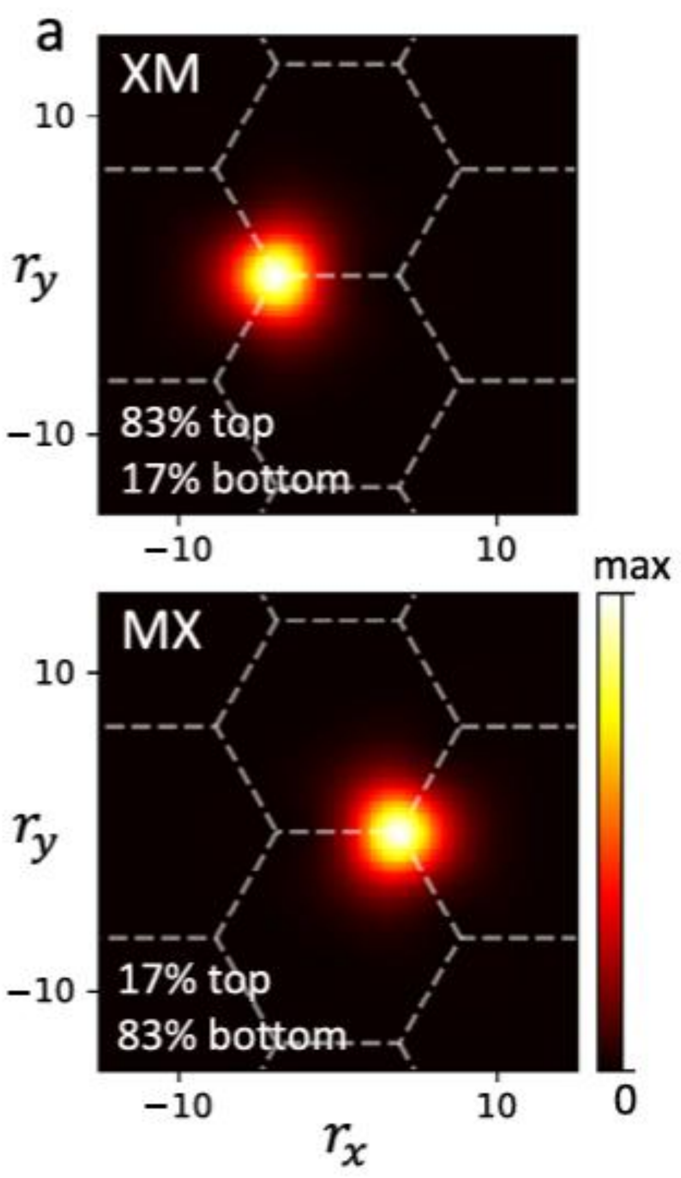
$$W^{(\widetilde{\boldsymbol{R}},a)}(\boldsymbol{r}) = \frac{1}{\sqrt{N_{\boldsymbol{k}}}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\widetilde{\boldsymbol{R}}} \varphi_{\boldsymbol{k}}^{(a)}(\boldsymbol{r})$$

$$\varphi_{\boldsymbol{k}}^{(a)}(\boldsymbol{r}) = \sum_{n=1,2} \widetilde{\psi}_{\boldsymbol{k},n}(\boldsymbol{r}) V_{\boldsymbol{k},n,a}$$

- Use layer polarization to disentangle hybridization:

$$\Pi_{\boldsymbol{k}} = \begin{pmatrix} \langle\widetilde{\psi}_{\boldsymbol{k},1}|\sigma_z|\widetilde{\psi}_{\boldsymbol{k},1}\rangle & \langle\widetilde{\psi}_{\boldsymbol{k},1}|\sigma_z|\widetilde{\psi}_{\boldsymbol{k},2}\rangle \\ \langle\widetilde{\psi}_{\boldsymbol{k},2}|\sigma_z|\widetilde{\psi}_{\boldsymbol{k},1}\rangle & \langle\widetilde{\psi}_{\boldsymbol{k},2}|\sigma_z|\widetilde{\psi}_{\boldsymbol{k},2}\rangle \end{pmatrix}$$

$$V_{\boldsymbol{k}}^{\dagger}\Pi_{\boldsymbol{k}}V_{\boldsymbol{k}} = \begin{pmatrix} \rho_{\boldsymbol{k}}^{1} & 0 \\ 0 & \rho_{\boldsymbol{k}}^{2} \end{pmatrix}$$



Hopping parameters

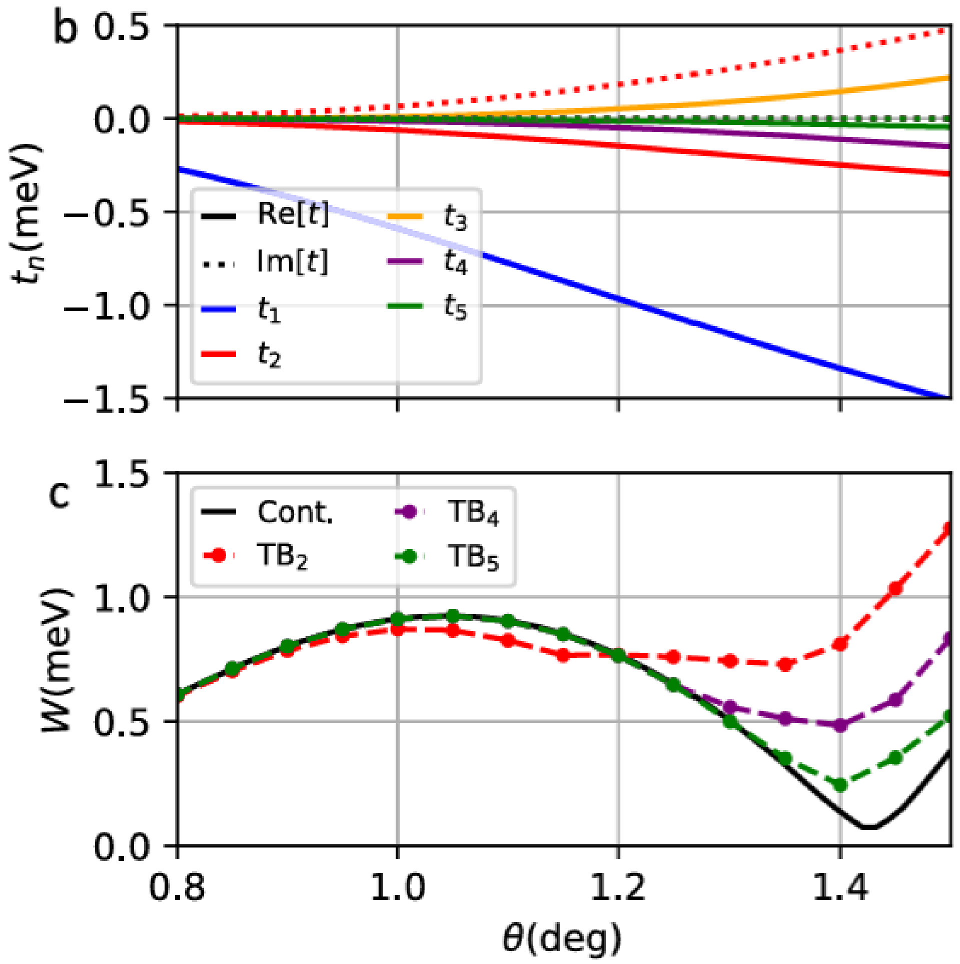
- Wannier states:

$$W^{(\widetilde{\boldsymbol{R}},a)}(\boldsymbol{r}) = \frac{1}{\sqrt{N_{\boldsymbol{k}}}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\widetilde{\boldsymbol{R}}} \varphi_{\boldsymbol{k}}^{(a)}(\boldsymbol{r})$$

$$\varphi_{\boldsymbol{k}}^{(a)}(\boldsymbol{r}) = \sum_{n=1,2} \widetilde{\psi}_{\boldsymbol{k},n}(\boldsymbol{r}) V_{\boldsymbol{k},n,a}$$

- Hopping amplitudes:

$$t_{ab}(\widetilde{\boldsymbol{R}}) = \int d^2\boldsymbol{r}\, [W^{(\widetilde{\boldsymbol{R}},a)}(\boldsymbol{r})]^* H_{\text{cont}} W^{(\boldsymbol{0},b)}(\boldsymbol{r})$$
$$= \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \sum_{n=1,2} e^{i\boldsymbol{k}\cdot\widetilde{\boldsymbol{R}}} V^*_{\boldsymbol{k},n,a} V_{\boldsymbol{k},n,b} \varepsilon_{\boldsymbol{k},n},$$



Three Wannier States