Transport in twisted bilayer graphene

- Introduction for twisted bilayer graphene (TBG)
- Non-linear Hall effect (NHE) at non-magic angle
- Quantum anomalous Hall (QAH) and semimetal at magic angle

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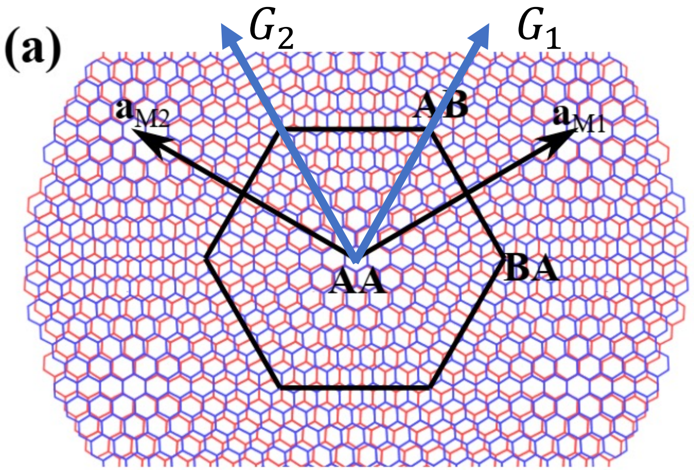
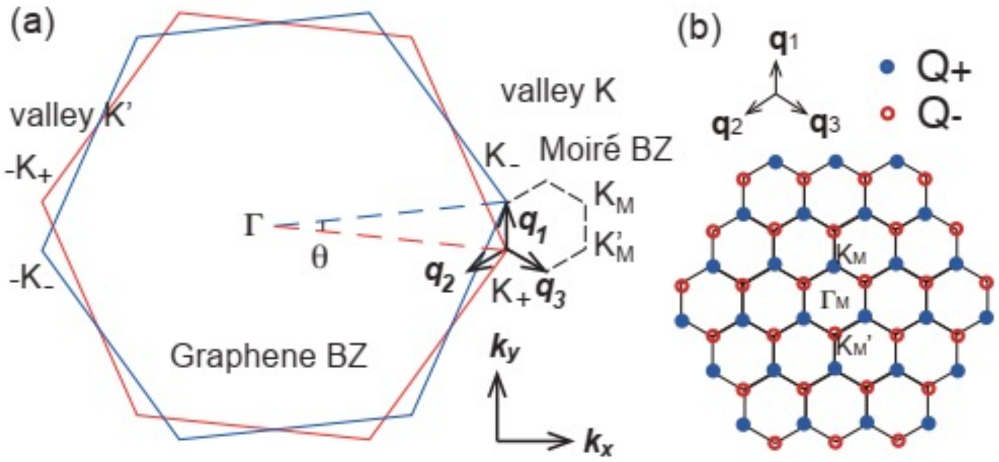
BM model for TBG



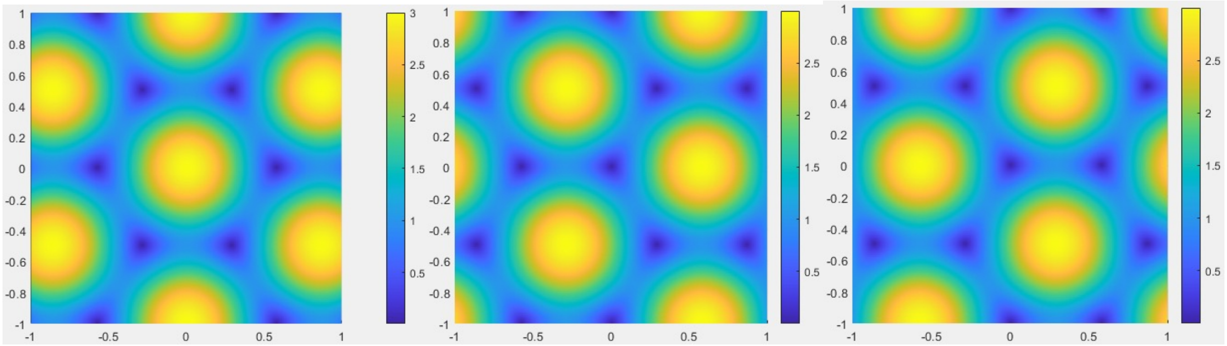


Moiré bands in twisted double-layer graphene, Rafi Bistritzer and Allan H. MacDonald. PNAS 108, 12233 (2011)

TBG I-V, B. Andrei Bernevig, Zhi-Da Song, etc. PRB (2021)…

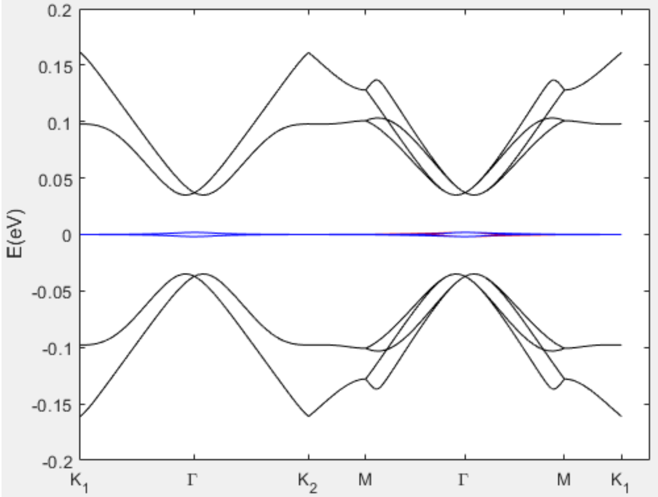
$$H(r) = -i v_F \begin{pmatrix} \partial_r \cdot \sigma & 0 \\ 0 & \partial_r \cdot \sigma \end{pmatrix} + \begin{pmatrix} 0 & T(r) \\ T^\dagger(r) & 0 \end{pmatrix}$$

$$T(r) = \sum_{j=1}^{3} e^{-i q_j \cdot r} \cdot \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi(j-1)}{3}} \\ u_1 e^{i\frac{2\pi(j-1)}{3}} & u_0 \end{pmatrix}$$



AA hopping | BA hopping | AB hopping

$$q_1 = \frac{G_2 + G_1}{3}, q_2 = \frac{G_2 - 2G_1}{3}, q_3 = \frac{G_1 - 2G_2}{3}$$



$$(\theta, v_F/a_0, u_0, u_1) = (1.08°, 2.38eV, 0.08eV, 0.11eV)$$

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Semiclassical Boltzmann equation

$$\frac{f-f_0}{-\tau} = \partial_t f + \dot{\boldsymbol{k}} \cdot \boldsymbol{\nabla}_{\boldsymbol{k}} f$$

$$\dot{\boldsymbol{k}} = q\boldsymbol{E}(t) = qE_k e^{iwt}$$

$$f^{(0)} = f_0 = \frac{1}{e^{\beta\varepsilon}+1}$$

$$f^{(1)} = \frac{-q\tau}{1+iw\tau} E_k e^{iwt} \partial_k f^{(0)}$$

$$f^{(2)} = \frac{(q\tau)^2 E_{k_1} E_{k_2} e^{i2wt}}{(1+i2w\tau)(1+iw\tau)} \partial_{k_1}\partial_{k_2} f^{(0)}$$

+

$$j_\alpha = q\int f(k)\, v_\alpha$$

$$v_\alpha \approx \partial_\alpha \varepsilon - q(\boldsymbol{E}\times\boldsymbol{\Omega})_\alpha$$

$$j_\alpha^{(0)} = q\int f^{(0)} \partial_\alpha \varepsilon = 0$$

$$j_\alpha^{(1)} = -q^2 \int f^{(0)} (\boldsymbol{E}\times\boldsymbol{\Omega})_\alpha + q\int f^{(1)} \partial_\alpha \varepsilon$$

$$j_\alpha^{(2)} = -q^2 \int f^{(1)} (\boldsymbol{E}\times\boldsymbol{\Omega})_\alpha + q\int f^{(2)} \partial_\alpha \varepsilon$$

$$\sigma_{\alpha\beta} = -q^2 \epsilon_{\alpha\beta\gamma} \int f^{(0)} \Omega_\gamma + \frac{q^2\tau}{1+iw\tau} \int f^{(0)} \partial_\alpha \partial_\beta \varepsilon$$

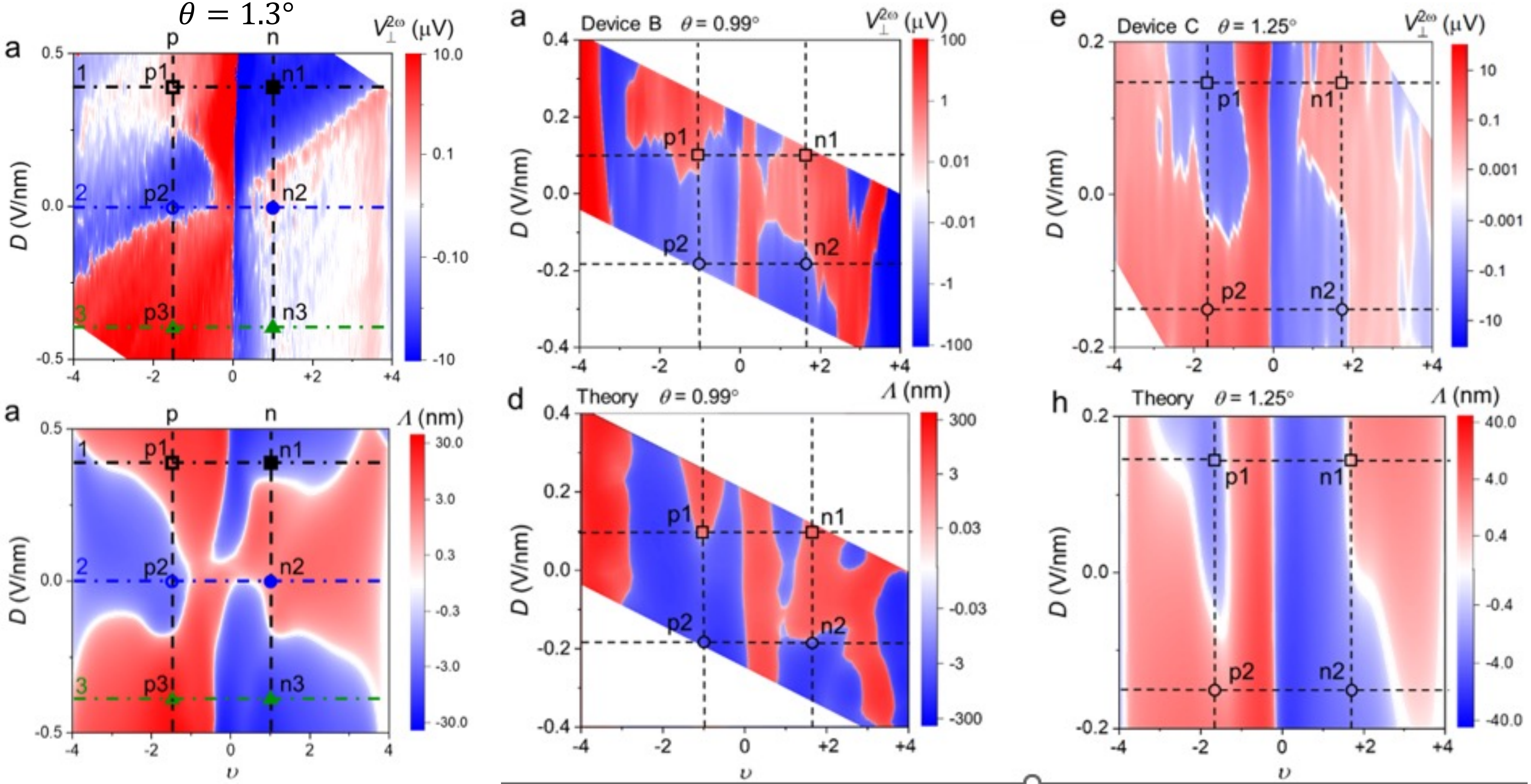
⇒

$$\chi_{\alpha\beta\gamma} = -\frac{q^3\tau}{1+iw\tau} \epsilon_{\alpha\beta\eta} \int f^{(0)} \partial_\gamma \Omega_\eta + \frac{q^3\tau^2}{(1+i2w\tau)(1+iw\tau)} \int f^{(0)} \partial_\alpha \partial_\beta \partial_\gamma \varepsilon + (\beta \leftrightarrow \gamma)$$

NHE tuning by gates

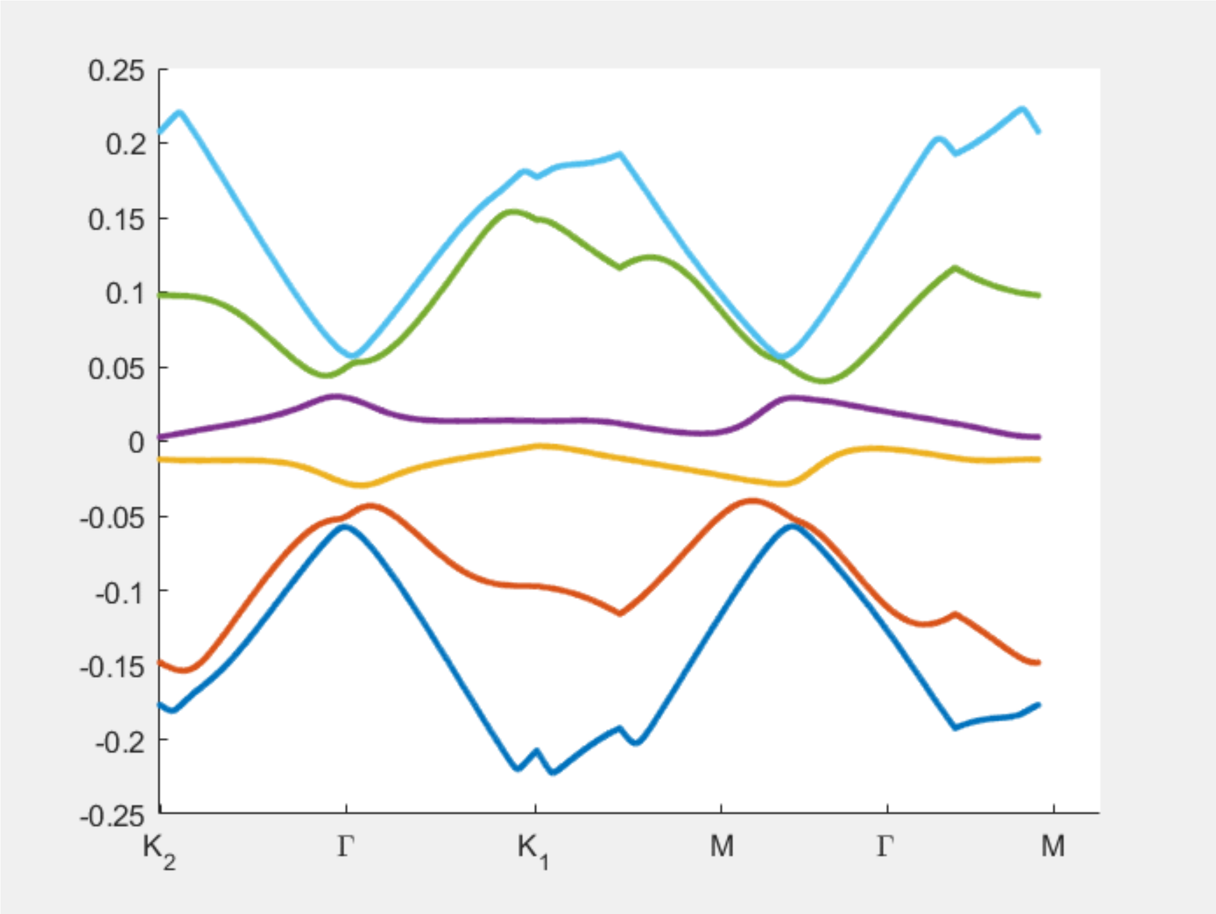
Intrinsic nonlinear Hall effect and gate-switchable Berry curvature sliding in twisted bilayer graphene, Meizhen Huang, Zefei Wu, Xu Zhang, etc. arXiv:2212.12666 (2022)

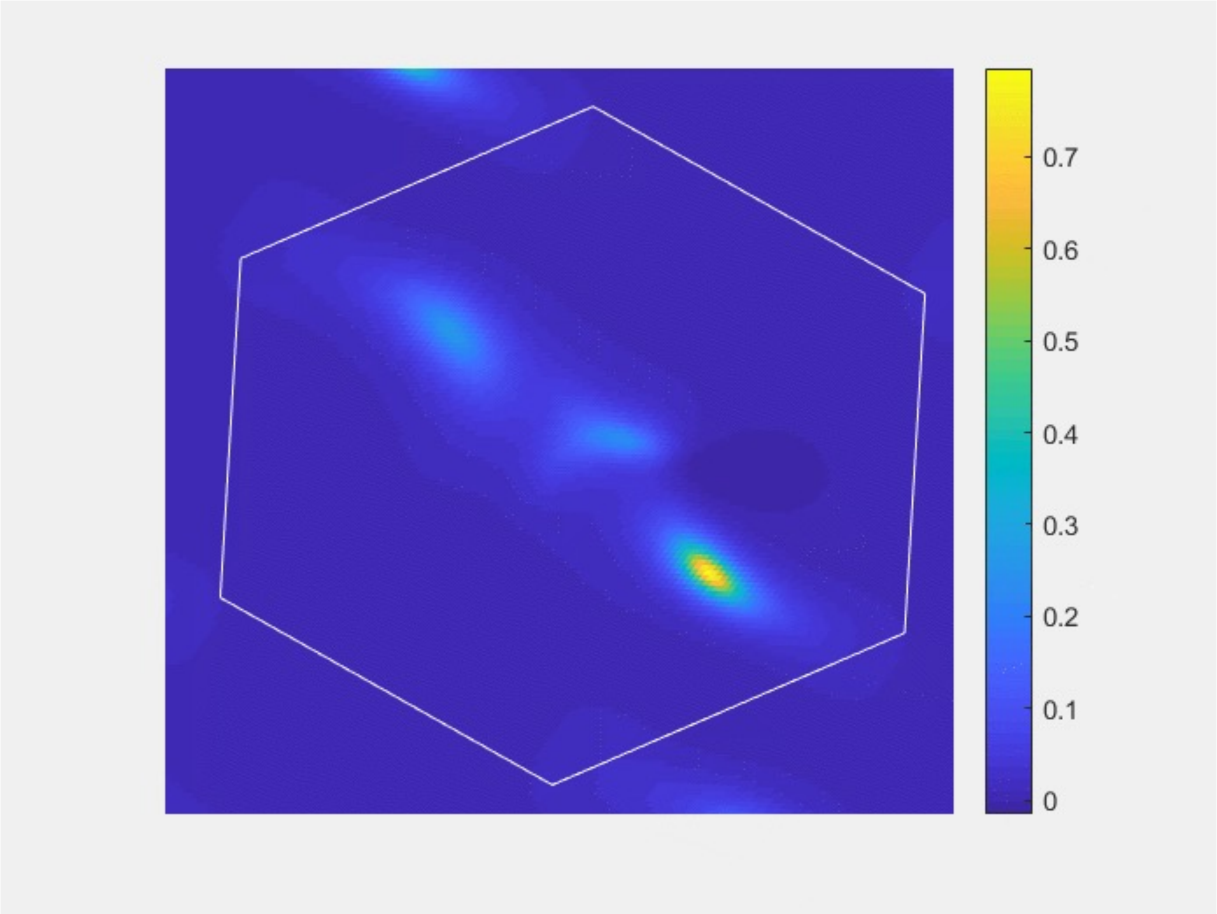
$\theta = 1.3°$



Berry curvature hotspot sliding

$\theta = 1.3°$, strain $\epsilon = 0.3\%$





$$\chi_{\alpha\beta\gamma} = -\frac{q^3\tau}{1+iw\tau}\epsilon_{\alpha\beta\eta}\int\left(\frac{\partial f_0}{\partial E}\right)\partial_\gamma E\cdot\Omega_\eta + (\beta\leftrightarrow\gamma)$$

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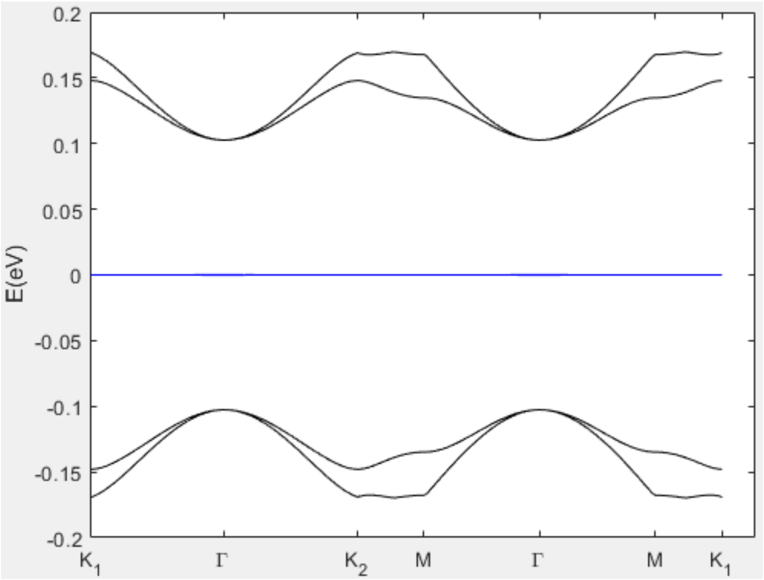
Chiral limit and symmetry



BM model review in momentum space

$$H^\tau(k) = v_F \begin{pmatrix} (k-K_-)\cdot\sigma & 0 \\ 0 & (k-K_+)\cdot\sigma \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} 0 & U^\tau \\ U^{\tau\dagger} & 0 \end{pmatrix}$$

$$U^\tau = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}} \\ u_1 e^{i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_1} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}} \\ u_1 e^{-i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_2}$$ ($u_0 = 0$ for chiral limit)

At chiral limit

$$\sigma_z H^\tau(k)\sigma_z = -H^\tau(k)$$

$$H^\tau(k)|\psi_E\rangle = E|\psi_E\rangle = 0$$ ($E = 0$ for chiral limit flat bands)

$$H^\tau(k)\sigma_z|\psi_E\rangle = -E\sigma_z|\psi_E\rangle = 0$$

Diagonalize flat bands according to eigenvalue of σ_z (Equivalent to apply an hBN perturbation which gives two bands Chern number ± 1)

$$\begin{pmatrix} \langle\psi_1|\sigma_z|\psi_1\rangle & \langle\psi_1|\sigma_z|\psi_2\rangle \\ \langle\psi_2|\sigma_z|\psi_1\rangle & \langle\psi_2|\sigma_z|\psi_2\rangle \end{pmatrix} \Rightarrow \begin{cases} |\psi_+\rangle = |\psi_1\rangle + \sigma_z|\psi_1\rangle \\ |\psi_-\rangle = |\psi_1\rangle - \sigma_z|\psi_1\rangle \end{cases} \Rightarrow \begin{pmatrix} \langle\psi_+|\sigma_z|\psi_+\rangle & \langle\psi_+|\sigma_z|\psi_-\rangle \\ \langle\psi_-|\sigma_z|\psi_+\rangle & \langle\psi_-|\sigma_z|\psi_-\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(Chern basis)

Chiral limit and symmetry

Projected Coulomb interaction at flat chiral limit

$C_{2z}P$ symmetry, $\lambda_{m,n,\tau}(k, k+q+G) = m \cdot n \cdot \lambda_{-m,-n,-\tau}(k, k+q+G)$

$\tilde{c}^{\dagger}_{k,-m,s,-\tau} = m c^{\dagger}_{k,m,s,-\tau}$

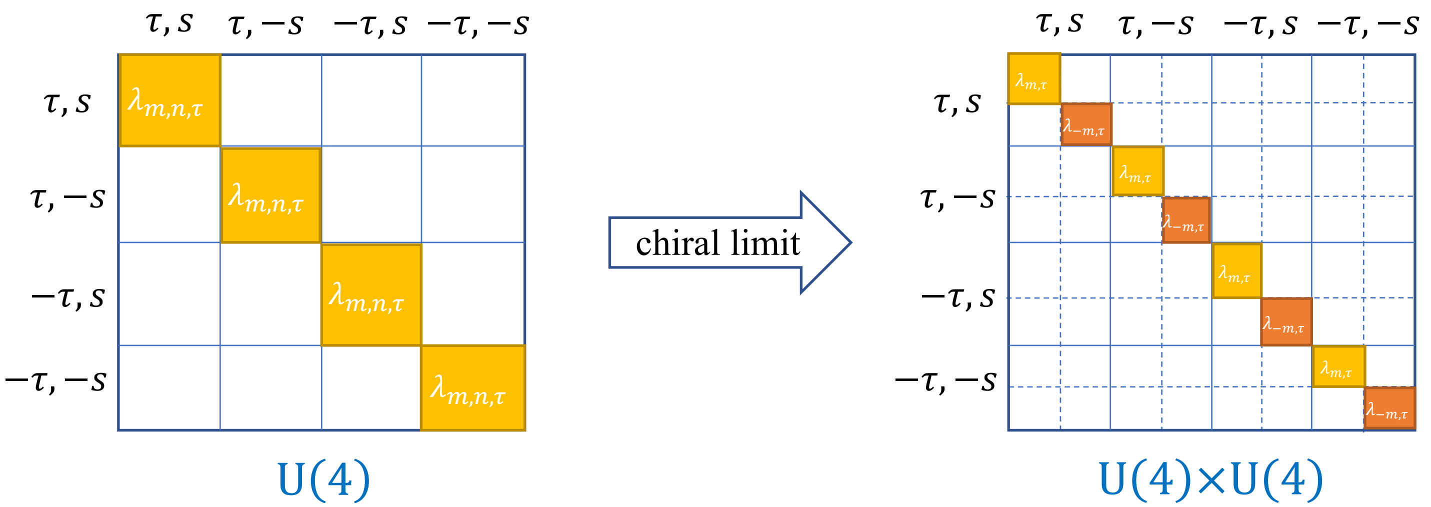
$$H = \frac{1}{2\Omega} \sum_{G} \sum_{q \in mBZ} V(q+G)\delta\rho_{q+G}\delta\rho_{-q-G}$$

$$\delta\rho_{q+G} = \sum_{k,m,n,s,\tau} \lambda_{m,n,\tau}(k, k+q+G)\left(c^{\dagger}_{k,m,s,\tau} c_{k+q,n,s,\tau} - \frac{\nu+4}{8}\delta_{q,0}\delta_{m,n}\right)$$

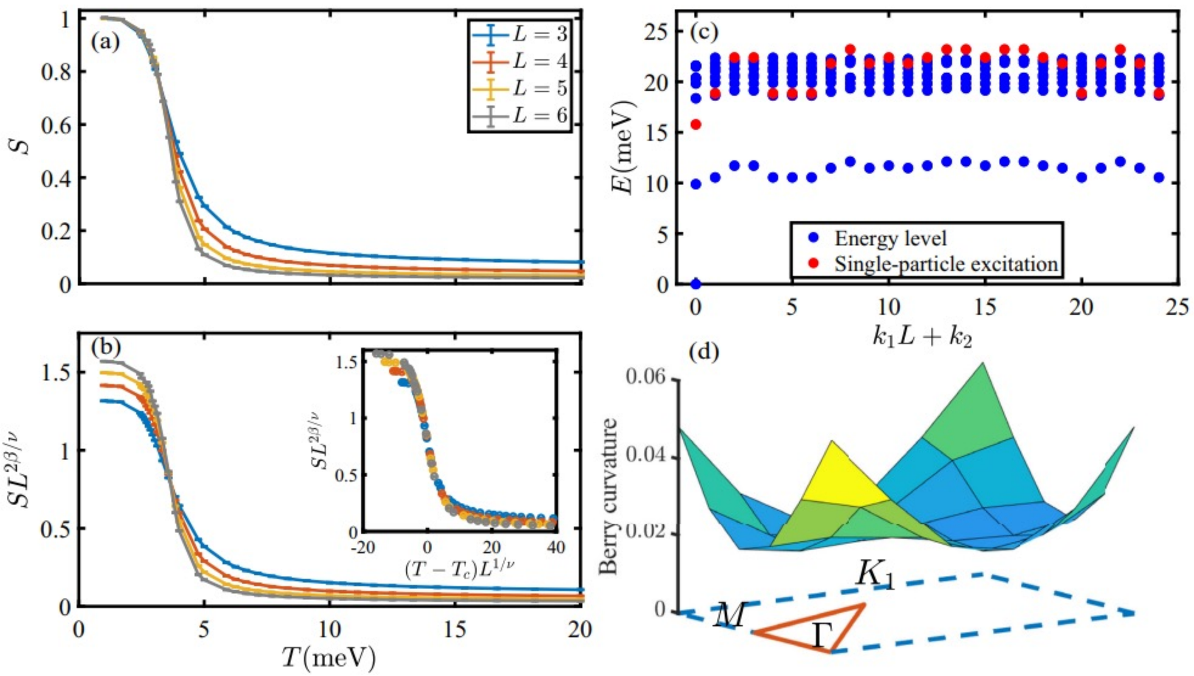
$$= \sum_{k,m,n} \lambda_{m,n,\tau}(k, k+q+G)\left(c^{\dagger}_{k,m,s,\tau} c_{k+q,n,s,\tau} + c^{\dagger}_{k,m,-s,\tau} c_{k+q,n,-s,\tau} + \tilde{c}^{\dagger}_{k,m,s,-\tau} \tilde{c}_{k+q,n,s,-\tau} + \tilde{c}^{\dagger}_{k,m,-s,-\tau} \tilde{c}_{k+q,n,-s,-\tau} - \frac{\nu+4}{2}\delta_{q,0}\delta_{m,n}\right)$$

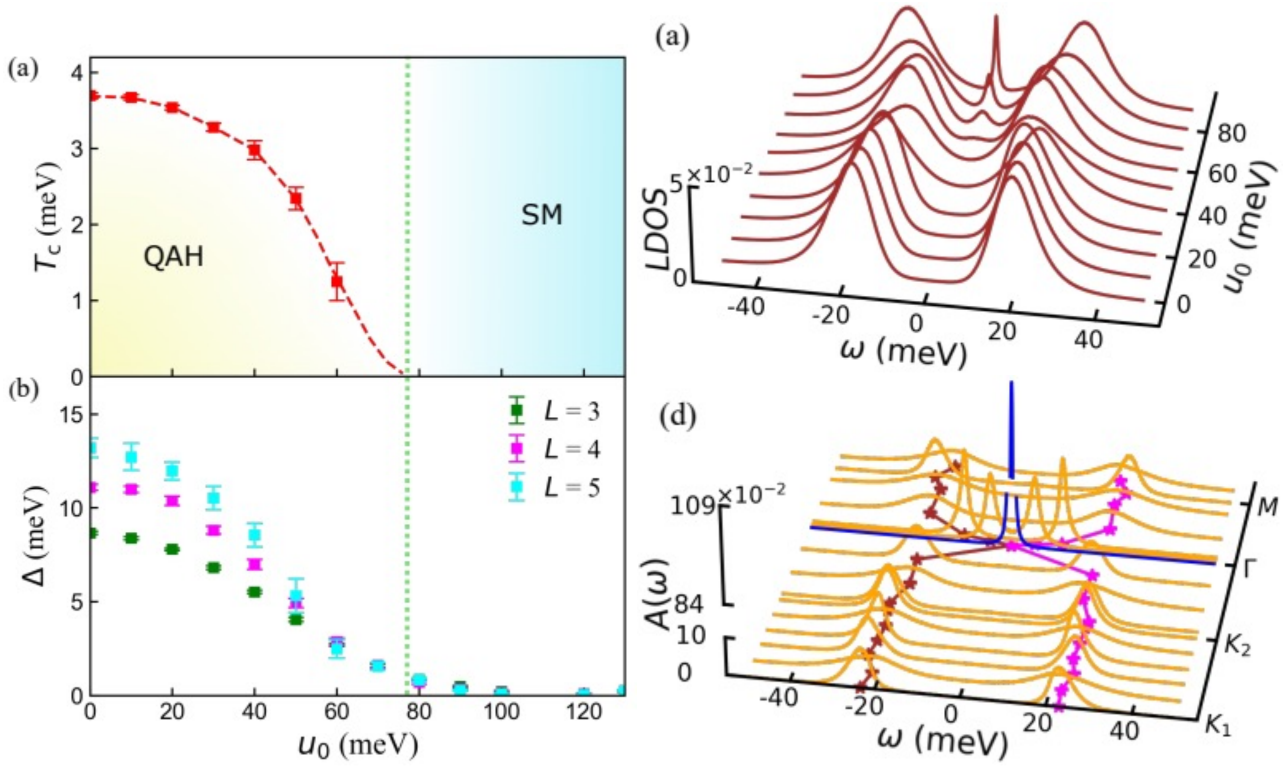
chiral limit
$\langle \psi_+ | \psi_- \rangle = 0$

$$= \sum_{k,m} \lambda_{m,\tau}(k, k+q+G)\left(c^{\dagger}_{k,m,s,\tau} c_{k+q,m,s,\tau} + c^{\dagger}_{k,m,-s,\tau} c_{k+q,m,-s,\tau} + \tilde{c}^{\dagger}_{k,m,s,-\tau} \tilde{c}_{k+q,m,s,-\tau} + \tilde{c}^{\dagger}_{k,m,-s,-\tau} \tilde{c}_{k+q,m,-s,-\tau} - \frac{\nu+4}{2}\delta_{q,0}\right)$$



Assume spin-valley polarizing at $\nu = \pm 3$





Flat-chiral limit $u_0 = 0$

Ground state: Quantum anomalous Hall

Flat band non-chiral $u_0 \neq 0$

Ground state: From Quantum anomalous Hall to semimetal

Thermodynamic Characteristic for a Correlated Flat-Band System with a Quantum Anomalous Hall Ground State, Gaopei Pan, Xu Zhang, etc. Phys. Rev. Lett. **130**, 016401 (2023)

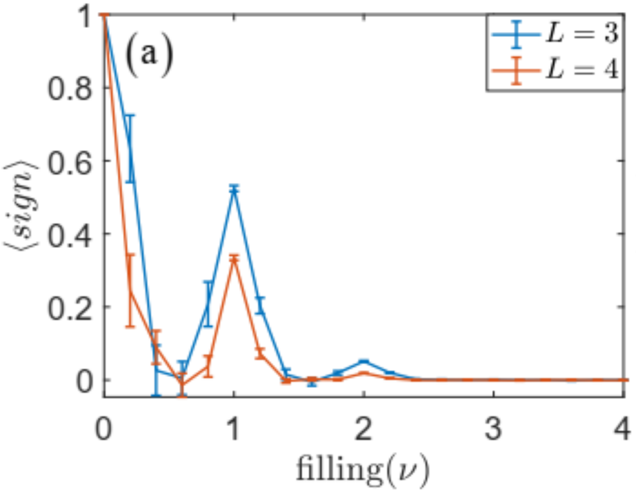
Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in magic-angle twisted bilayer graphene, Cheng Huang, Xu Zhang, etc. arXiv:2304.14064 (2023)

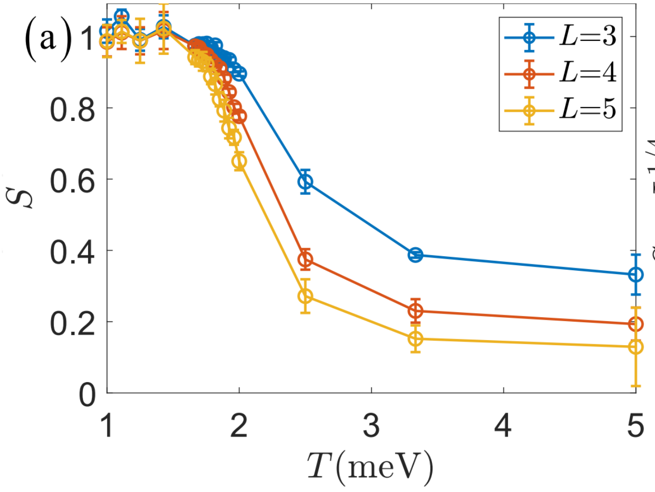
Chiral-flat band TBG at $v = \pm 1$

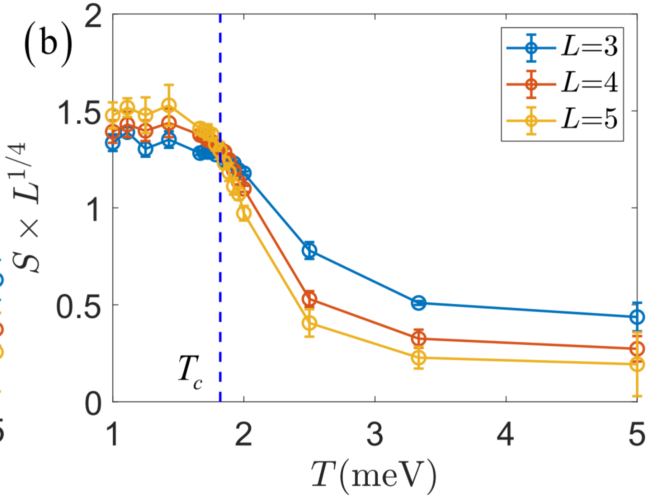
Polynomial sign bounds behavior at low temperature

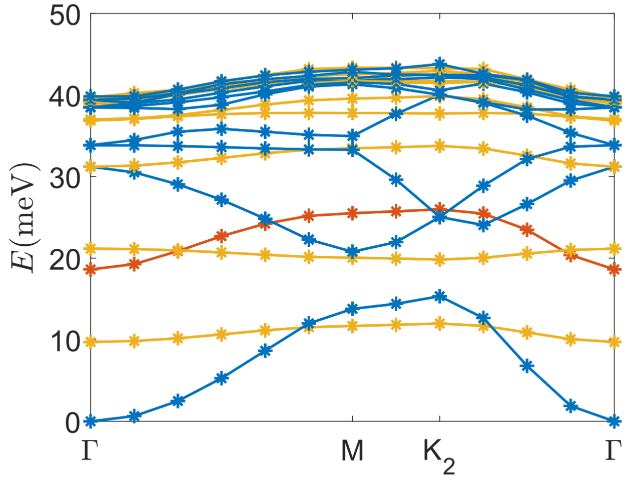
$$\langle sign\rangle \geq \frac{g_{v=1}}{g_{v=0}} = \frac{\frac{(N+3)^2(N+2)^3(N+1)^2}{3!\,3!} + \frac{(N+3)(N+2)(N+1)}{3}}{\frac{(N+3)^2(N+2)^4(N+1)^2}{3!\,3!\,2!\,2!} + \frac{(N+3)^2(N+2)^2(N+1)^2}{3!\,3} + 2} \propto N^{-1}$$

Filling(ν)	Chiral($\gamma = 0$)
0	1
± 1	N^{-1}
± 2	N^{-2}
± 3	N^{-5}
± 4	N^{-8}









Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, Xu Zhang, Gaopei Pan, etc. Phys. Rev. B 107, L241105 (2023)

Non-chiral simulation is in process…

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Conclusions

- 1. Berry curvature hotspot is easy to tune in flat band materials, so that non-linear Hall signal can be sensitive to gate voltage (e.g., TBG at non-magic angle).
- 2. TBG at magic angle, assuming spin-valley polarizing at filling $\nu = \pm 3$, evolves from QAH to semimetal departing from chiral limit.
- 3. TBG at magic angle, assuming flat-chiral limit at filling $\nu = \pm 1$, is QAH ground state with Chern number 1. Simulation for non-chiral case is in process.

Thanks!