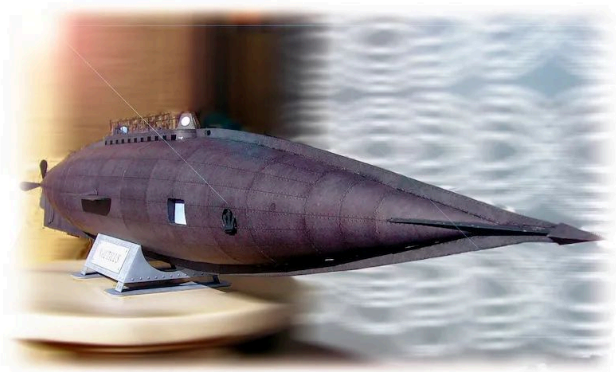
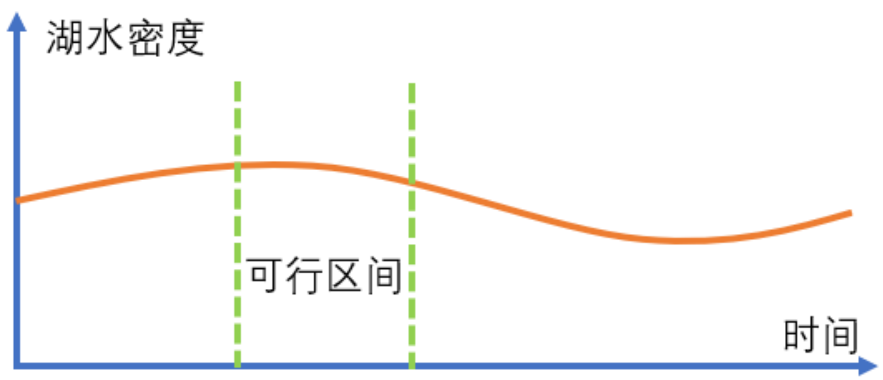
Detective Dr. Dragon on the Polynomial Sign Problem in Twisted Bilayer Graphene

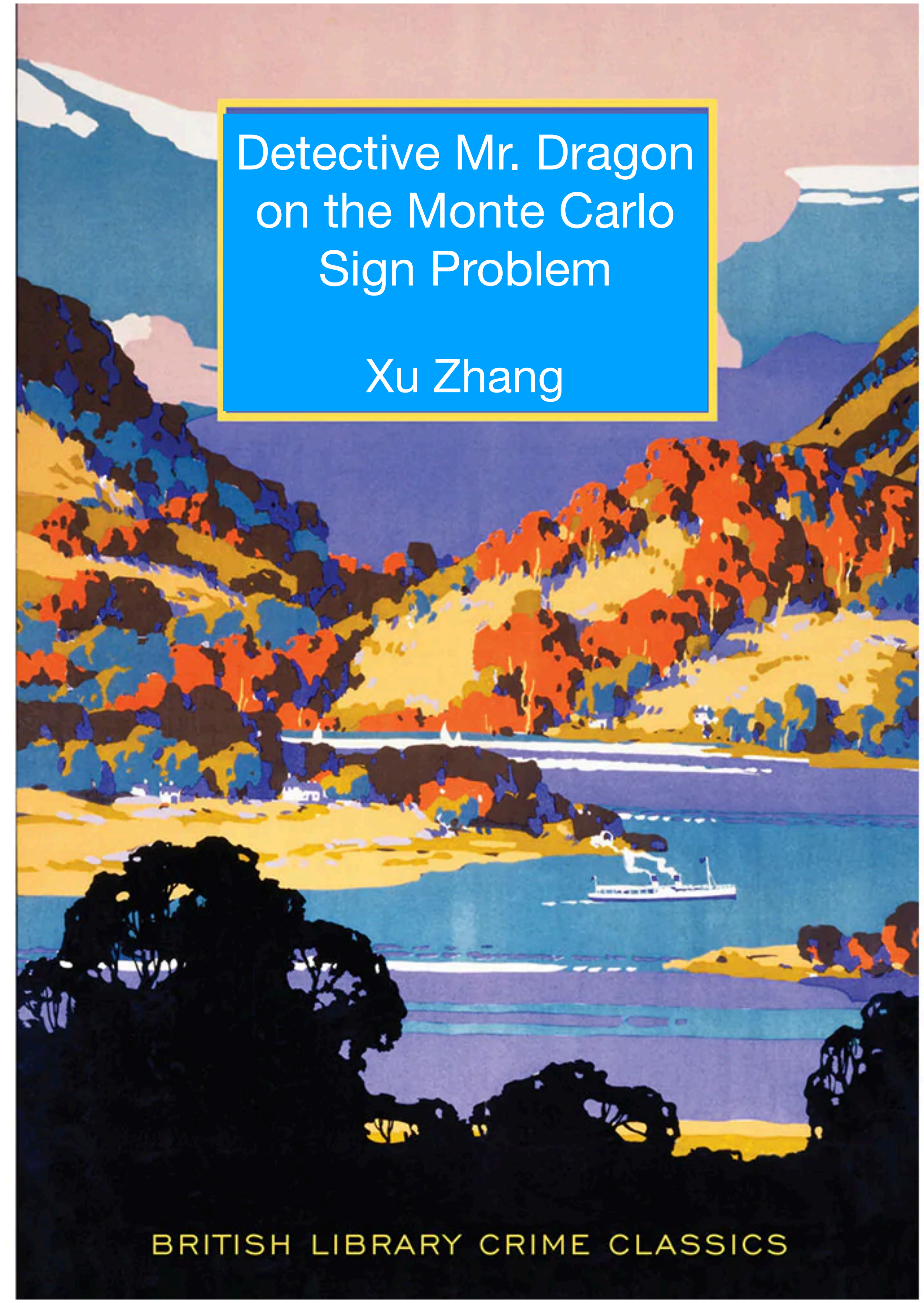
ZI YANG MENG
孟子杨
https://quantummc.xyz/

Xu Zhang

Caption Nemo and submarine Nautilus







$$\langle \rho \rangle_{V_i} = \frac{\sum_i V_i \rho_i}{\sum_i V_i} = \frac{\frac{\sum_i |V_i| (\pm \rho_i)}{\sum_i |V_i|}}{\frac{\sum_i |V_i| (\pm 1)}{\sum_i |V_i|}} = \frac{\langle \pm \rho_i \rangle_{|V_i|}}{\langle \pm 1 \rangle_{|V_i|}}$$

$\langle \pm 1 \rangle \sim e^{-N}$ **Sign problem and Sign bound**

- Twenty Thousand Leagues Under the Seas, Jules Verne
- Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)
- Xu Zhang et al., Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, PRB 107, L241105 (2023)

Xu Zhang

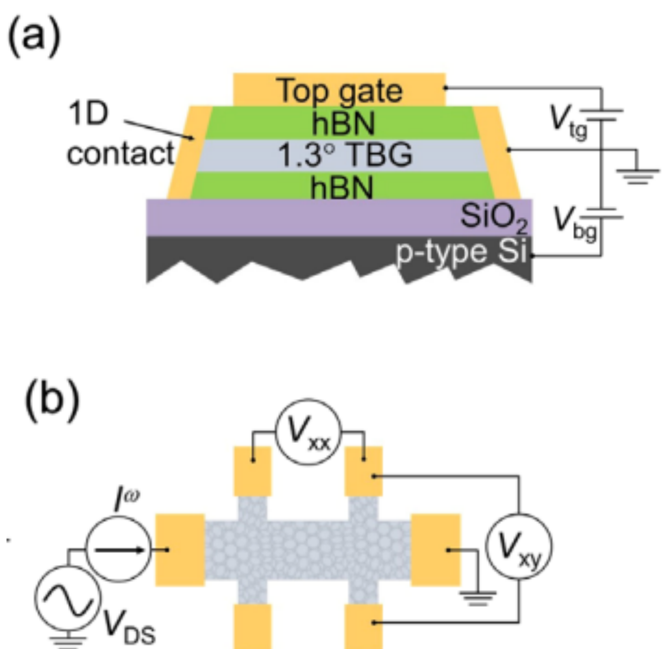
PHYSICAL REVIEW LETTERS

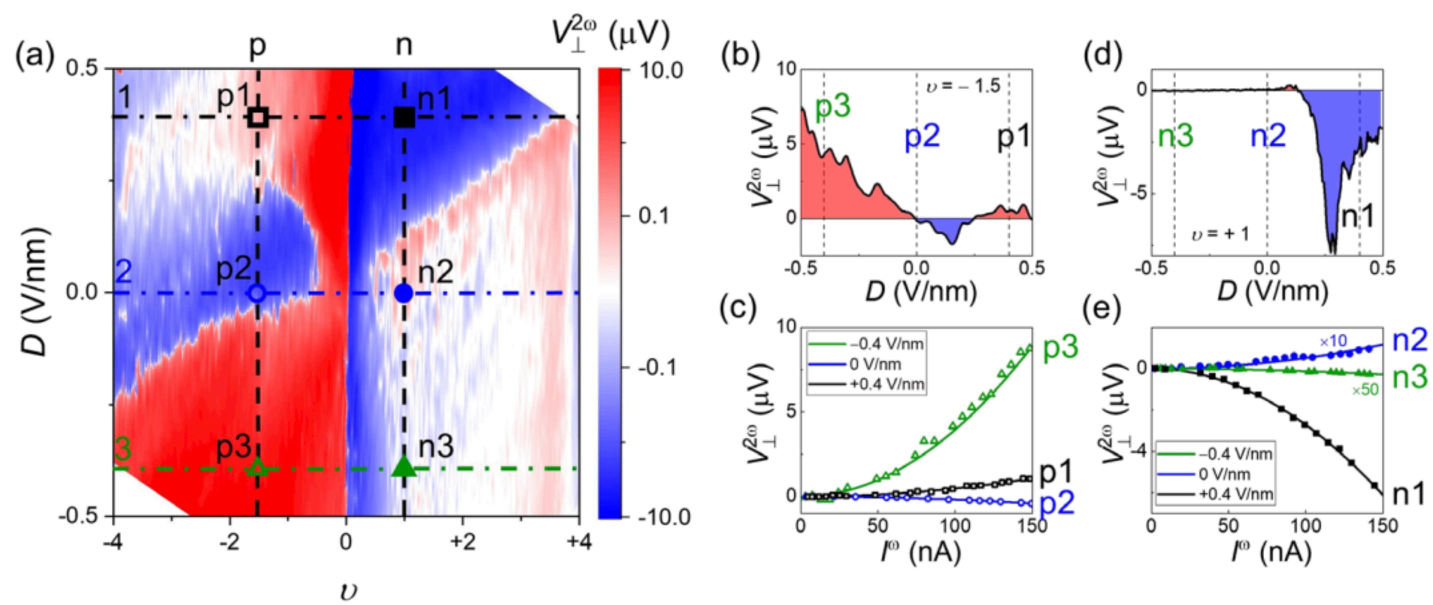
Editors' Suggestion

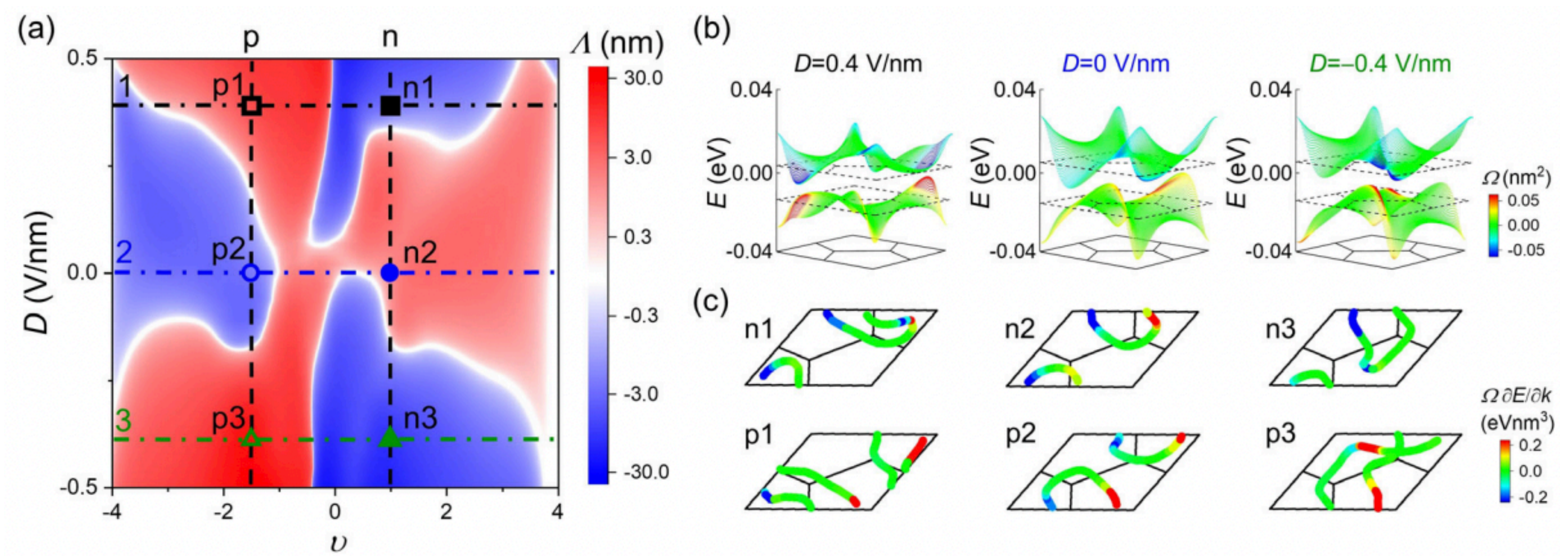
Intrinsic Nonlinear Hall Effect and Gate-Switchable Berry Curvature Sliding in Twisted Bilayer Graphene

Meizhen Huang, Zefei Wu, Xu Zhang, Xuemeng Feng, Zishu Zhou, Shi Wang, Yong Chen, Chun Cheng, Kai Sun, Zi Yang Meng, and Ning Wang

Phys. Rev. Lett. **131**, 066301 – Published 11 August 2023

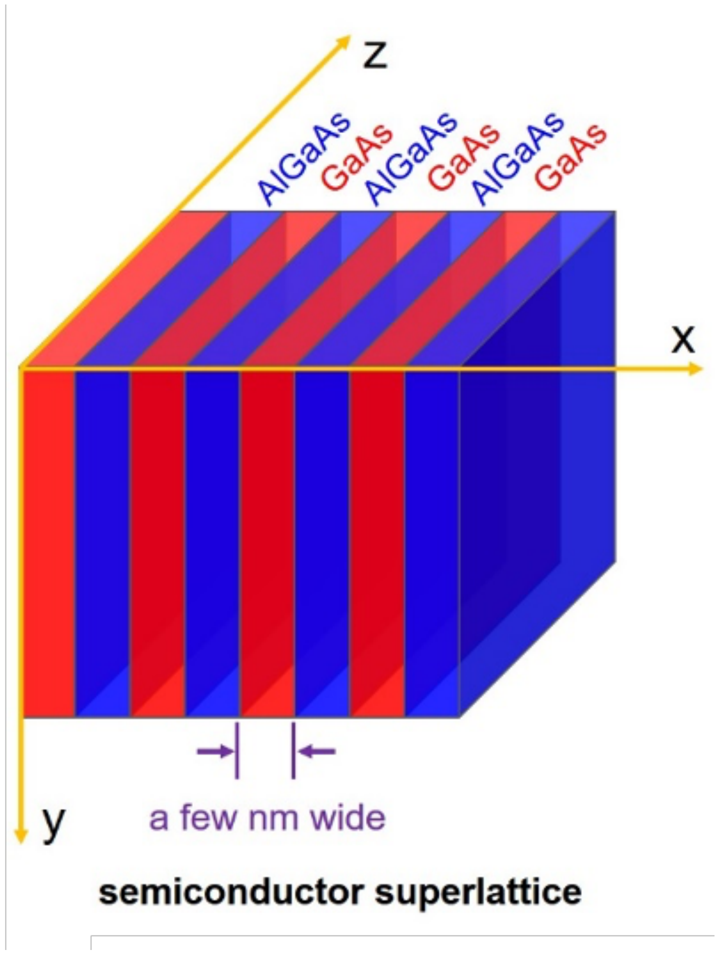






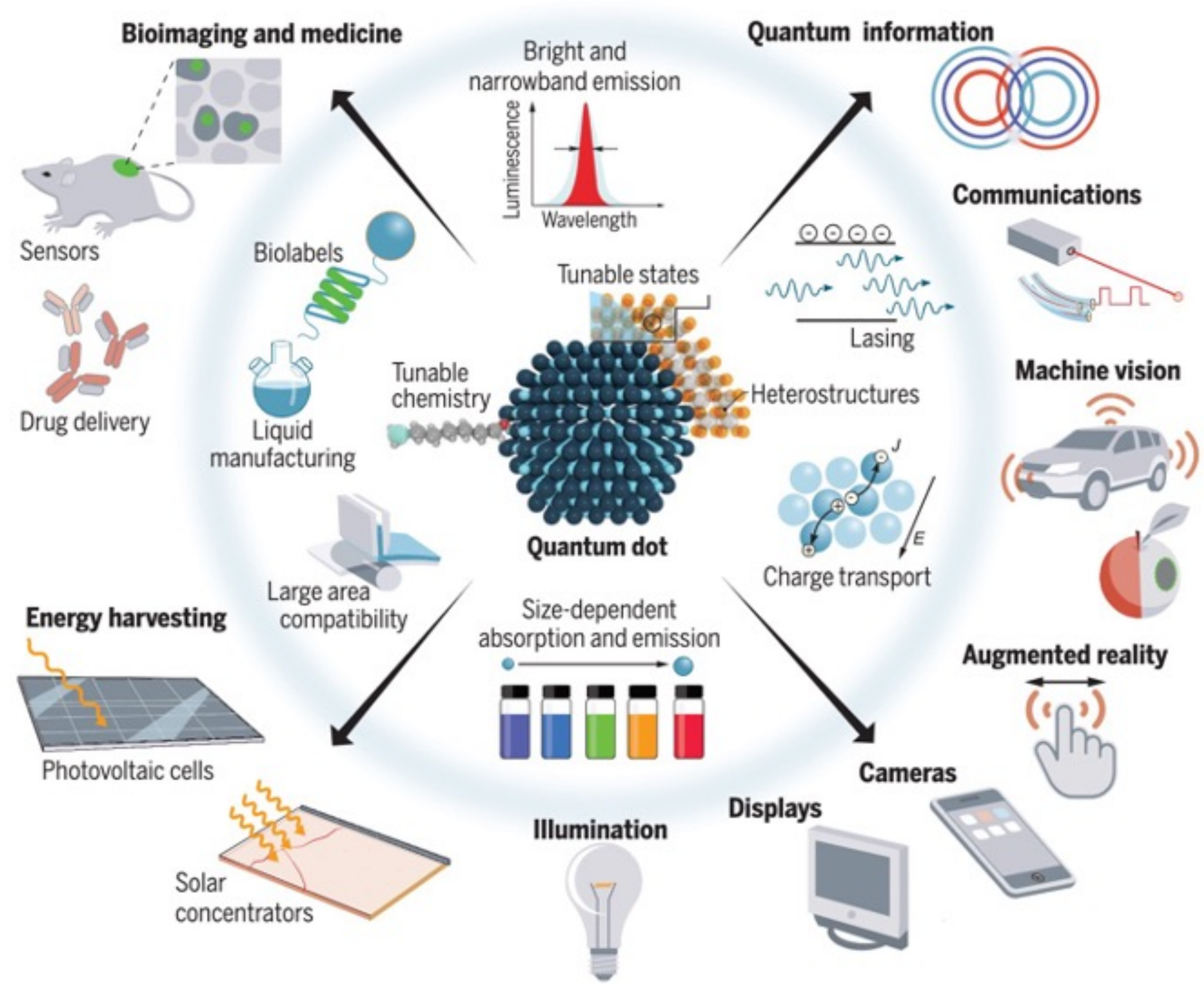
Superlattices are widely used as electric and optical devices

In semiconductor industry



Wikipedia

In semiconductor quantum dots / wires technologies



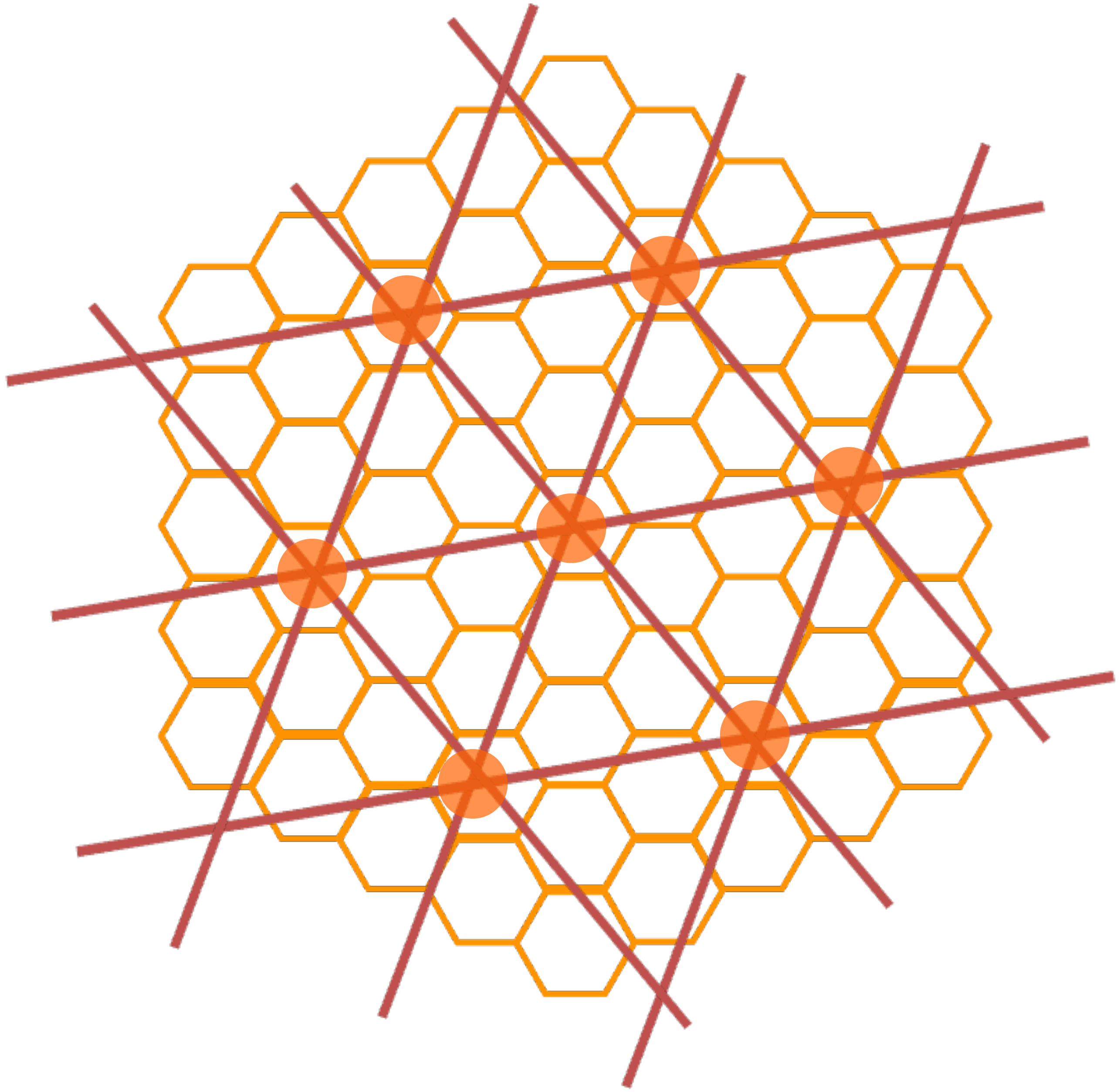
Garcia de Arquer et al., Science (2021)

- Periodic in growth direction (mainly 1D)
- Based on free electron band structure

- **Quantum moiré materials are new superlattices in 2D**
- **Based on many-body effects with novel properties (such as superconductivity)**

Quantum moiré materials are superlattice of 2D materials (e.g. graphene)

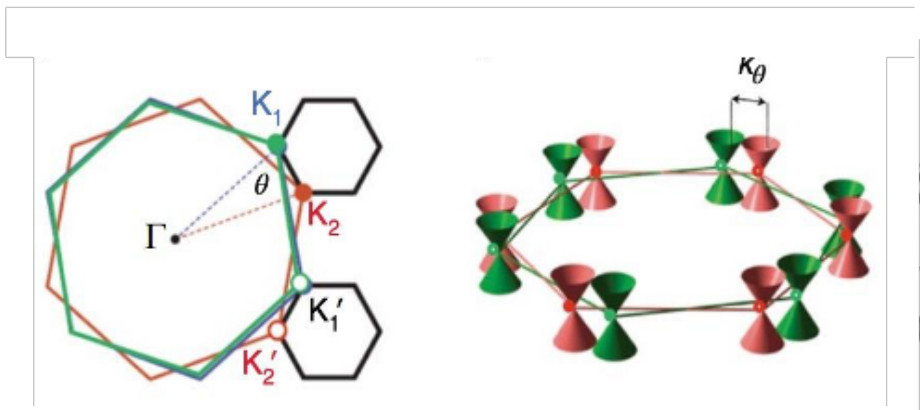
Moiré: stack, twist & new physics emerges
crystal from crystals
ideal playground & challenge for quantum many-body physics

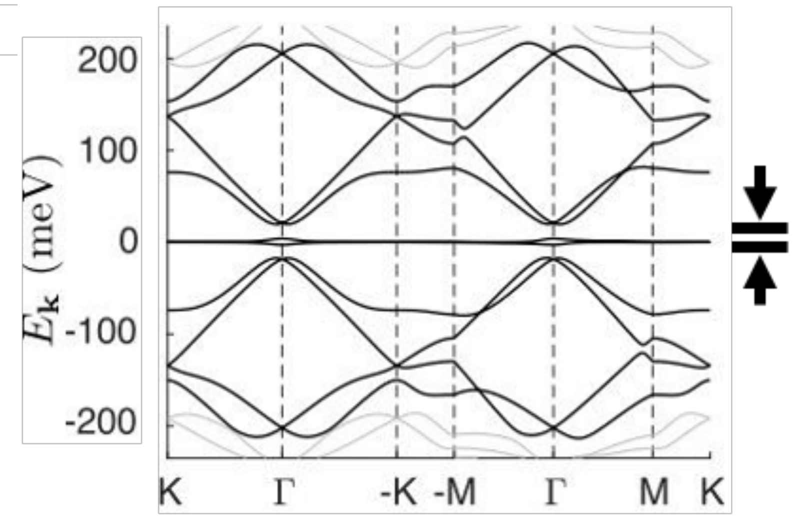


20° **rotation**

Quantum moiré materials exhibit many-body phenomena

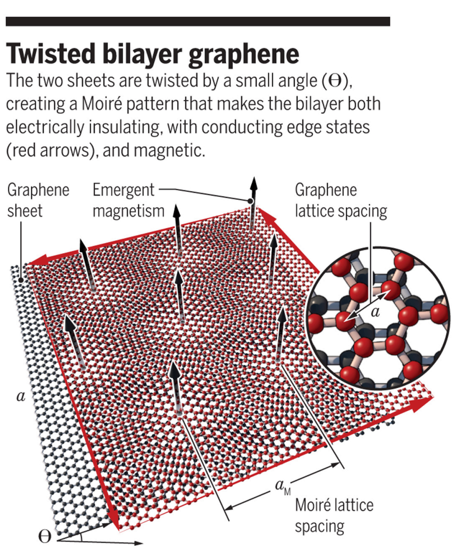
Flat band (fragile) **topology** + long-range Coulomb **interaction**

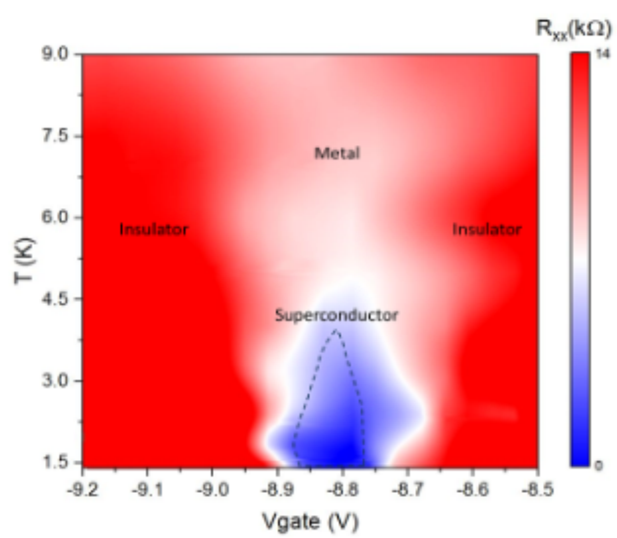


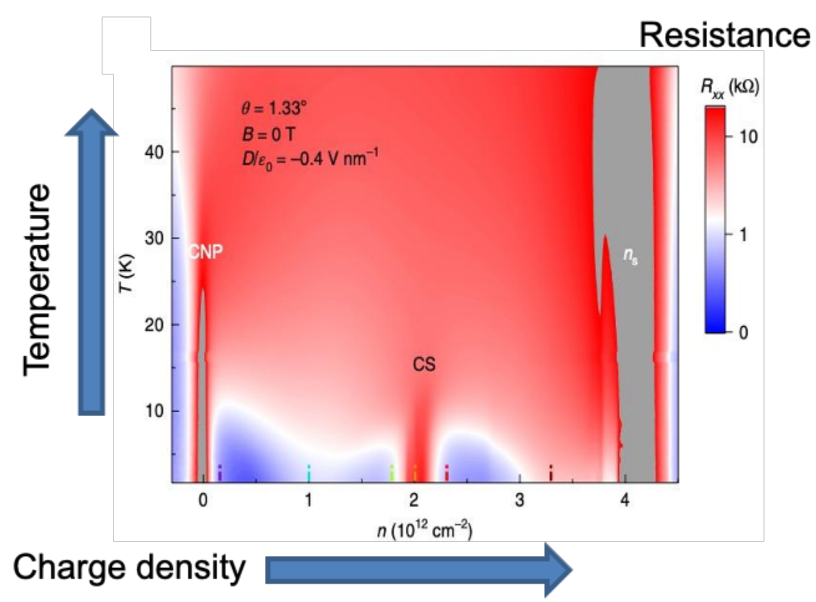


Trambly, et al. Nano Letter 2010
Bistritzer & MacDonald, PNAS 2011

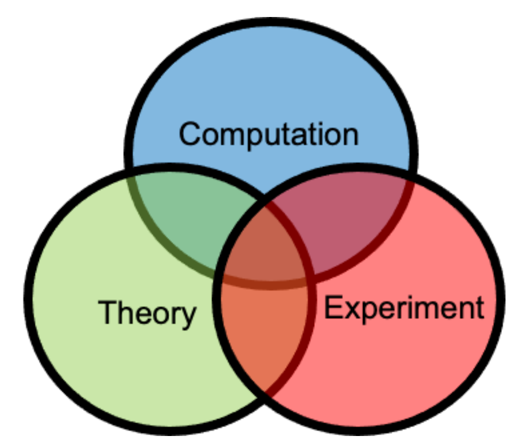
Multiple parameters (angle, filling, temperature, field) ⟶ novel **phase diagrams**







Rich and difficult physics requires joint efforts



Cao, et al. Nature 2018
Cao, et al. Nature 2018
Lu, et al. Nature 2019
…

TMDC: WSe2

Ning Wang, Nanoscale Horiz. 2020

TDBG

Shen, …, **Meng**, et al. Nature Physics 2019

In collaborations with

Xu Zhang 张栩（HKU）
Bin-Bin Chen 陈斌斌 (HKU)
Cheng Huang 黄程 (HKU)
Gaopei Pan 潘高培 (Würzburg)

Meizhen Huang 黄美珍 (HKUST)
Ning Wang 王宁 (HKUST)
Berthold Jaeck (HKUST)
Xi Dai 戴希 (HKUST)

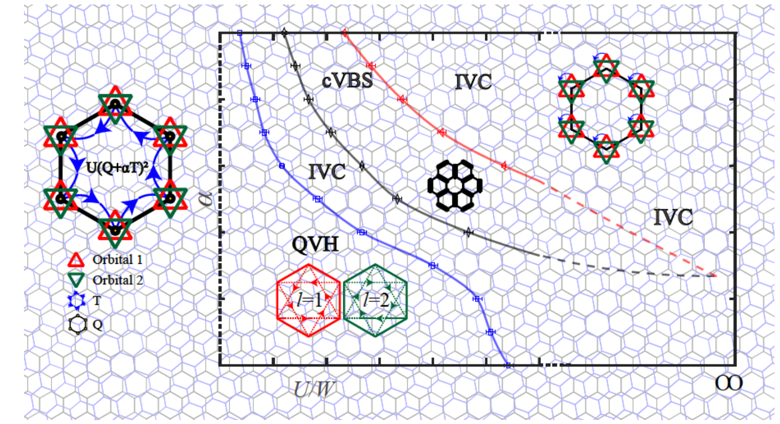
Yuan Da Liao (Fudan)
Xiao Yan Xu (SJTU)
Xiyue Lin (ITP)
Wei Li (ITP)
Tao Shi (ITP)

Heqiu Li 李河虬 (Toronto)
Kai Sun 孙锴 (Michigan)
Rafael Fernandes (Minnesota)

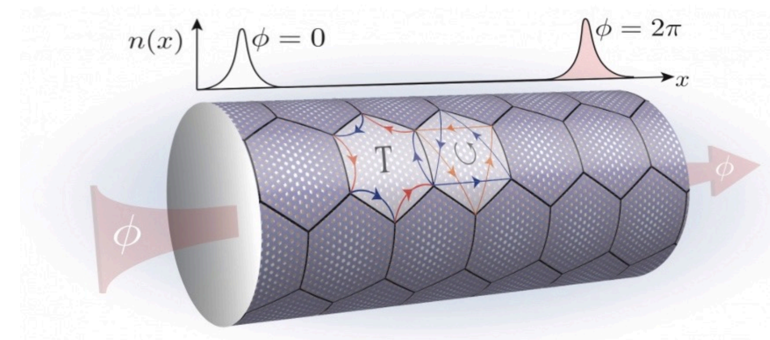
Clara N. Breiø (NBI)
Brian M. Andersen (NBI)

Content

1. Real-space models and QMC / TRG phase diagram

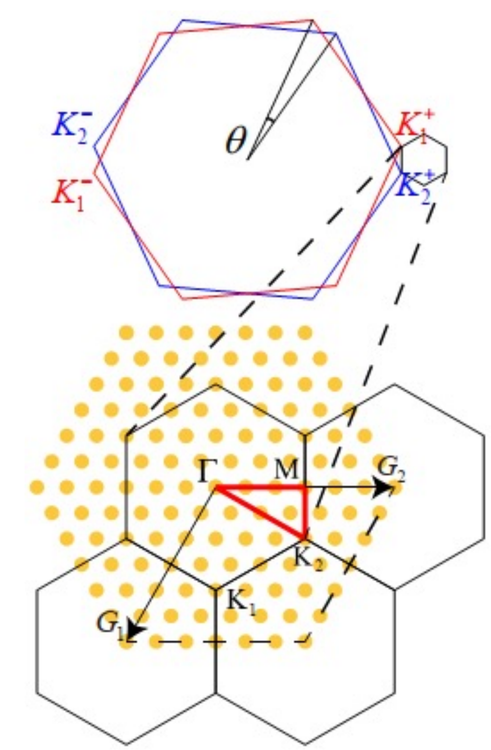


- PRL 123, 157601 (2019) [valence bond solid]
- PRX 11, 011014 (2021) [intervalley coherent insulator]
- Nat. Commun. 12, 5480 (2021) [quantum anomalous Hall]
- PRL 128, 157201 (2022) [exciton proliferation]
- ……

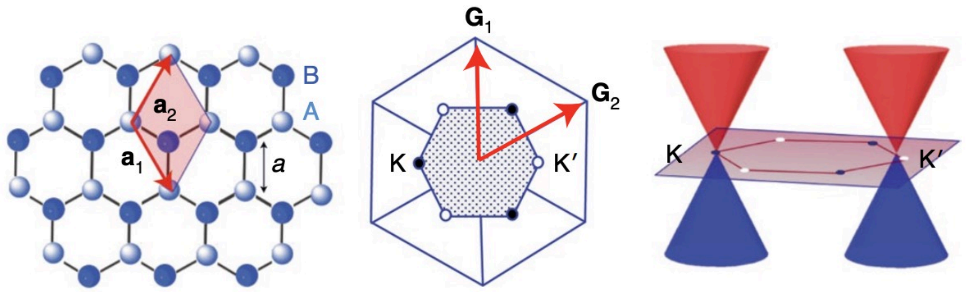


2. Momentum-space QMC for long-range Coulomb and quantum metric

- CPL 38, 077305 (2021) [momentum-space QMC]
- PRB 105, L121110 (2022) [valley waves]
- PRB 106, 184517 (2022) Editors' Suggestion [superconductivity]
- PRL 130, 016401 (2023) [Thermodynamic responses]
- PRB 107, L241105 (2023) [Polynomial sign and Topo. Mott]
- PRL 131, 066301 (2023) Editors' Suggestion [non-linear Hall]
- ……



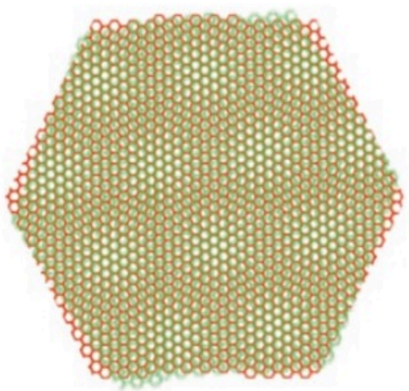
TBG — Setting

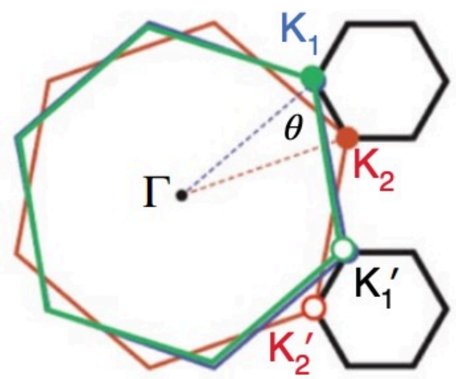


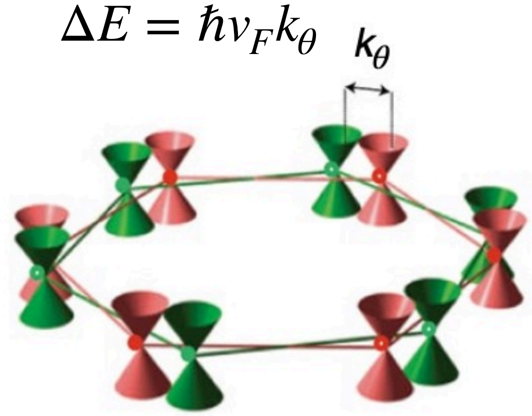
Andrei, E.Y., MacDonald, A.H. Nat Mater 19, 1265 (2020)

interlayer tunnelling produces avoided crossings

$L \approx a_0/(2\sin(\theta/2))$ $k_\theta \approx 2K\sin(\theta/2)$ $\Delta E = \hbar v_F k_\theta$

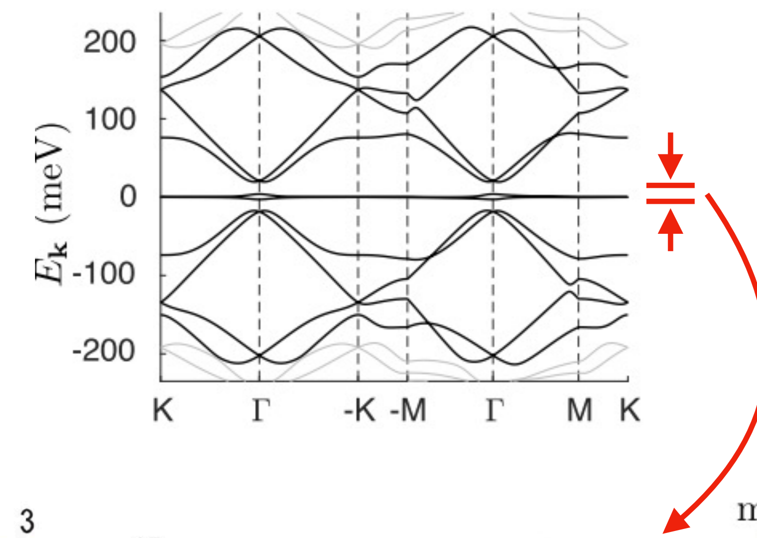




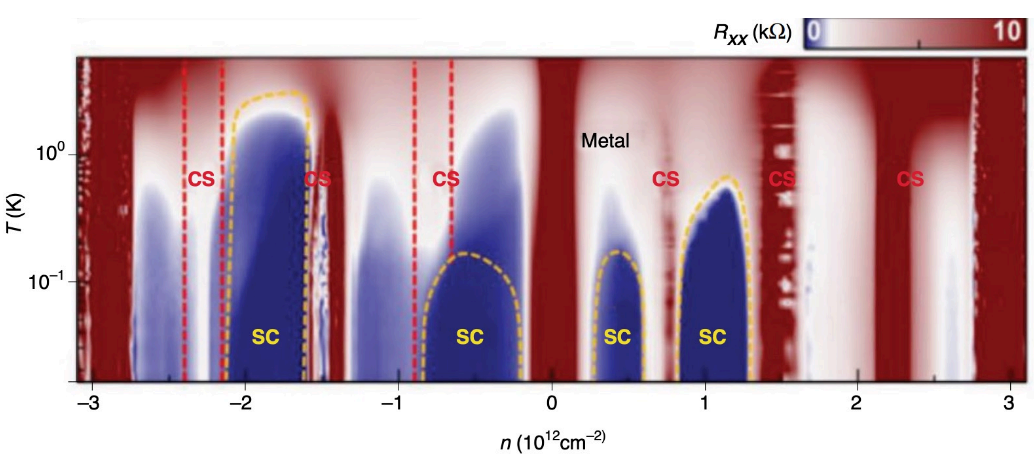


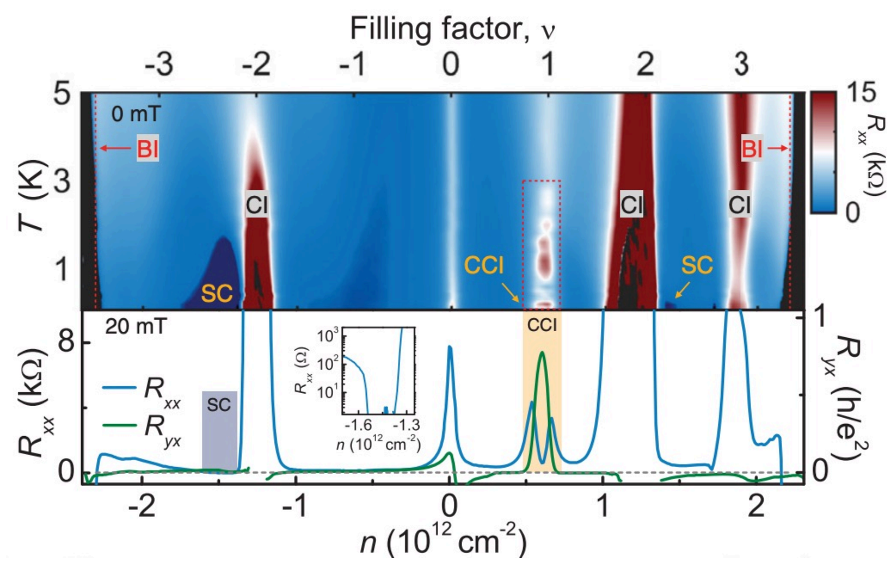
$\theta > 10^\circ$ $\Delta E > 1$ eV isolated graphene

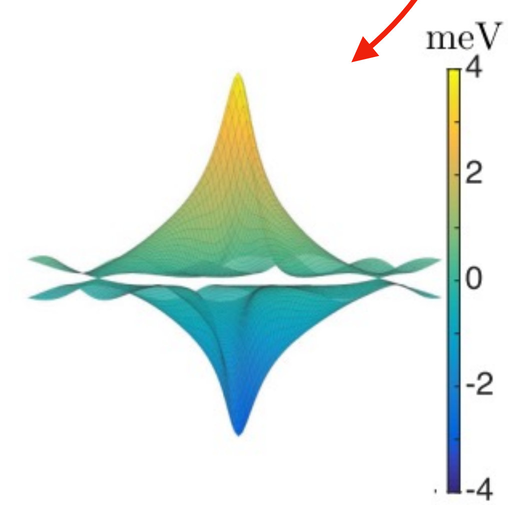
$\theta \sim 1^\circ$ layers hybridization
strong tunnelings couple Dirac cones
flat bands and strong correlation



Lu, Stepanov, …, MacDonald, Efetov, Nature 574, 653 (2019)



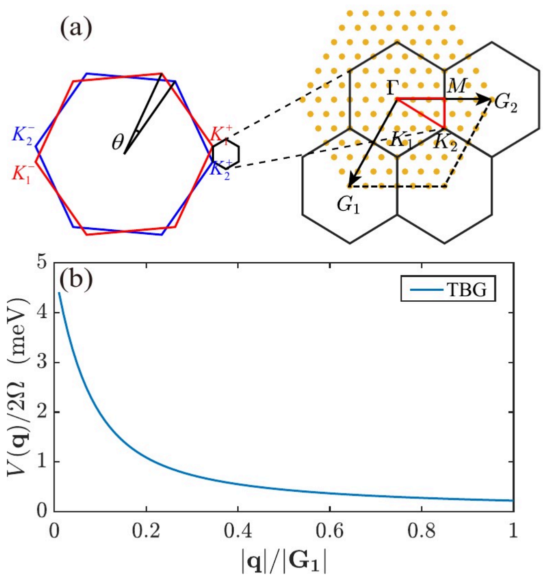


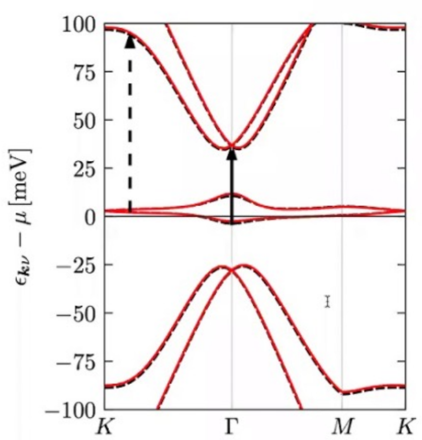


Stepanov, …, Bernevig, Efetov, PRL 127, 197701 (2021) Po, … , Vishwanath, PRB 99, 195455 (2019)

TBG — Setting, Questions

$$H = \underbrace{\sum_{m\mathbf{k}s\tau}(\epsilon_{m\mathbf{k}\tau}-\mu)d^{+}_{m\mathbf{k}s\tau}d_{m\mathbf{k}s\tau}}_{H_0} + \underbrace{\frac{1}{2S}\sum_{\{m_i\}}\sum_{ss'\tau\tau'}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}} V^{\tau\tau'\tau'\tau}_{m_1,m_2,m_3,m_4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\; d^{+}_{m_1\mathbf{k}_1-\mathbf{q}s\tau}d^{+}_{m_2\mathbf{k}_2+\mathbf{q}s'\tau'}d_{m_3\mathbf{k}_2s'\tau'}d_{m_4\mathbf{k}_1s\tau}}_{H_{int}}$$





$$V^{\tau\tau'\tau'\tau}_{m_1,m_2,m_3,m_4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}) = \sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G})\; \lambda_{m_1m_4;\tau}(\mathbf{k}_1-\mathbf{q},\mathbf{k}_1+\mathbf{G})\lambda^{*}_{m_3m_2;\tau'}(\mathbf{k}_2,\mathbf{k}_2+\mathbf{q}+\mathbf{G})$$

$\mathbf{k}_1, \mathbf{k}_2, \mathbf{q} \in$ mBZ

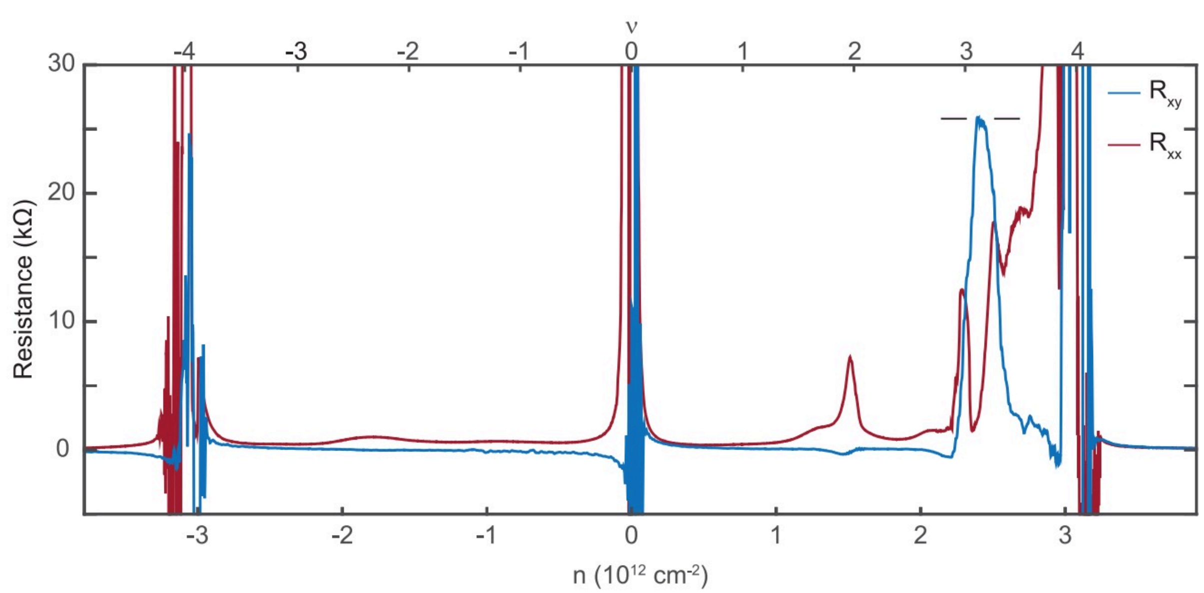
$\mathbf{G} = n_1\mathbf{G}_1 + n_2\mathbf{G}_2$

Gate-screened Coulomb potential

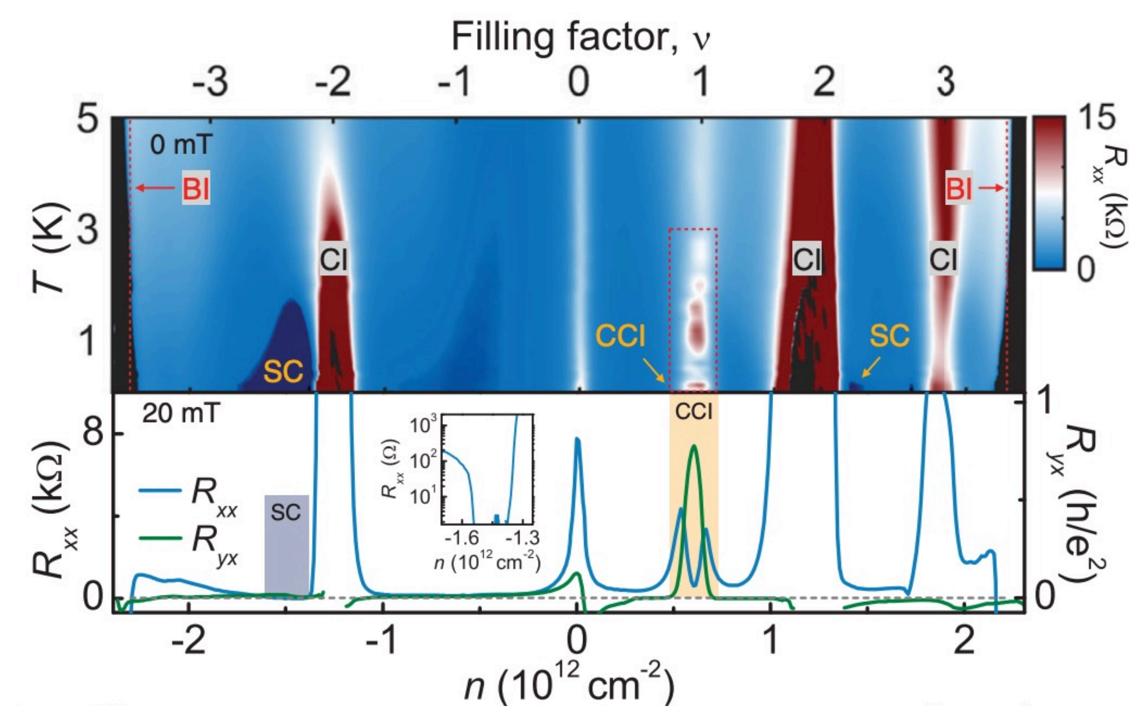
$$V(\mathbf{q}) = \frac{e^2}{2\varepsilon\varepsilon_0 q}(1-e^{-2qd_s})$$

form factors from Bloch WF

$$\lambda_{m_1,m_2,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u_{\mathbf{k},m_1} | u_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$



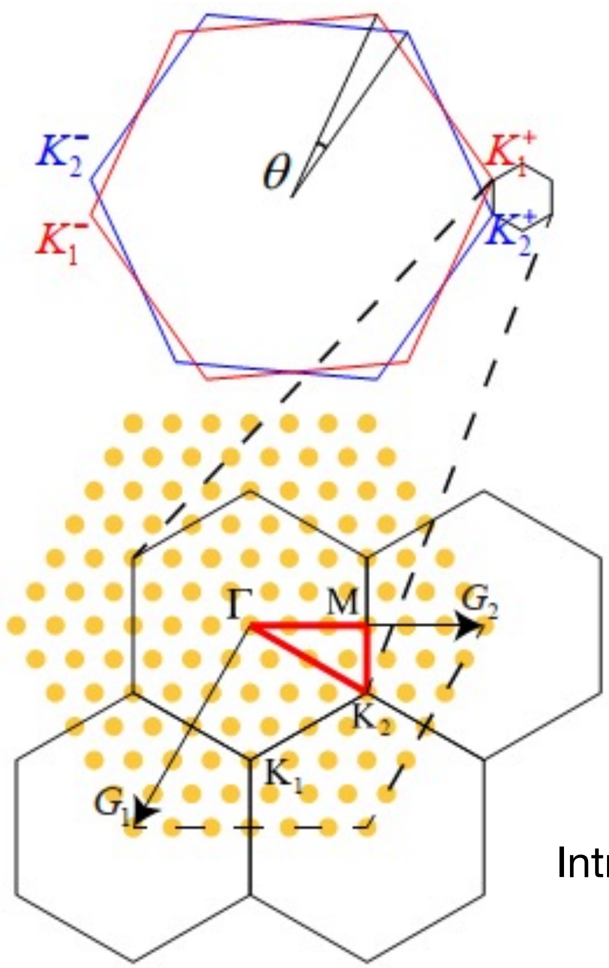
Serlin… Young, Science 367, 900 (2020)



Stepanov … Efetov, PRL 127, 197701 (2021)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

Xu Zhang(张栩)[1†], Gaopei Pan(潘高培)[2,3†], Yi Zhang(张焱)[4],
Jian Kang(康健)[5], and Zi Yang Meng(孟子杨)[1,2*]



$$H = H_0 + H_{int}$$

CPL 38, 077305 (2021) Express Letter

- Trambly de Laissardiere et al., Nano Lett. 2010
- Bistritzer & MacDonald, PNAS 2011 BM Hamiltonian

$$H^{\tau}_{0,\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} \begin{pmatrix} -\hbar v_F(\mathbf{k}-\mathbf{K}_1^\tau)\cdot\boldsymbol{\sigma}^\tau & U_0 \\ U_0^\dagger & -\hbar v_F(\mathbf{k}-\mathbf{K}_2^\tau)\cdot\boldsymbol{\sigma}^\tau \end{pmatrix} + \begin{pmatrix} 0 & U_1^\tau \delta_{\mathbf{k},\mathbf{k}'-\tau\mathbf{G}_1} \\ U_1^{\tau\dagger}\delta_{\mathbf{k},\mathbf{k}'+\tau\mathbf{G}_1} & 0 \end{pmatrix} + \begin{pmatrix} 0 & U_2^\tau \delta_{\mathbf{k},\mathbf{k}'-\tau(\mathbf{G}_1+\mathbf{G}_2)} \\ U_2^{\tau\dagger}\delta_{\mathbf{k},\mathbf{k}'+\tau(\mathbf{G}_1+\mathbf{G}_2)} & 0 \end{pmatrix}$$

$\tau = \pm$ valley

v_F Dirac velocity

$\mathbf{K}^\tau_{1,2}$ Dirac points

$\sigma^\tau = (\tau\sigma_x, \sigma_y)$ A/B sublattice

$$\mathbf{G}_1 = \left(-\frac{2\pi}{\sqrt{3}L_M}, -\frac{2\pi}{L_M}\right)$$
$$\mathbf{G}_2 = \left(\frac{4\pi}{\sqrt{3}L_M}, 0\right)$$

Intra-sublattice, interlayer hopping

$$U_0 = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}$$

Inter-sublattice, interlayer hopping

$\theta = 1.08°$ 1st magic angle

$u_1 = 110$ meV

$u_0 = 0$ chiral limit

$u_0 \sim 60$ meV, realistic cases

$\hbar v_F / a_0 = 2377.45$ meV

$L_M \approx a_0/(2\sin(\theta/2)) \sim 10$ nm

Similar for matrices U_1, U_2

$$H_0 = \sum_{m=\pm 1} \sum_{\mathbf{k},\tau,s} \epsilon_{m,\tau}(\mathbf{k})\, d^\dagger_{\mathbf{k},m,\tau,s}\, d_{\mathbf{k},m,\tau,s}$$

- Fermionic Monte Carlo Study of a Realistic Model of Twisted Bilayer Graphene, Johannes S. Hofmann, et al., PRX 12, 011061 (2022)

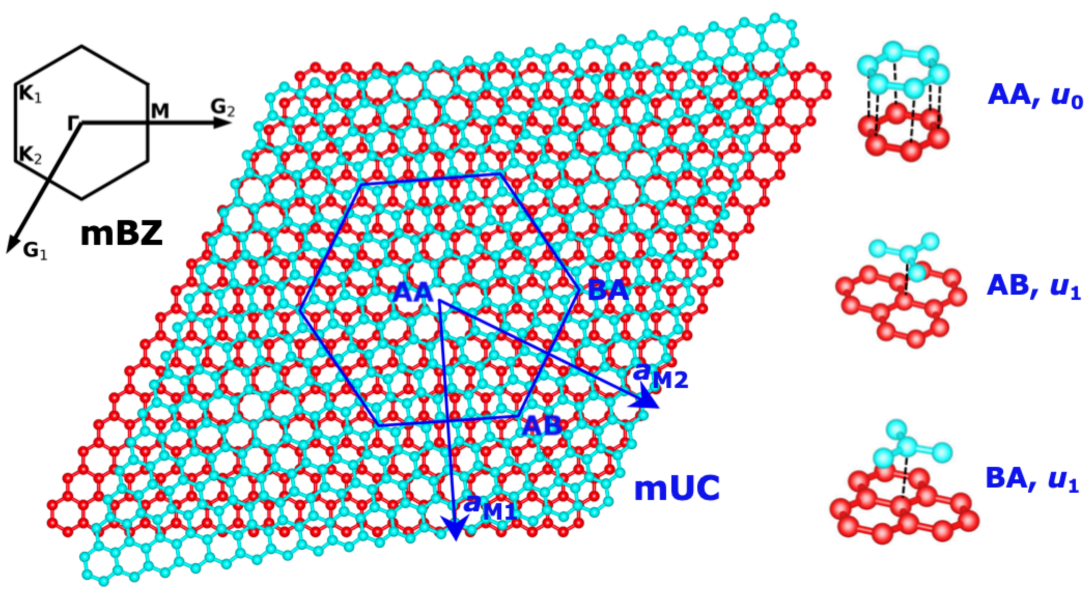
Intra-sublattice, interlayer hopping

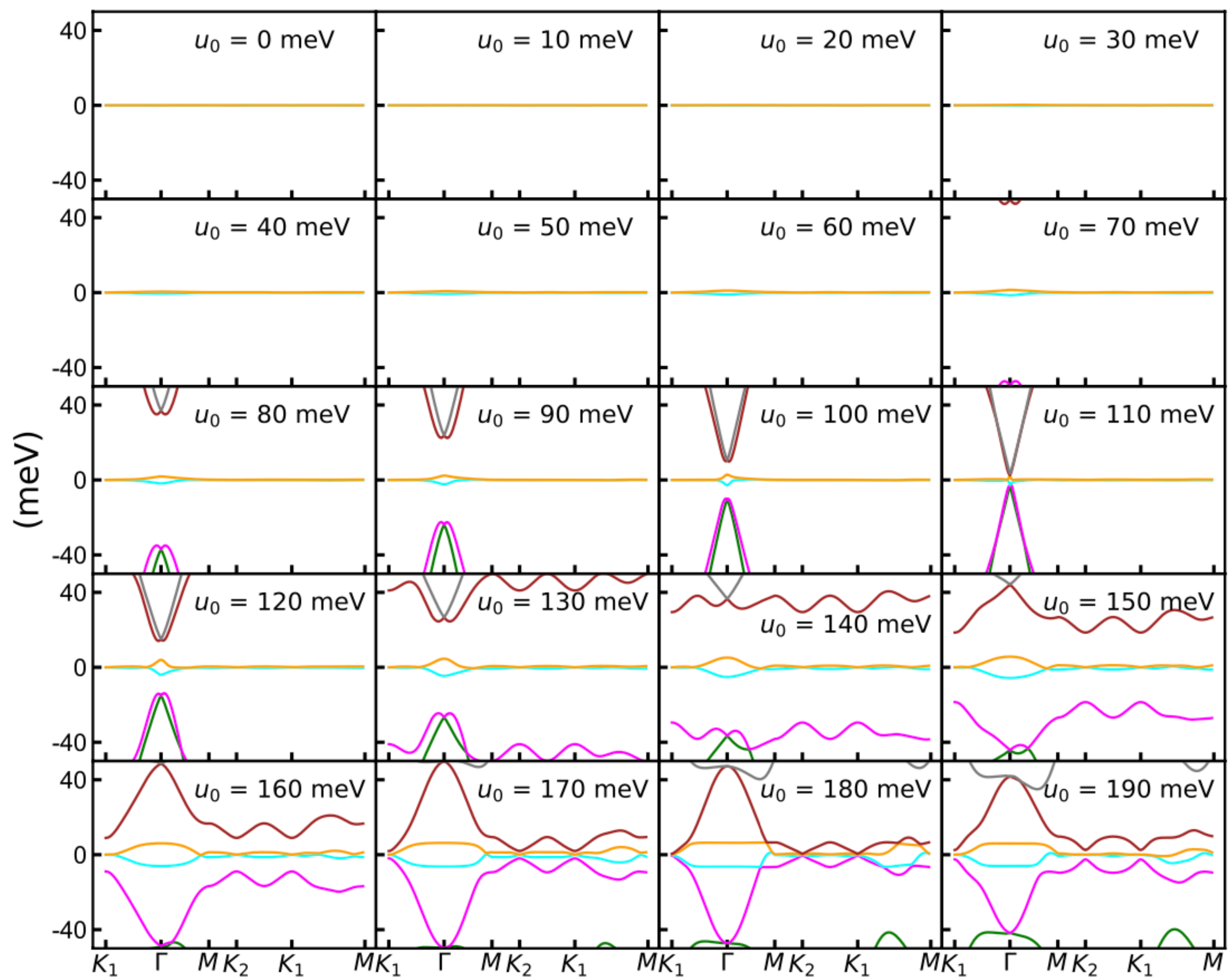
$$U_0 = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}$$

Inter-sublattice, interlayer hopping

Similar for matrices $U_1, \ U_2$

$$H_0 = \sum_{m=\pm 1} \sum_{\mathbf{k},\tau,s} \epsilon_{m,\tau}(\mathbf{k}) \ d^{\dagger}_{\mathbf{k},m,\tau,s} \ d_{\mathbf{k},m,\tau,s}$$





- Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in twisted bilayer graphene
  Cheng Huang, Xu Zhang, Gaopei Pan, Heqiu Li, Kai Sun, Xi Dai, Zi Yang Meng,
  arXiv: 2304.14064

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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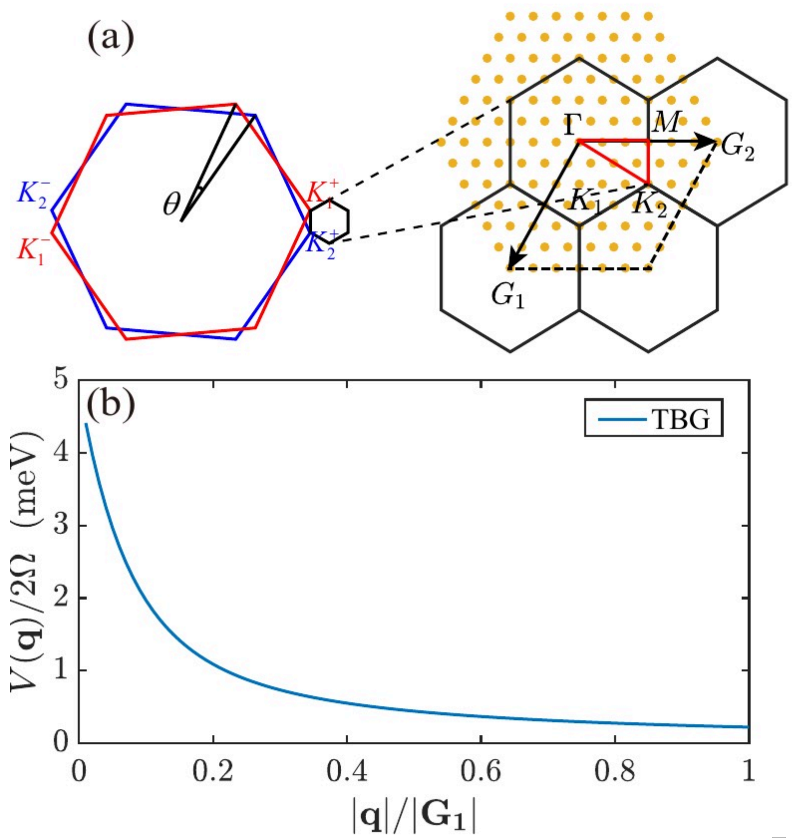
CPL 38, 077305 (2021) Express Letter



$$H = H_0 + H_{int}$$

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

$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{\mathbf{k}\in mBZ, m_1, m_2, \tau, s} \lambda_{m_1,m_2,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})\ (d^\dagger_{\mathbf{k},m_1,\tau,s}\ d_{\mathbf{k}+\mathbf{q},m_2,\tau,s} - \frac{\nu+4}{8}\delta_{\mathbf{q},0}\ \delta_{m_1,m_2})$$

$$\lambda_{m_1,m_2,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u_{\mathbf{k},m_1} | u_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$ overlap of H_0 eigenstate

$$V(\mathbf{q}) = \frac{e^2}{4\pi\varepsilon}\int d^2\mathbf{r}(\frac{1}{\mathbf{r}} - \frac{1}{\sqrt{\mathbf{r}^2+d^2}})\ e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{e^2}{2\varepsilon}\frac{1}{q}(1-e^{-qd})$$

Single gate

$$\frac{d}{2} = 20 \text{ nm}$$

$$\varepsilon = 7\varepsilon_0$$

$$\Omega = N_{\mathbf{k}}\frac{\sqrt{3}}{2}L_M^2 \qquad N_{\mathbf{k}} = 6\times6,\ 9\times9,\ 12\times12$$

$$= \sum_{\mathbf{G},\mathbf{q}\in mBZ}\frac{V(\mathbf{q}+\mathbf{G})}{2}[(\delta\rho_{-\mathbf{q}-\mathbf{G}}+\delta\rho_{\mathbf{q}+\mathbf{G}})^2 - (\delta\rho_{-\mathbf{q}-\mathbf{G}}-\delta\rho_{\mathbf{q}+\mathbf{G}})^2]$$

Fermionic Monte Carlo Study of a Realistic Model of Twisted Bilayer Graphene, Johannes S. Hofmann, et al., PRX 12, 011061 (2022)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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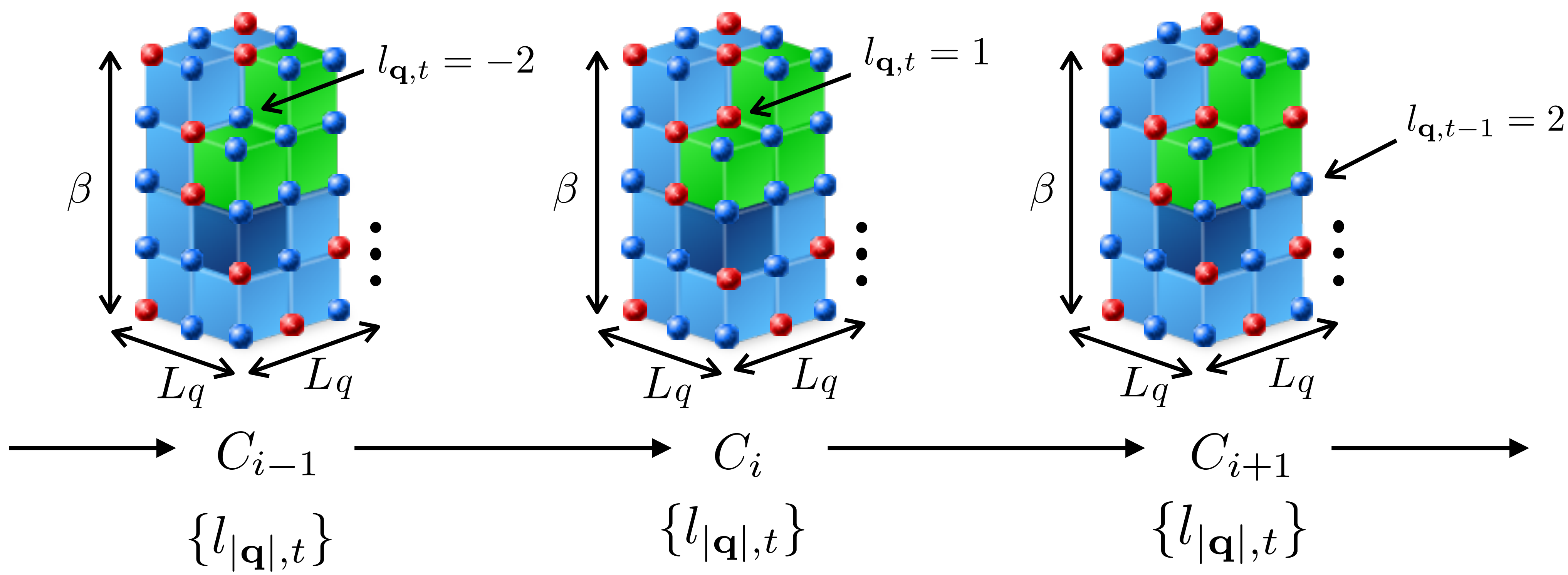
CPL 38, 077305 (2021) Express Letter

$$Z = \mathrm{Tr}\left\{ \prod_t e^{-\Delta\tau H_{\mathrm{int}}(t)} \right\}$$

$$= \mathrm{Tr}\left\{ \prod_t \exp\left\{ -\Delta\tau \frac{1}{4\Omega} \sum_{|\boldsymbol{q}+\boldsymbol{G}|\neq 0} V(\boldsymbol{q}+\boldsymbol{G}) \cdot \left[\left(\delta\rho_{-\boldsymbol{q}-\boldsymbol{G}} + \delta\rho_{\boldsymbol{q}+\boldsymbol{G}}\right)^2 - \left(\delta\rho_{-\boldsymbol{q}-\boldsymbol{G}} - \delta\rho_{\boldsymbol{q}+\boldsymbol{G}}\right)^2 \right] \right\} \right\}$$

$$\approx \sum_{\{l_{|\boldsymbol{q}|,t}\}} \prod_t \left[\prod_{|\boldsymbol{q}+\boldsymbol{G}|\neq 0} \frac{1}{16} \gamma\left(l_{|\boldsymbol{q}|_1,t}\right) \gamma\left(l_{|\boldsymbol{q}|_2,t}\right) \right] \cdot \mathrm{Tr}\left\{ \prod_t \left\{ \prod_{|\boldsymbol{q}+\boldsymbol{G}|\neq 0} \exp\left[i\eta\left(l_{|\boldsymbol{q}|_1,t}\right) A_{\boldsymbol{q}} \left(\delta\rho_{-\boldsymbol{q}} + \delta\rho_{\boldsymbol{q}}\right) \right] \cdot \exp\left[\eta\left(l_{|\boldsymbol{q}|_2,t}\right) A_{\boldsymbol{q}} \left(\delta\rho_{-\boldsymbol{q}} - \delta\rho_{\boldsymbol{q}}\right) \right] \right\} \right\}$$

$$e^{\alpha \hat{O}^2} = \frac{1}{4} \sum_{l=\pm 1,\pm 2} \gamma(l) e^{\sqrt{\alpha}\eta(l)\hat{o}} + O\left(\alpha^4\right) \qquad A_{\boldsymbol{q}+\boldsymbol{G}} = \sqrt{\frac{\Delta\tau}{4} \frac{V(\boldsymbol{q}+\boldsymbol{G})}{\Omega}} \qquad \{l_{|\boldsymbol{q}|_1,t}, l_{|\boldsymbol{q}|_2,t}, l_{0,t}\}$$



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Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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Jian Kang(康健)[5], and Zi Yang Meng(孟子杨)[1,2*]

CPL 38, 077305 (2021) Express Letter

$C_{2z}T$ symmetry $\lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) = \lambda^*_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})$

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

$$\begin{aligned}
\delta\rho_{\mathbf{q}+\mathbf{G},-\tau} &= \sum_{\mathbf{k},m,n} \lambda_{m,n,-\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(c^\dagger_{\mathbf{k},m,-\tau}c_{\mathbf{k}+\mathbf{q},n,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= \sum_{\mathbf{k},m,n} -m\times n\times \lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(c_{\mathbf{k}+\mathbf{q},-n,-\tau}c^\dagger_{\mathbf{k},-m,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= \sum_{\mathbf{k},m,n} -\lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(\tilde{c}^\dagger_{\mathbf{k}+\mathbf{q},n,-\tau}c_{\mathbf{k},m,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= \sum_{\mathbf{k},m,n} -\lambda^*_{n,m,\tau}(\mathbf{k},\mathbf{k}-\mathbf{q}-\mathbf{G})(\tilde{c}^\dagger_{\mathbf{k},n,-\tau}c_{\mathbf{k}-\mathbf{q},m,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= -\delta\rho_{-\mathbf{q}-\mathbf{G},\tau}
\end{aligned}$$

$$\tilde{c}_{\mathbf{k},m,-\tau} = m\times c^\dagger_{\mathbf{k},-m,-\tau}$$

$$\mathrm{Tr}\{\prod_t B(\{l_{|\mathbf{q}|,t}\})\} = \sum_{\{l_{|\mathbf{q}|,t}\}} D_\tau(\{l_{|\mathbf{q}|,t}\})D_{-\tau}(\{l_{|\mathbf{q}|,t}\}) = \sum_{\{l_{|\mathbf{q}|,t}\}} D_\tau(\{l_{|\mathbf{q}|,t}\})D^*_\tau(\{l_{|\mathbf{q}|,t}\})$$

No sign-problem

decoupled Hamiltonian is traceless anti-Hermitian matrix ⟶

Degrees of freedom	Kinetic terms	Sign structure
Single valley single spin	No	Real
Single valley double spin	No	Non-negative
Double valley single spin	Flat bands	Non-negative
Double valley double spin	Flat bands	Non-negative

Fermionic Monte Carlo Study of a Realistic Model of Twisted Bilayer Graphene, Johannes S. Hofmann, et al., PRX 12, 011061 (2022)

Dynamical properties of collective excitations in twisted bilayer graphene

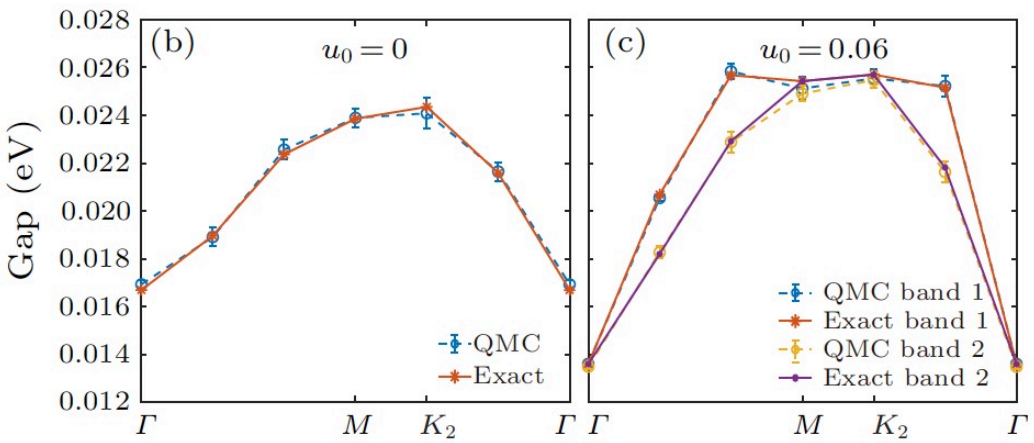
Gaopei Pan[1,2] Xu Zhang[3] Heqiu Li[4,5] Kai Sun,[4,*] and Zi Yang Meng[3,†]

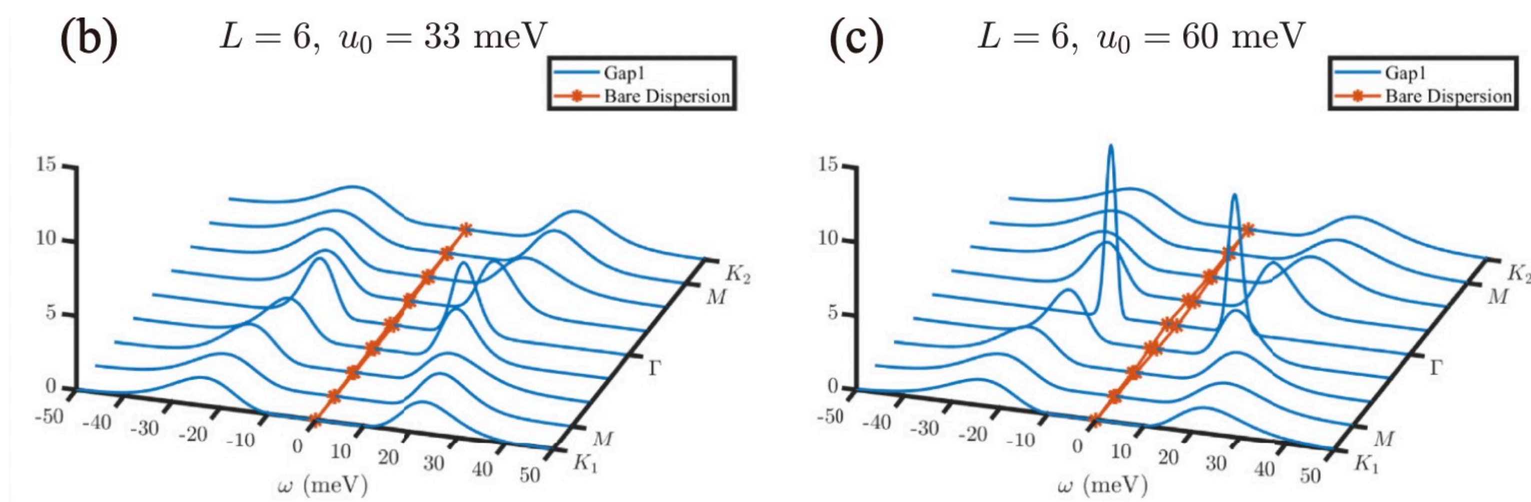
CPL 38, 077305 (2021) Express Letter

single-particle excitations

PRB 105, L121110 (2022)

$T = 0.667$ meV





$$\mathcal{O}_a(\boldsymbol{q},\tau) \equiv \sum_{\boldsymbol{k}} d^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) M_a d_{\boldsymbol{k}}(\tau)$$

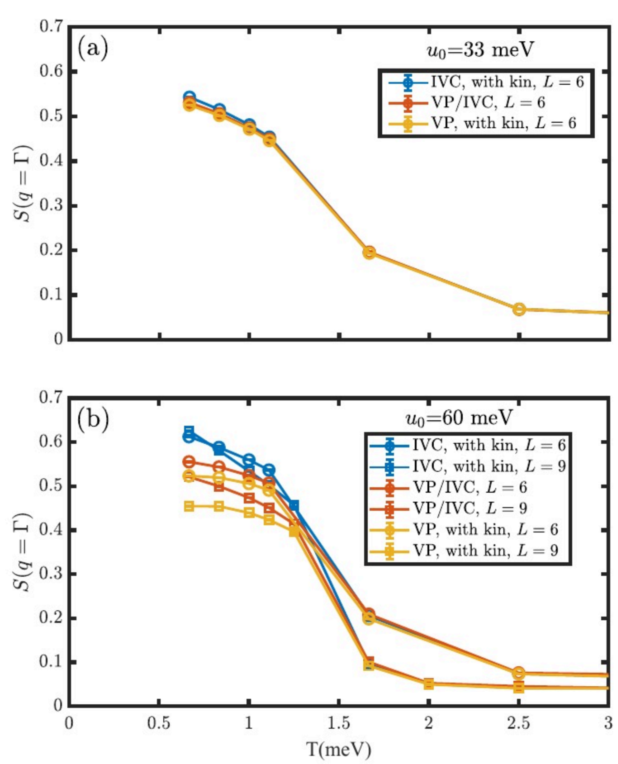
Bosonic collective excitations

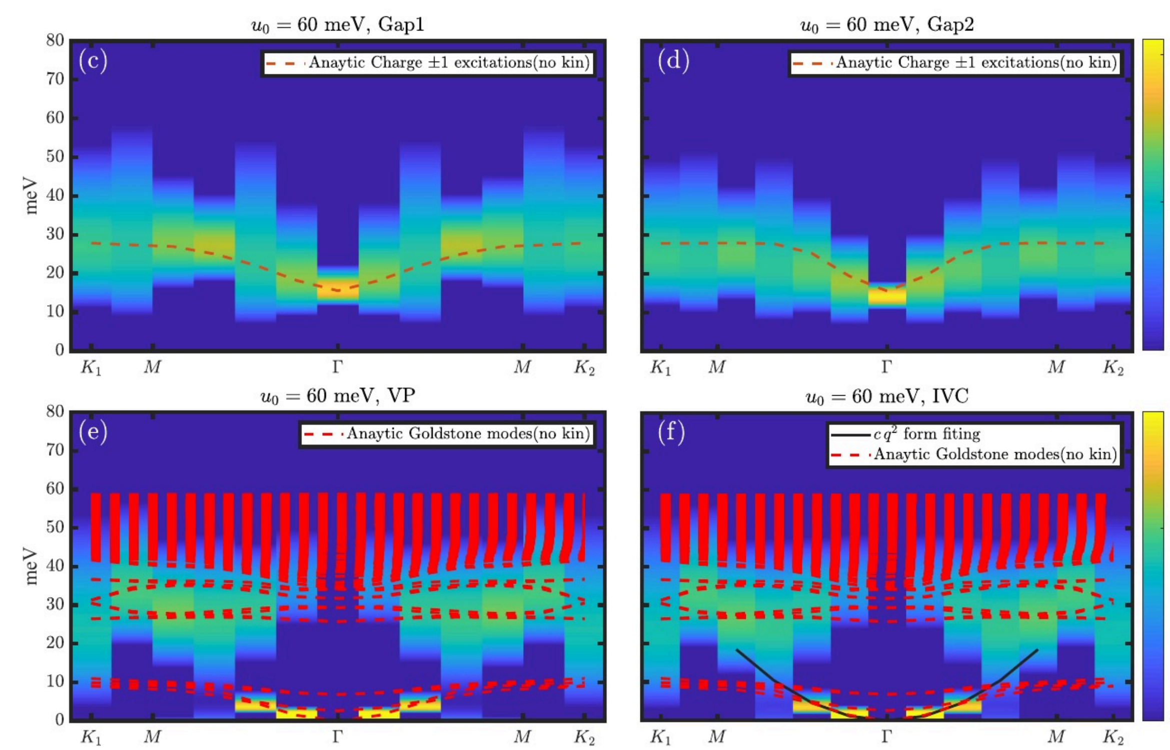
$$M_a = \tau_z \eta_0$$

for valley polarized state

$$M_a = \tau_x \eta_y \ \text{or} \ \tau_y \eta_y$$

for intervalley coherent state





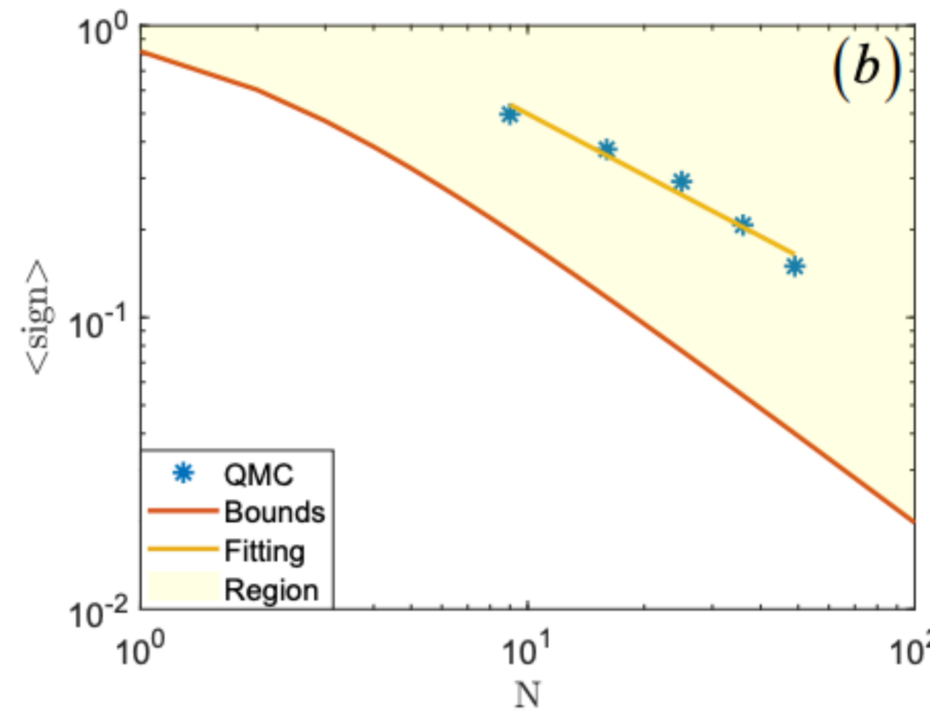
PHYSICAL REVIEW B **106**, 035121 (2022)

Fermion sign bounds theory in quantum Monte Carlo simulation

Xu Zhang [1], Gaopei Pan [2,3], Xiao Yan Xu [4,*] and Zi Yang Meng [1,†]

$$H = \frac{1}{2\Omega} \sum_{\mathbf{q},\mathbf{G},|\mathbf{q}+\mathbf{G}|\neq 0} V(\mathbf{q}+\mathbf{G})\delta\rho_{\mathbf{q}+\mathbf{G}}\delta\rho_{-\mathbf{q}-\mathbf{G}}$$

$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{\mathbf{k},m_1,m_2} \lambda_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(d^\dagger_{\mathbf{k},m_1} d_{\mathbf{k}+\mathbf{q},m_2} - \tfrac{1}{2}\delta_{q,0}\delta_{m_1,m_2}).$$



PHYSICAL REVIEW B **104**, L241104 (2021)

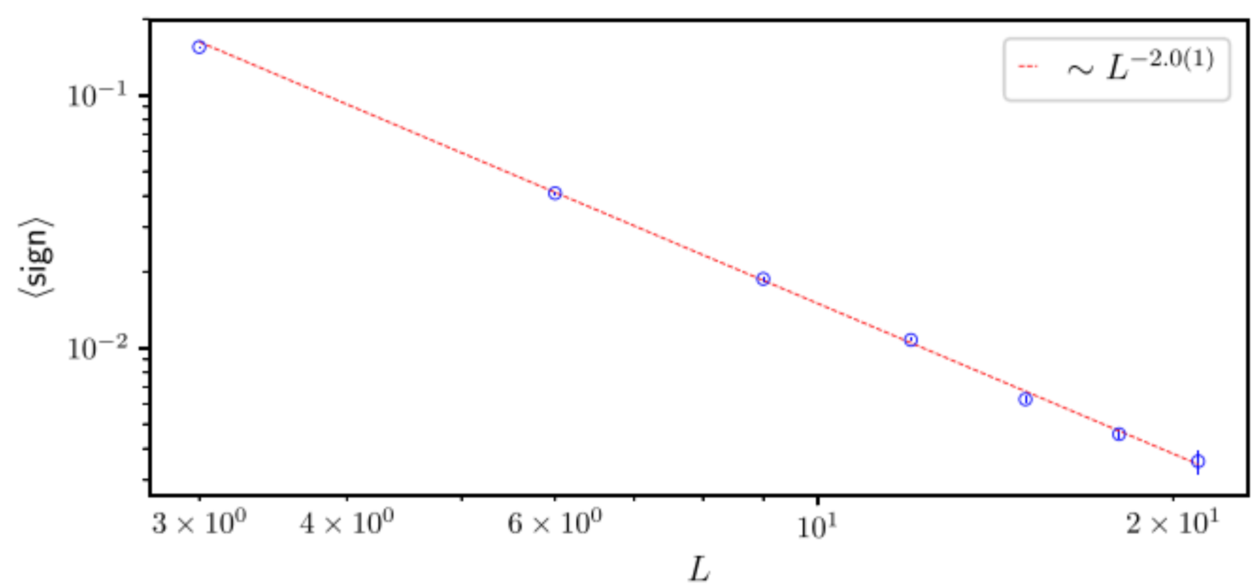
Letter

Projection of infinite-U Hubbard model and algebraic sign structure

Yunqing Ouyang [1,2] and Xiao Yan Xu [3,4,*]

$$H = U_p \sum_{\hexagon} (Q_{\hexagon} + \alpha T_{\hexagon})^2$$

$$e^{-\Delta_\tau U_{\rm p}(\tilde{Q}_{\rm p}-\nu_{\rm p})^2}\Big|_{U_{\rm p}\to+\infty} = \frac{1}{M}\sum_{s_{\rm p}=1}^{M} e^{\frac{i2\pi z s_{\rm p}}{M}(\tilde{Q}_{\rm p}-\nu_{\rm p})}$$



Detective Dr. Dragon on the Monte Carlo Sign Problem

Xu Zhang

$$\langle \hat{O} \rangle = \frac{\sum_l W_l \langle \hat{O} \rangle_l}{\sum_l W_l} = \frac{\frac{\sum_l |\mathrm{Re}(W_l)| \frac{W_l \langle \hat{O} \rangle_l}{|\mathrm{Re}(W_l)|}}{\sum_l |\mathrm{Re}(W_l)|}}{\frac{\sum_l W_l}{\sum_l |\mathrm{Re}(W_l)|}} \equiv \frac{\langle \hat{O} \rangle_{|\mathrm{Re}(W_l)|}}{\langle \mathrm{sign} \rangle}$$

$$\langle sign \rangle \sim e^{-\beta N}$$

$$\langle sign \rangle = \frac{\sum_l W_l}{\sum_l |Re(W_l)|} = \frac{\langle W \rangle}{\langle |Re(W)| \rangle} \qquad \langle |Re(W)| \rangle \le \langle |W| \rangle \le \sqrt{\langle |W|^2 \rangle}$$

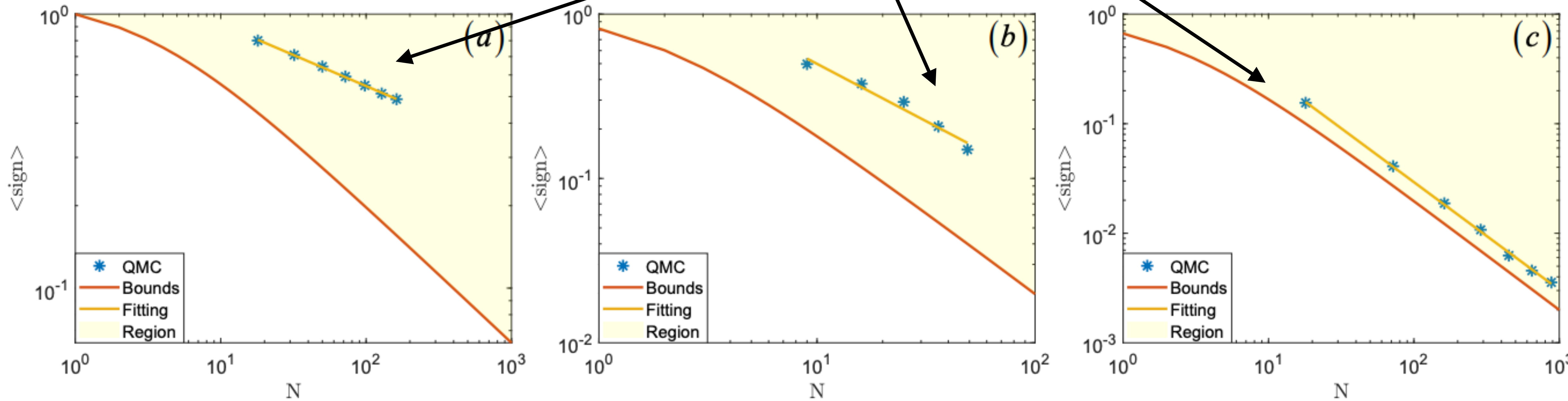
$$\langle sign \rangle \ge \frac{\langle W \rangle}{\langle |W| \rangle} = \frac{Z_W}{Z_{|W|}} = \frac{g_W}{g_{|W|}} e^{-\beta(\langle E \rangle_W - \langle E \rangle_{|W|})}$$

$$\langle sign \rangle \ge \frac{\langle W \rangle}{\sqrt{\langle |W|^2 \rangle}} = \frac{Z_W}{\sqrt{Z_{|W|^2}}} = \frac{g_W}{\sqrt{g_{|W|^2}}} e^{-\beta(\langle E \rangle_W - \langle E \rangle_{|W|^2}/2)}$$

Correlated flat-bands have sign bound

- Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)
- Xu Zhang et al., Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, PRB 107, L241105 (2023)

$$\langle sign \rangle = \frac{\langle W \rangle}{\langle |Re(W)| \rangle}$$



momentum space model

$$\langle sign \rangle \geq \langle sign_{bound} \rangle = \frac{\langle W \rangle}{\sqrt{\langle |W|^2 \rangle}} \sim \frac{1}{\sqrt{N}}$$

target, one valley

reference, two valley, charge neutrality point

momentum space model

$$\langle sign \rangle \geq \langle sign_{bound} \rangle \sim \frac{1}{N}$$

real space model

$$\langle sign \rangle \geq \langle sign_{bound} \rangle = \frac{\langle W \rangle}{\langle |W| \rangle} \sim \frac{1}{N}$$

$$H = U \sum_{\hexagon} \left(Q_{\hexagon} + \alpha T_{\hexagon} - \nu\right)^2$$

$$Q_{\hexagon} = \frac{1}{3} \sum_{\sigma,\tau} \sum_{l=1}^{6} c^{\dagger}_{R+\delta_l,\sigma,\tau} c_{R+\delta_l,\sigma,\tau} - 4$$

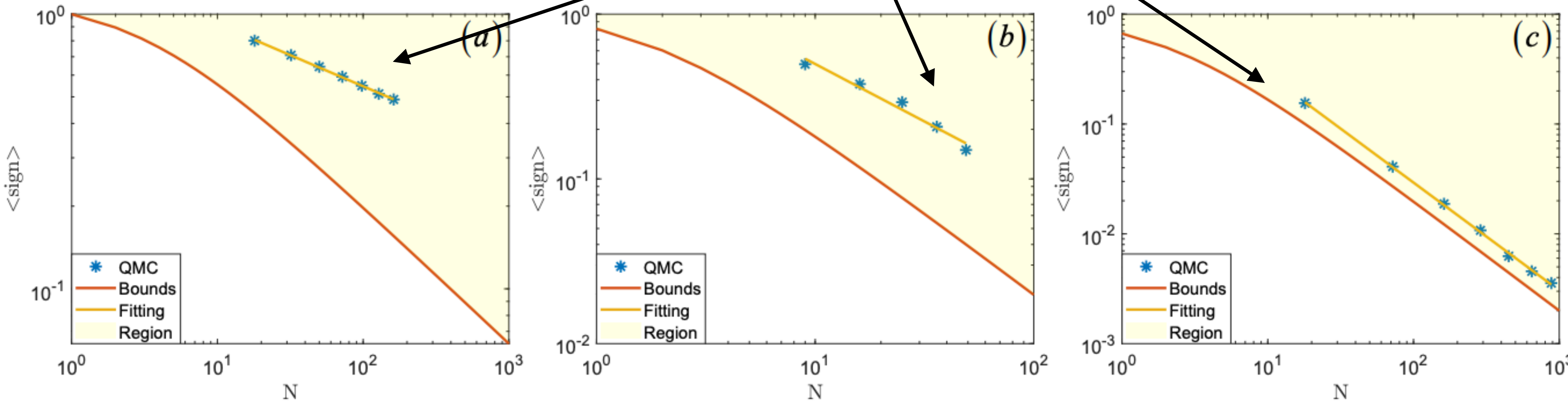
$$T_{\hexagon} = \sum_{\sigma,\tau} \sum_{l=1}^{6} \left[(-1)^l c^{\dagger}_{R+\delta_{l+1},\sigma,\tau} c_{R+\delta_l,\sigma,\tau} + h.c.\right]$$

$\nu = \pm 2$ target

$\nu = 0$ charge neutrality point, reference

📍 Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)

$$\langle sign \rangle = \frac{\langle W \rangle}{\langle |Re(W)| \rangle}$$



momentum space model

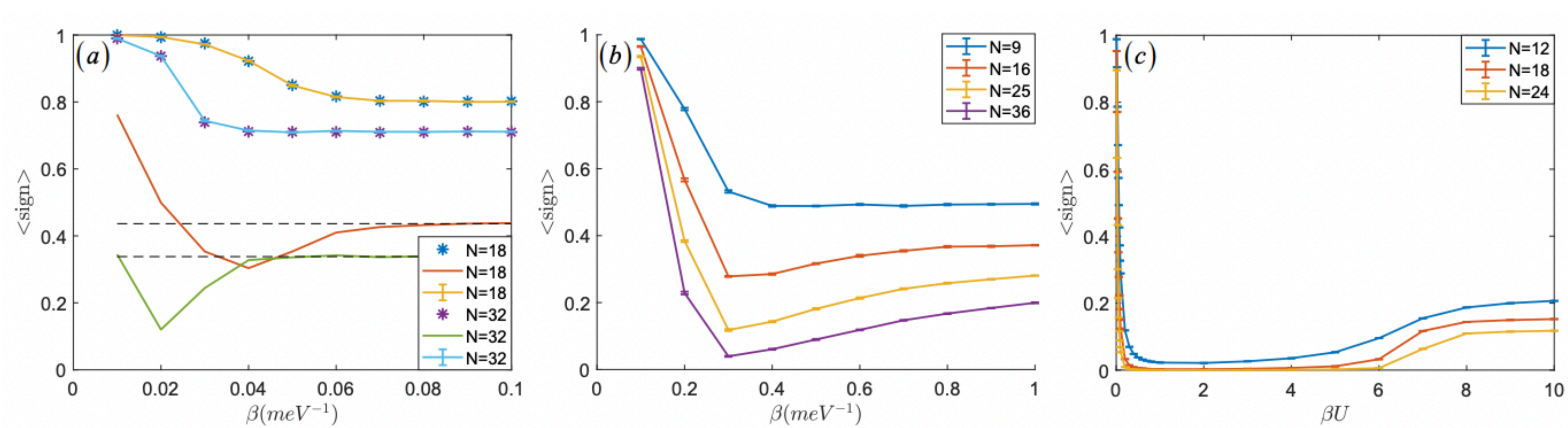
momentum space model

real space model

$$\langle sign \rangle \geq \langle sign_{bound} \rangle = \frac{\langle W \rangle}{\sqrt{\langle |W|^2 \rangle}} \sim \frac{1}{\sqrt{N}}$$

$$\langle sign \rangle \geq \langle sign_{bound} \rangle \sim \frac{1}{N}$$

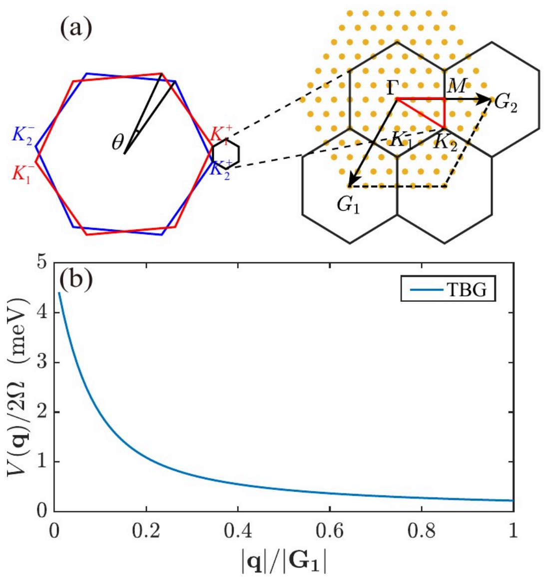
$$\langle sign \rangle \geq \langle sign_{bound} \rangle = \frac{\langle W \rangle}{\langle |W| \rangle} \sim \frac{1}{N}$$

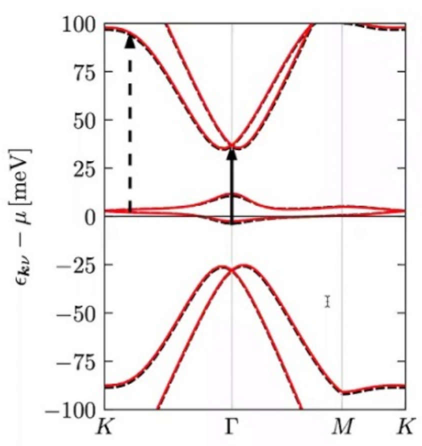


Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)

TBG — Setting, Question 1

$$H = \underbrace{\sum_{m\mathbf{k}s\tau}(\epsilon_{m\mathbf{k}\tau} - \mu)d^{+}_{m\mathbf{k}s\tau}d_{m\mathbf{k}s\tau}}_{H_0} + \underbrace{\frac{1}{2S}\sum_{\{m_i\}}\sum_{ss'\tau\tau'}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}} V^{\tau\tau'\tau'\tau}_{m_1,m_2,m_3,m_4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\; d^{+}_{m_1\mathbf{k}_1-\mathbf{q}s\tau}d^{+}_{m_2\mathbf{k}_2+\mathbf{q}s'\tau'}d_{m_3\mathbf{k}_2s'\tau'}d_{m_4\mathbf{k}_1s\tau}}_{H_{int}}$$





$$V^{\tau\tau'\tau'\tau}_{m_1,m_2,m_3,m_4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}) = \sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G})\;\lambda_{m_1m_4;\tau}(\mathbf{k}_1-\mathbf{q},\mathbf{k}_1+\mathbf{G})\lambda^{*}_{m_3m_2;\tau'}(\mathbf{k}_2,\mathbf{k}_2+\mathbf{q}+\mathbf{G})$$

$\mathbf{k}_1, \mathbf{k}_2, \mathbf{q} \in$ mBZ

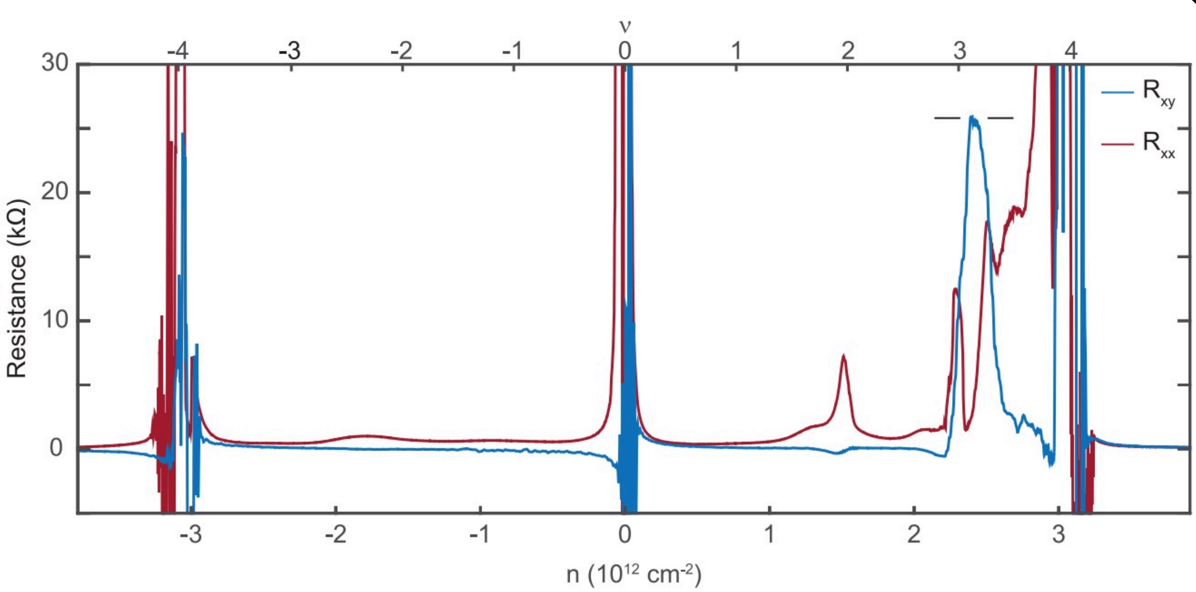
$\mathbf{G} = n_1\mathbf{G}_1 + n_2\mathbf{G}_2$

form factors from Bloch WF

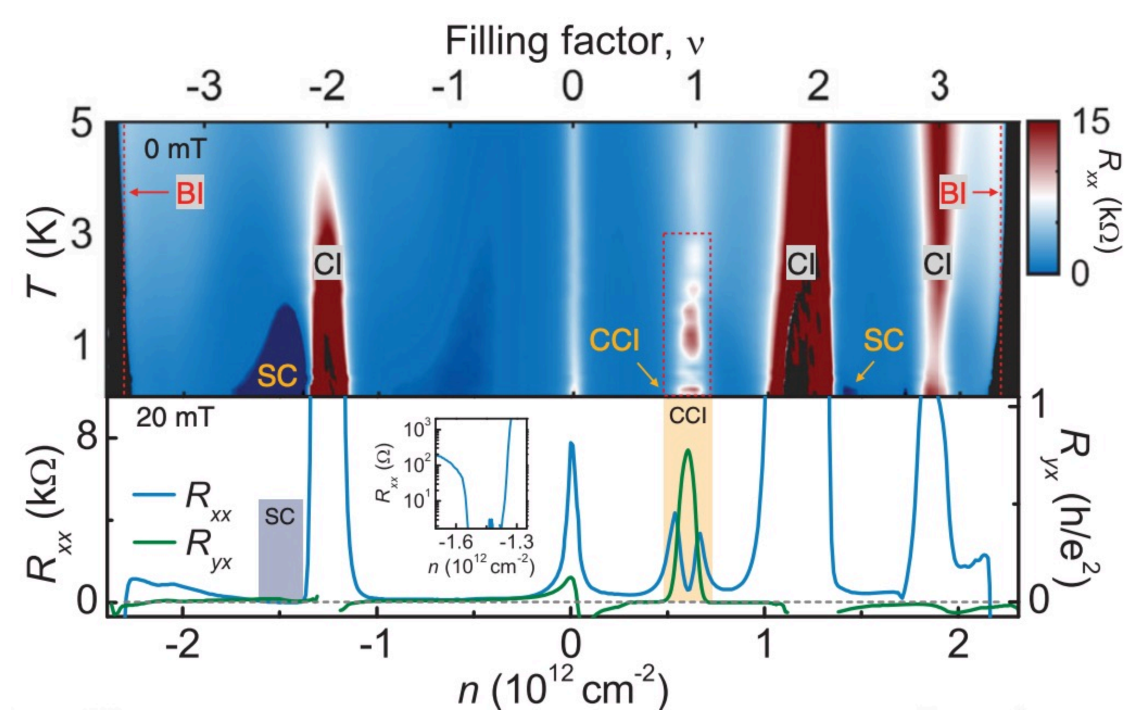
$$\lambda_{m_1,m_2,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u_{\mathbf{k},m_1} | u_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$

Gate-screened Coulomb potential

$$V(\mathbf{q}) = \frac{e^2}{2\varepsilon\varepsilon_0 q}(1 - e^{-2qd_s})$$



Serlin… Young, Science 367, 900 (2020)



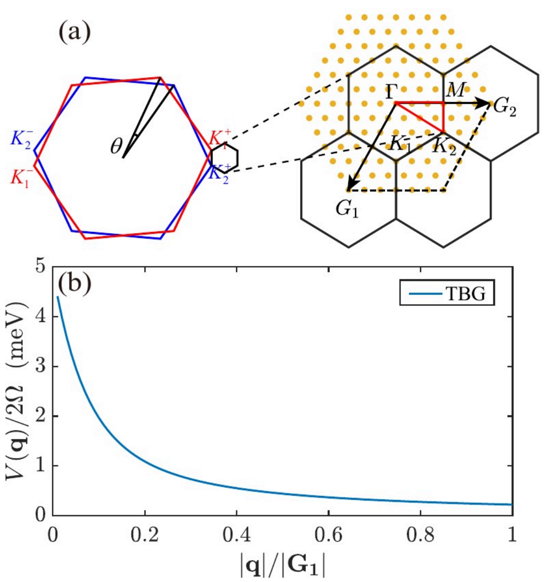
Stepanov … Efetov, PRL 127, 197701 (2021)

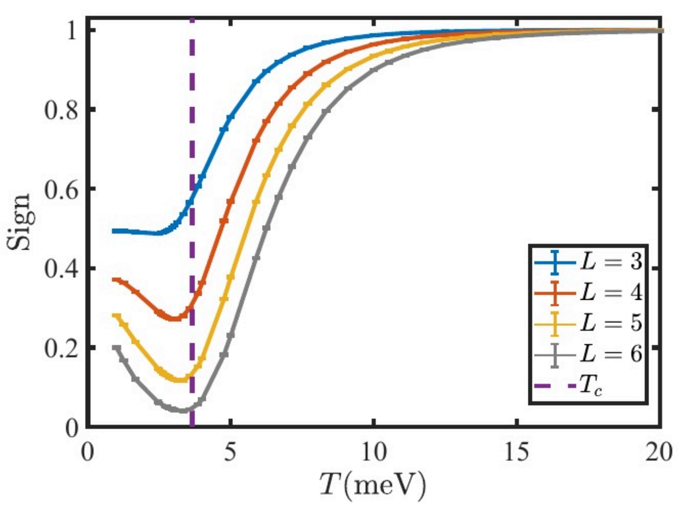
Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

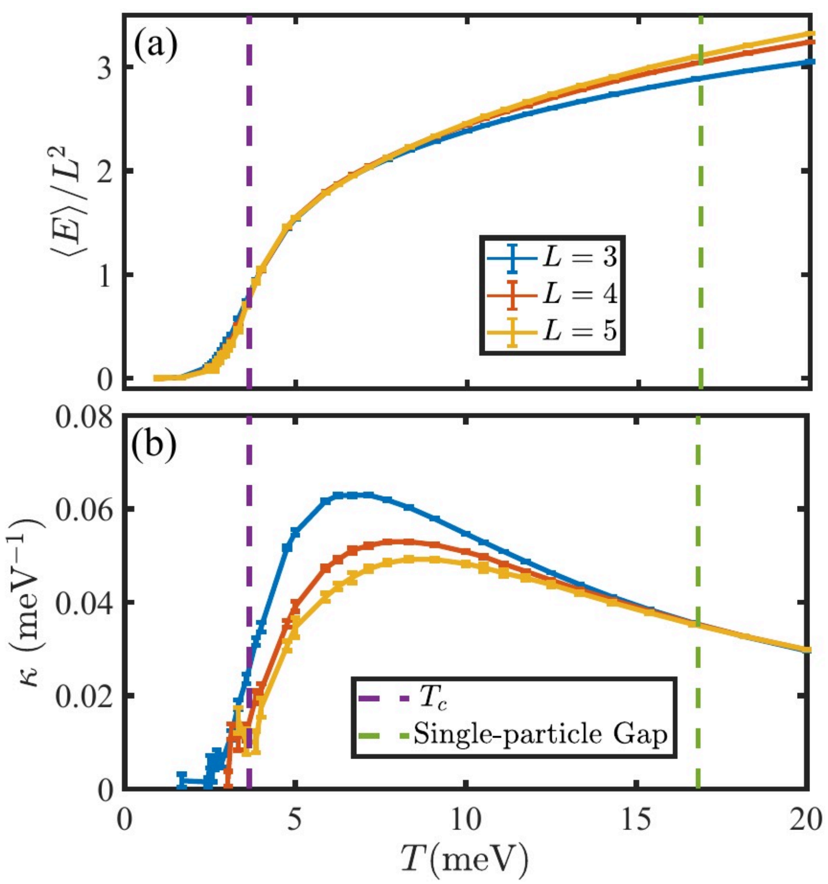
Gaopei Pan,[1,2] Xu Zhang,[3] Hongyu Lu,[3] Heqiu Li,[4] Bin-Bin Chen,[3] Kai Sun,[5,*] and Zi Yang Meng[3,†]

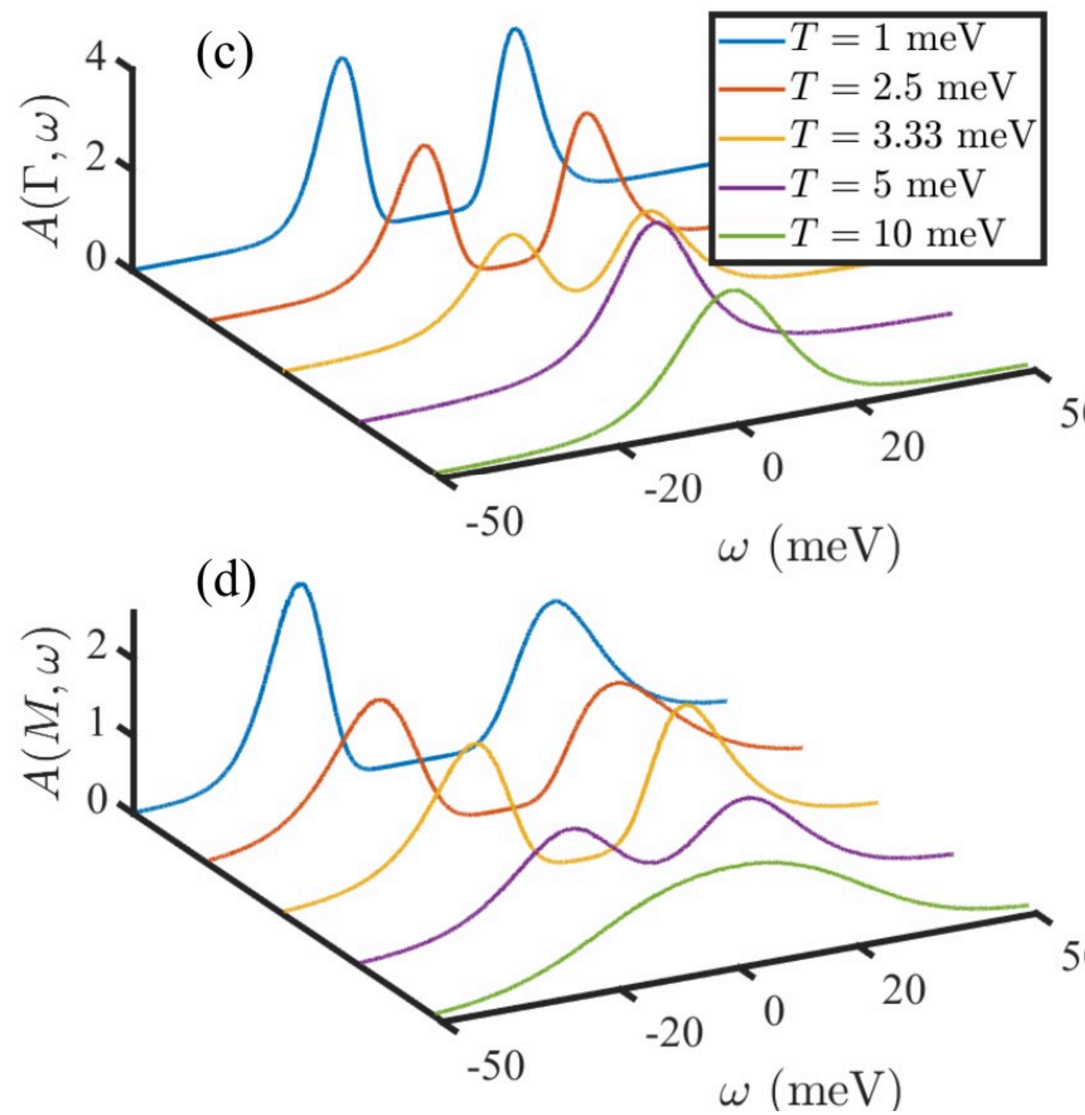
PRL 130, 016401 (2023)

momentum-space QMC
Single valley and single spin









$T_c = 3.65(5)$ meV

$$\kappa = \frac{\partial n}{\partial \mu} = \frac{\langle N^2\rangle - \langle N\rangle^2}{TN}$$

measured via quantum capacitance

measured via STM

Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

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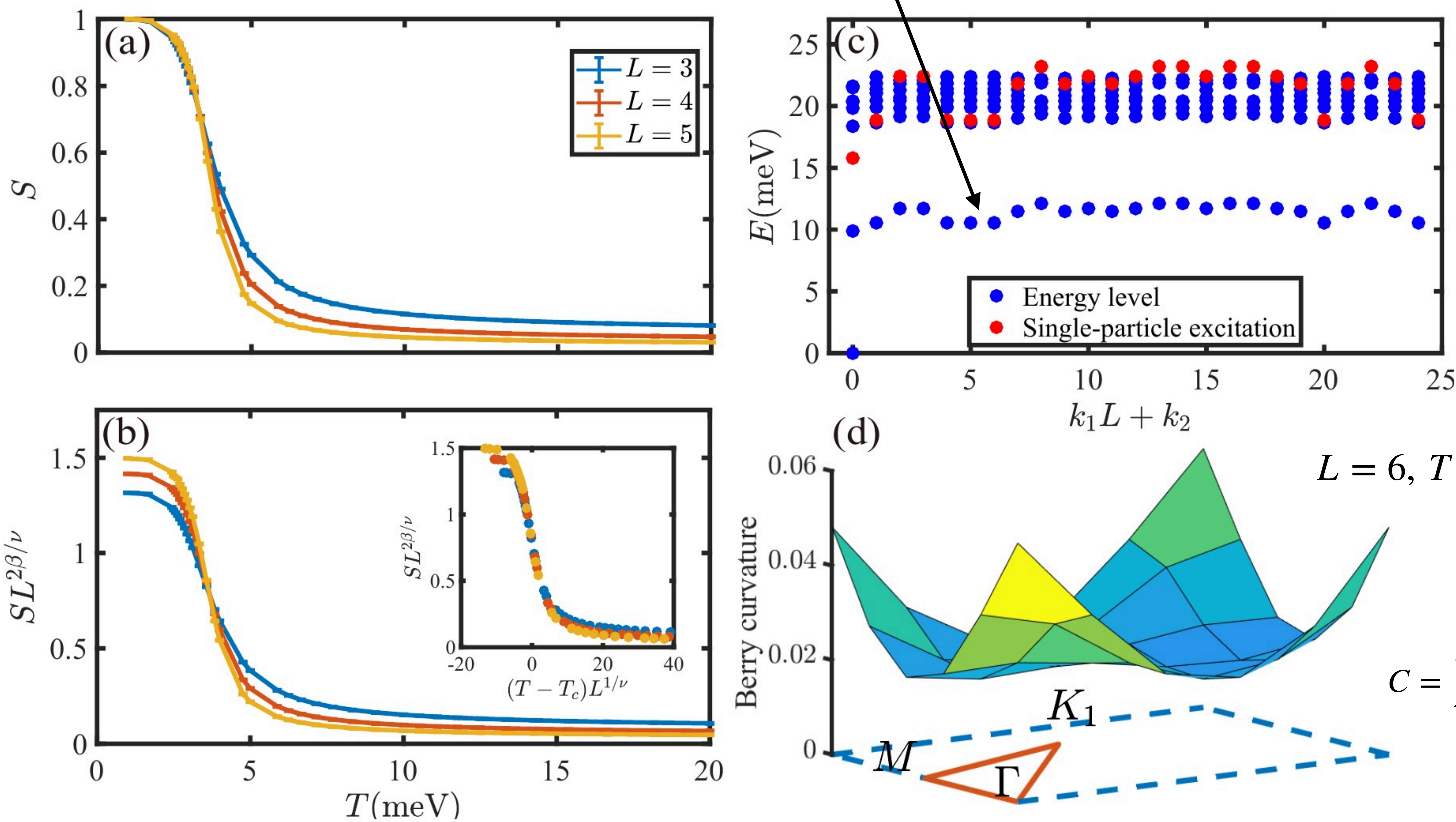
PRL 130, 016401 (2023)

momentum-space QMC & exact diagonalization

$$S = \frac{1}{N^2}\langle (N_+ - N_-)^2 \rangle$$

Gapped excitons restore time-reversal

$L = 5$



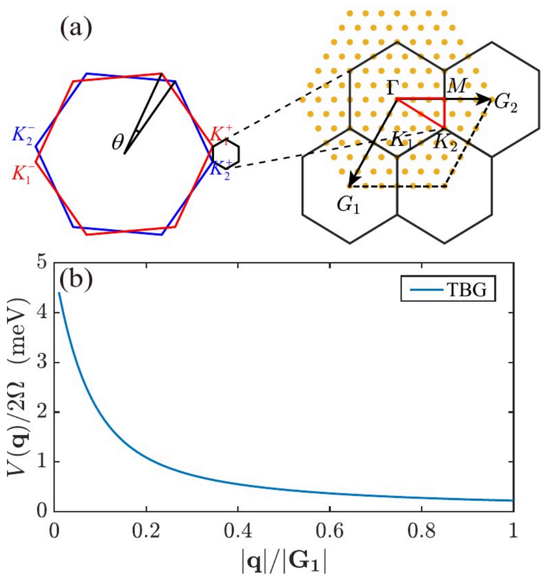
$L = 6,\ T = 1.25$ meV

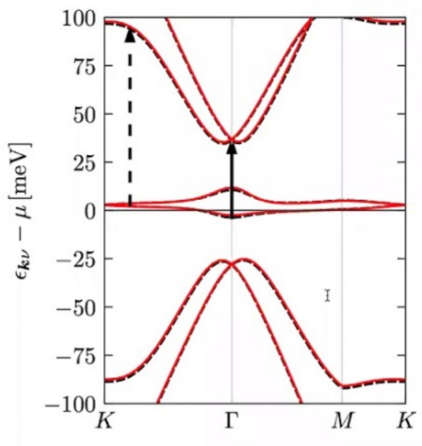
$C = \sum F_{\square} = 1$

$T_c = 3.65(5)$ meV

TBG — Setting, Question 2

$$H = \underbrace{\sum_{m\mathbf{k}s\tau}(\epsilon_{m\mathbf{k}\tau} - \mu)d^{+}_{m\mathbf{k}s\tau}d_{m\mathbf{k}s\tau}}_{H_0} + \underbrace{\frac{1}{2S}\sum_{\{m_i\}}\sum_{ss'\tau\tau'}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}} V^{\tau\tau'\tau'\tau}_{m_1,m_2,m_3,m_4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\ d^{+}_{m_1\mathbf{k}_1-\mathbf{q}s\tau}d^{+}_{m_2\mathbf{k}_2+\mathbf{q}s'\tau'}d_{m_3\mathbf{k}_2s'\tau'}d_{m_4\mathbf{k}_1s\tau}}_{H_{int}}$$





$$V^{\tau\tau'\tau'\tau}_{m_1,m_2,m_3,m_4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}) = \sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G})\ \lambda_{m_1m_4;\tau}(\mathbf{k}_1-\mathbf{q},\mathbf{k}_1+\mathbf{G})\lambda^{*}_{m_3m_2;\tau'}(\mathbf{k}_2,\mathbf{k}_2+\mathbf{q}+\mathbf{G})$$

$\mathbf{k}_1, \mathbf{k}_2, \mathbf{q} \in$ mBZ

$\mathbf{G} = n_1\mathbf{G}_1 + n_2\mathbf{G}_2$

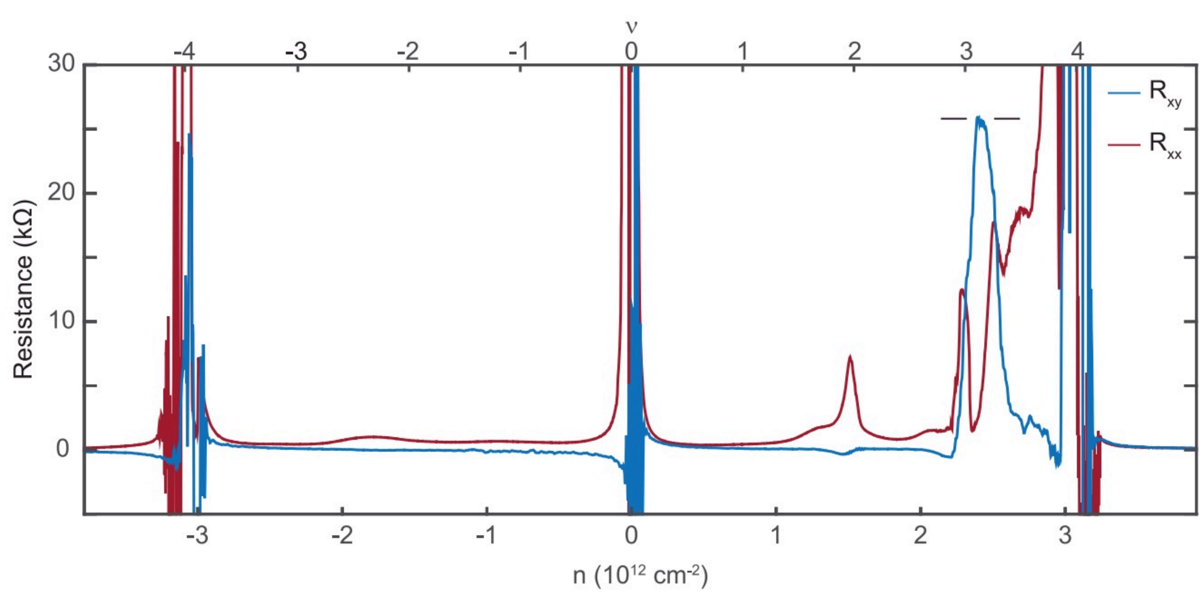
form factors from Bloch WF

$$\lambda_{m_1,m_2,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u_{\mathbf{k},m_1} | u_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$

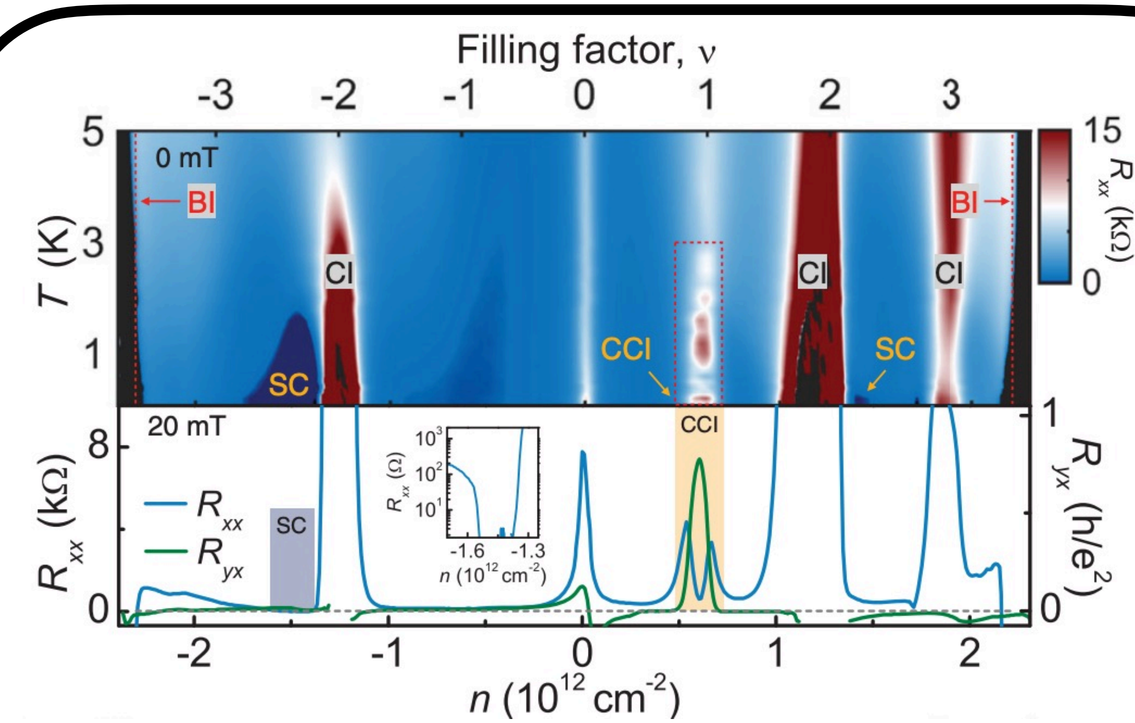
Single-gate-screened Coulomb potential

$$V(\mathbf{q}) = \frac{e^2}{2\varepsilon\varepsilon_0 q}(1 - e^{-2qd_s})$$

Yi Zhang … Fuchun Zhang, PRB 102, 035136 (2020)



Serlin… Young, Science 367, 900 (2020)



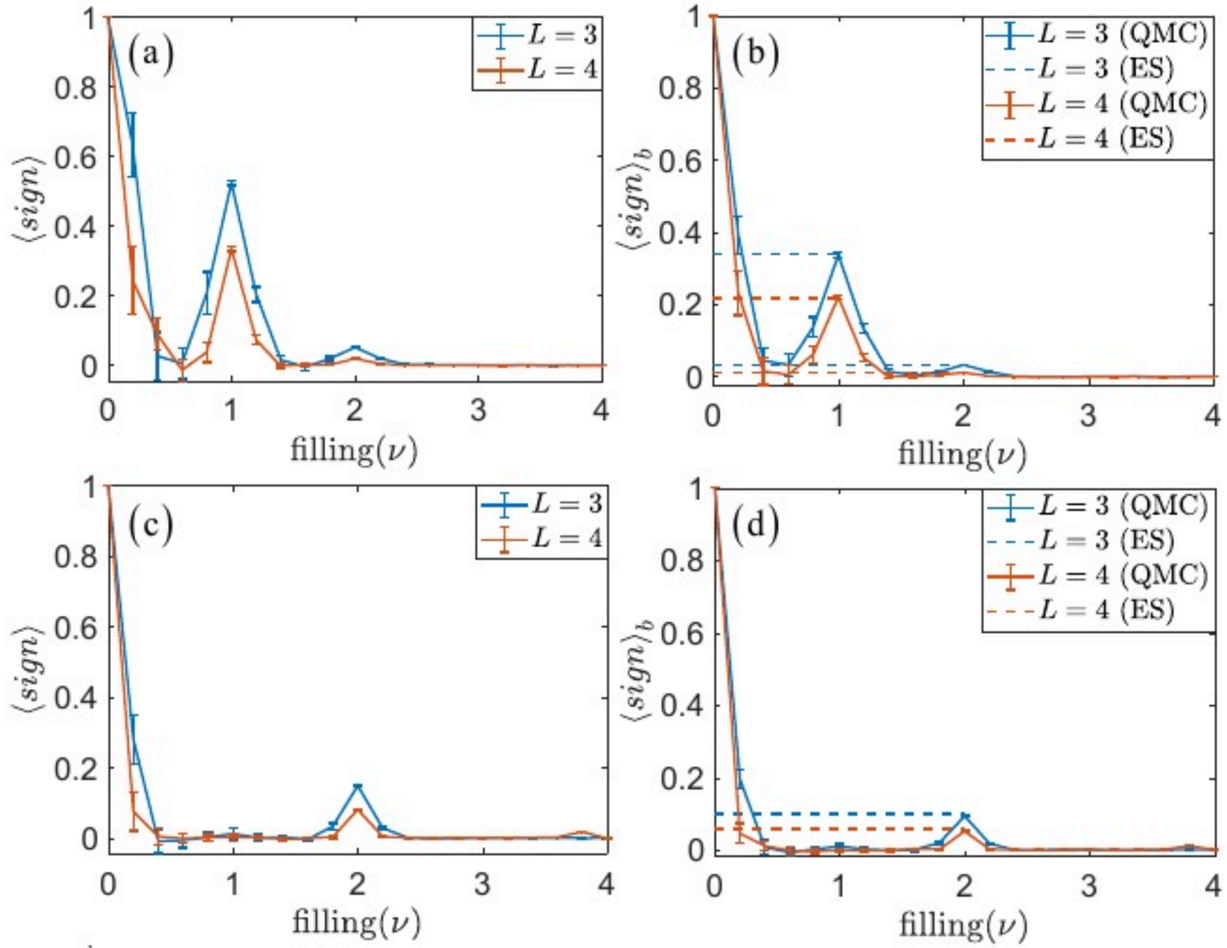
Stepanov … Efetov, PRL 127, 197701 (2021)

Polynomial Sign Problem and Topological Mott Insulator emerging in Twisted Bilayer Graphene

Xu Zhang,[1] Gaopei Pan,[2,3] Bin-Bin Chen,[1] Heqiu Li,[4] Kai Sun,[5,*] and Zi Yang Meng[1,†]

Phys. Rev. B 107, L241105 (2023)

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



$$\langle sign \rangle \geq \frac{g_{\nu=1}}{g_{\nu=0}} = \frac{\frac{(N+3)^2(N+2)^3(N+1)^2}{(3!)^2}}{\frac{(N+3)^2(N+2)^4(N+1)^2}{(3!)^2(2!)^2}} \sim \frac{N^7}{N^8} = N^{-1}$$

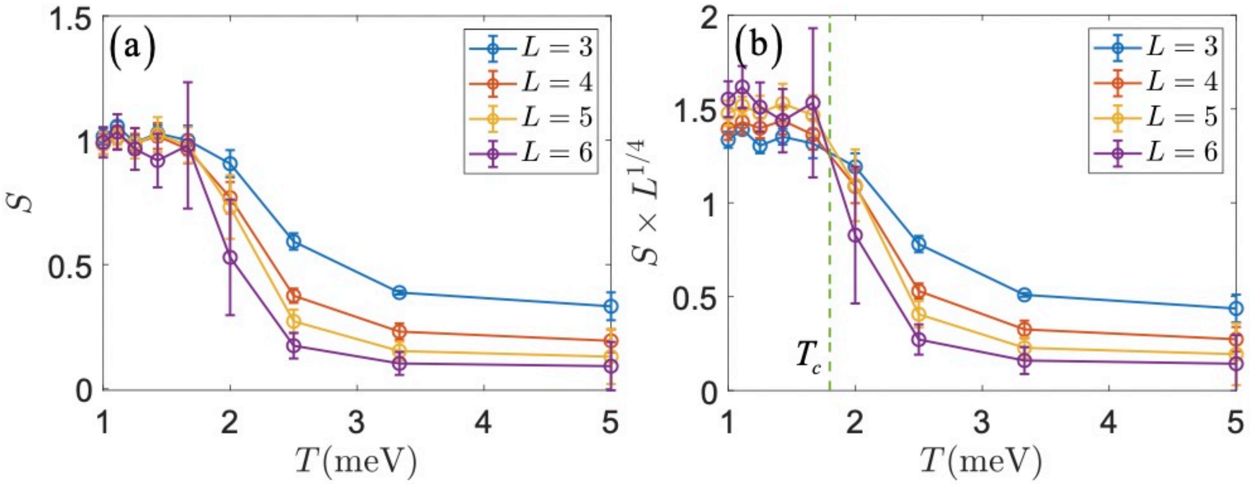
$$g_{\nu=1} = 2g_{C_+=3,C_-=0} + 2g_{C_+=2,C_-=1} = \frac{(N+3)(N+2)(N+1)}{3} + \frac{(N+3)^2(N+2)^3(N+1)^2}{(3!)^2}$$

$$g_{\nu=0} = 2g_{C_+=4,C_-=0} + 2g_{C_+=3,C_-=1} + g_{C_+=2,C_-=2} = 2 + \frac{(N+3)^2(N+2)^2(N+1)^2}{(3!)^2} + \frac{(N+3)^2(N+2)^4(N+1)^2}{(3!)^2(2!)^2}$$

Polynomial Sign Problem and Topological Mott Insulator emerging in Twisted Bilayer Graphene

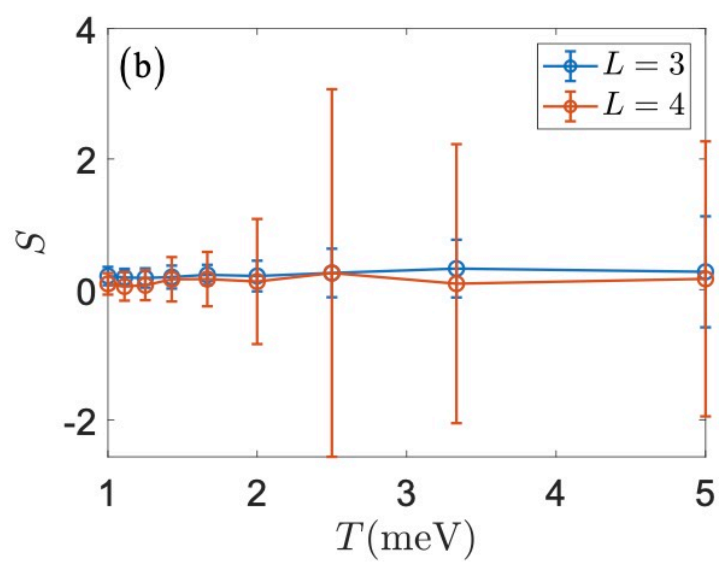
Xu Zhang,[1] Gaopei Pan,[2,3] Bin-Bin Chen,[1] Heqiu Li,[4] Kai Sun,[5,*] and Zi Yang Meng[1,†]

$\nu = 1$



$T_c = 1.8$ meV

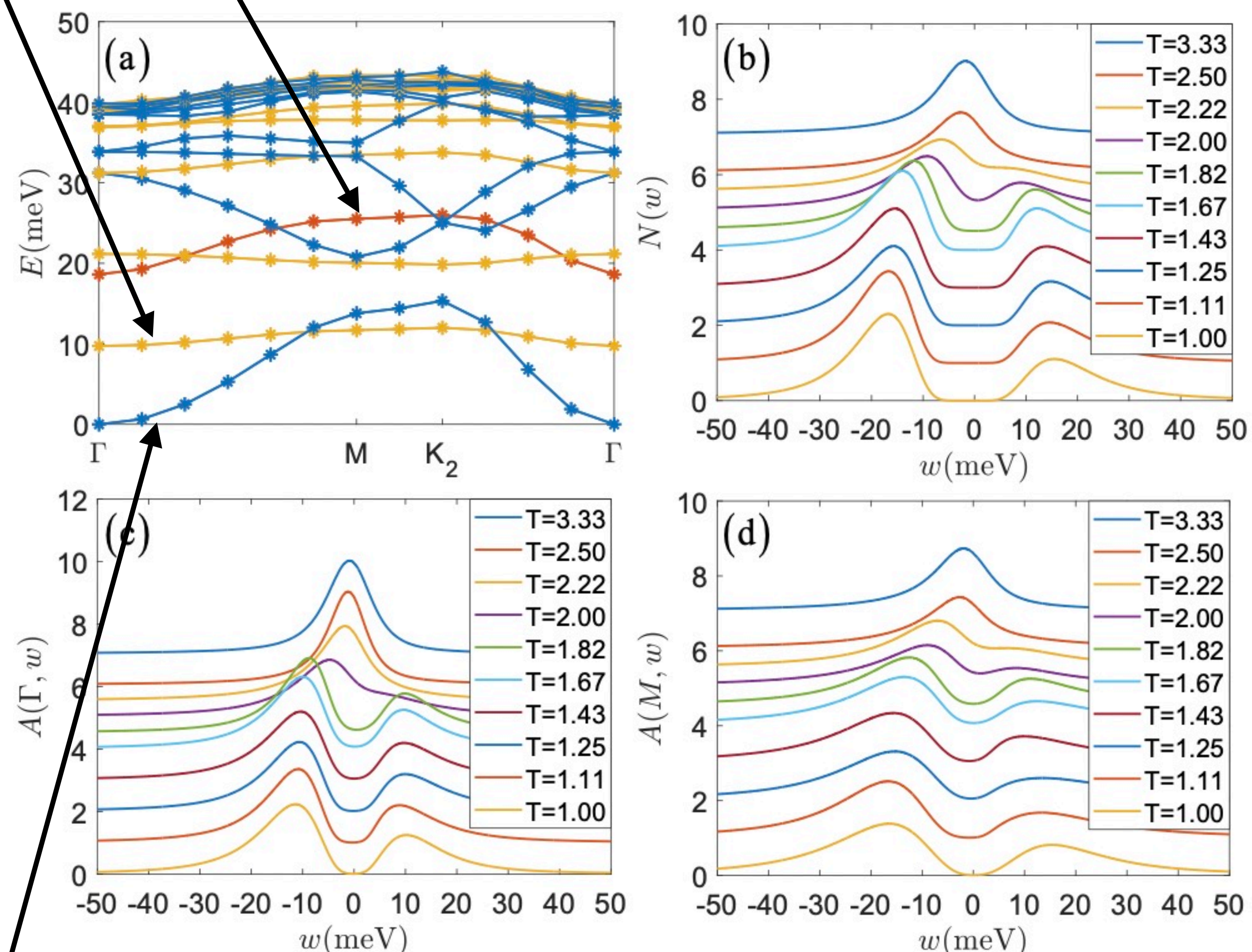
$\nu = 2$



$\nu = 1$

Gapped excitons

Gapped single-particle excitations



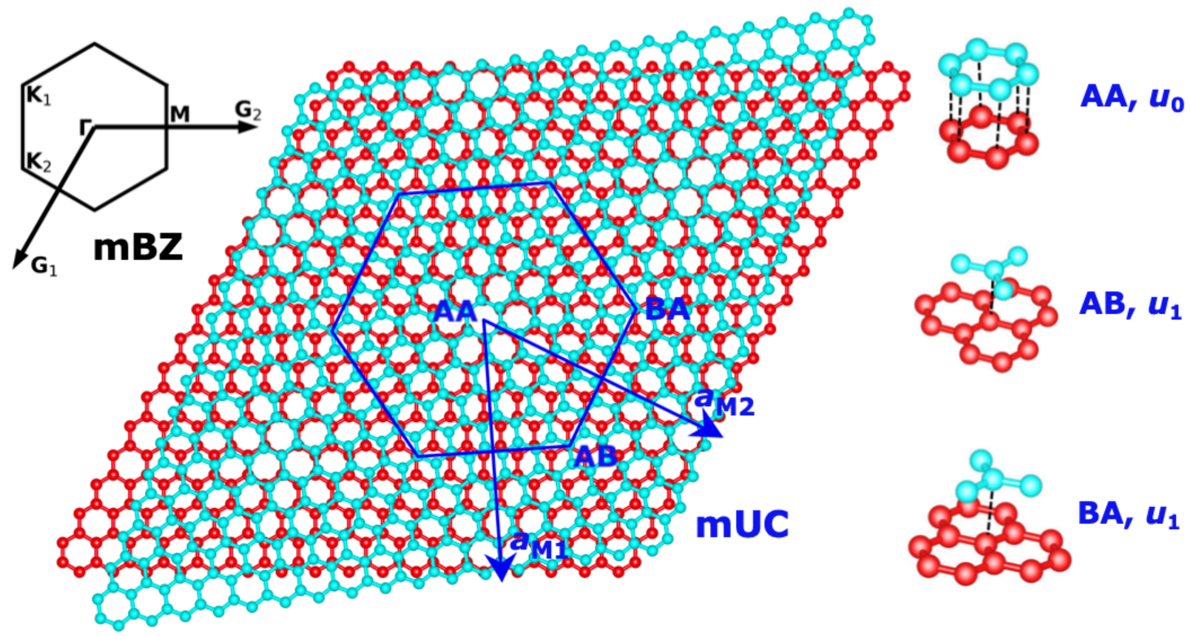
Gapless excitons,
Spin-valley continuous symmetry
Orbital ferromagnetism

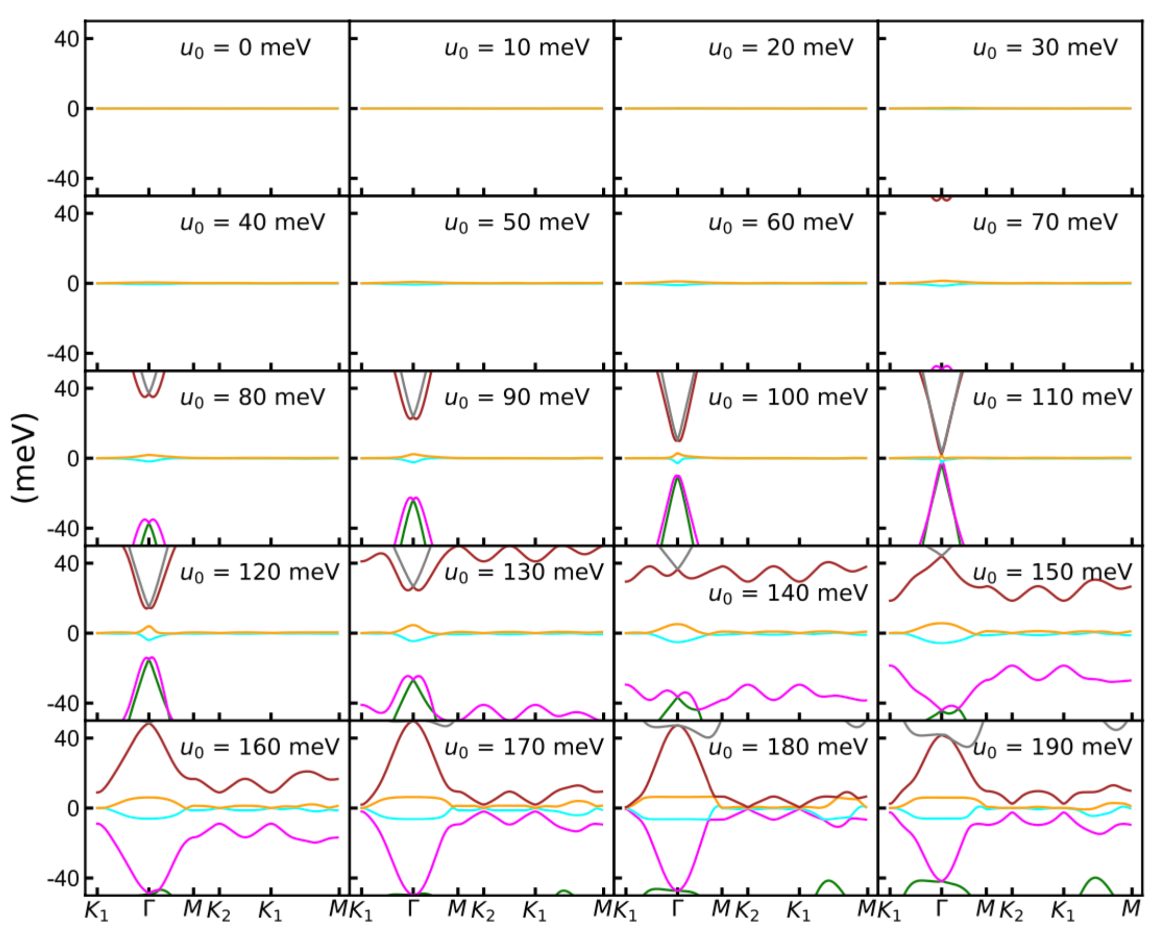
Phys. Rev. B 107, L241105 (2023)

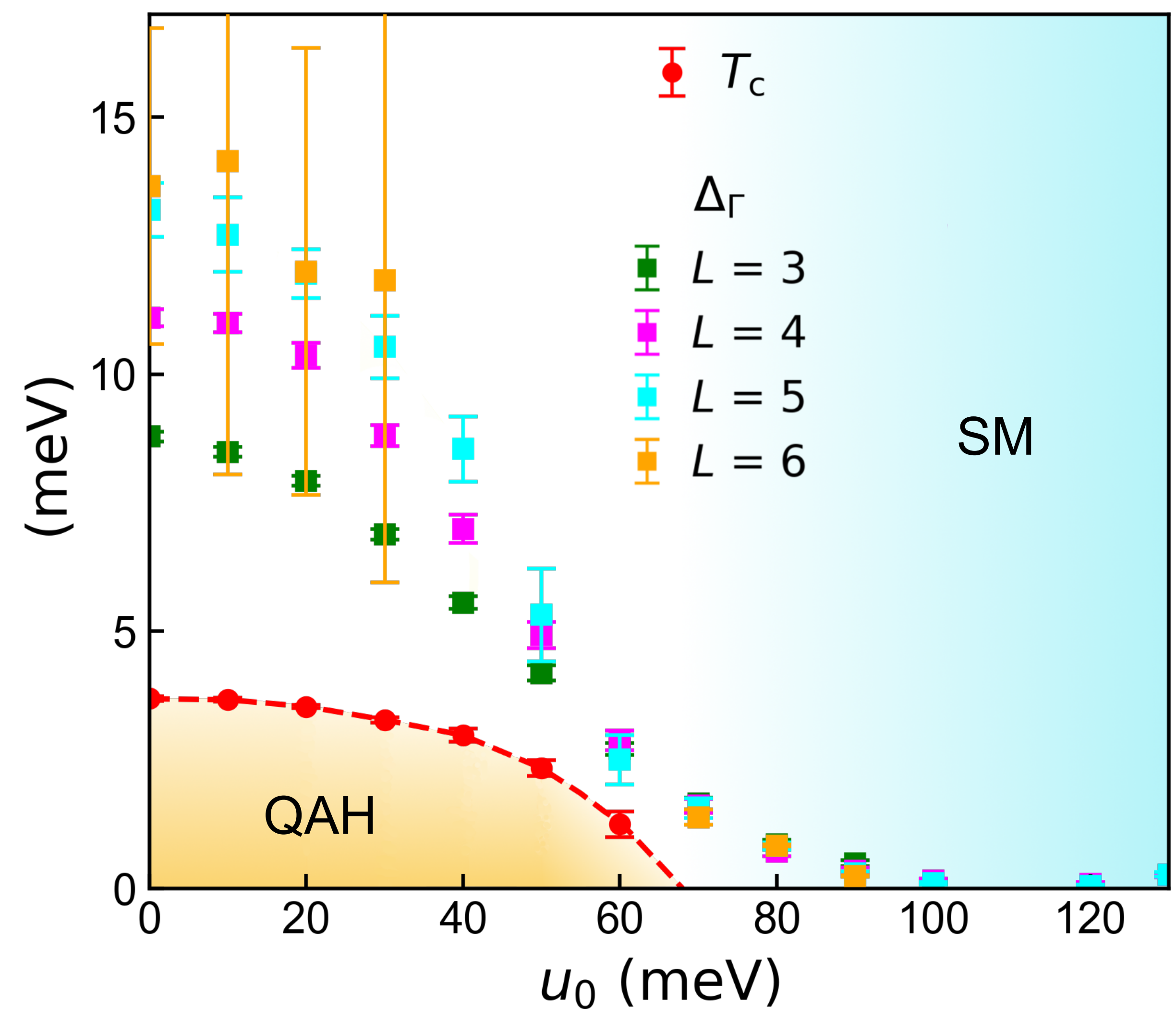
Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in magic-angle twisted bilayer graphene

Cheng Huang,[1] Xu Zhang,[1] Gaopei Pan,[2,3] Heqiu Li,[4] Kai Sun,[5,*] Xi Dai,[6,†] and Ziyang Meng[1,‡]

arXiv: 2304.14064







Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in magic-angle twisted bilayer graphene

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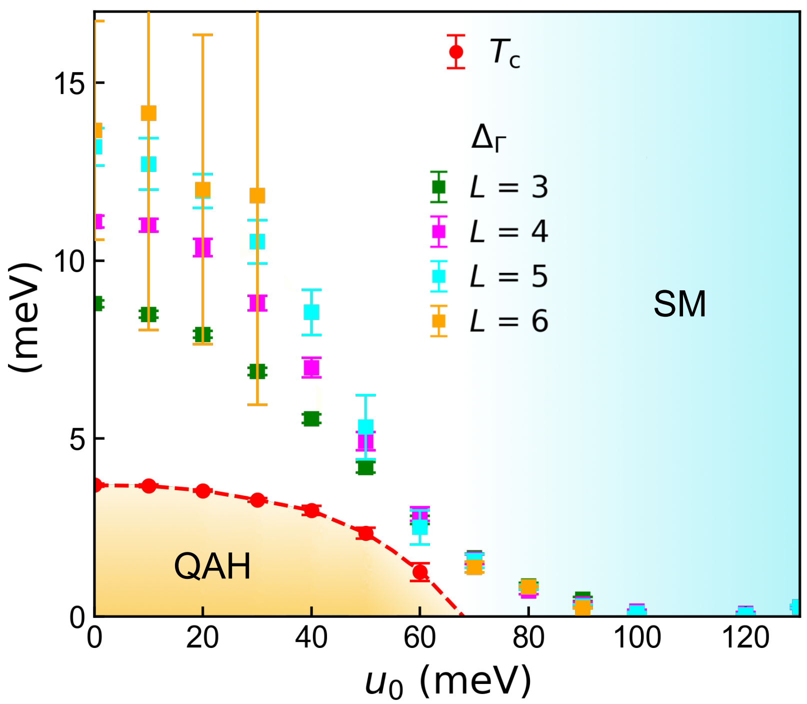
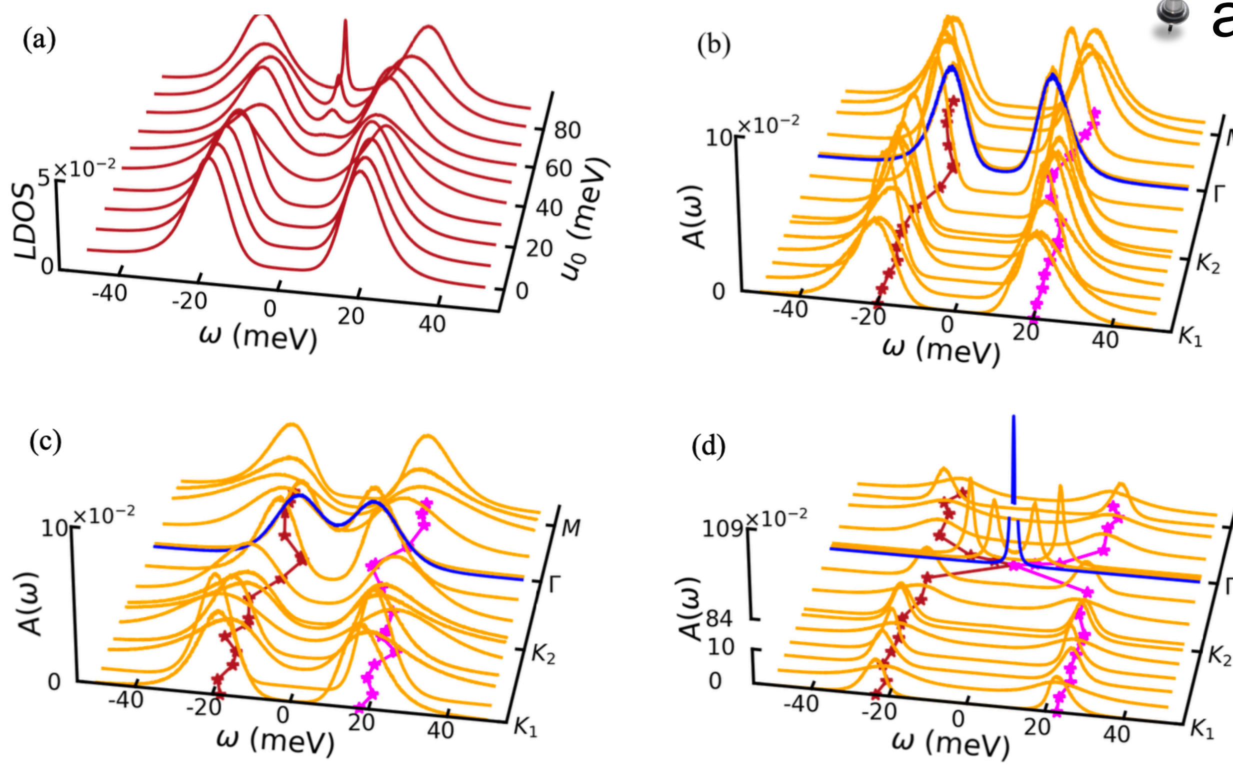
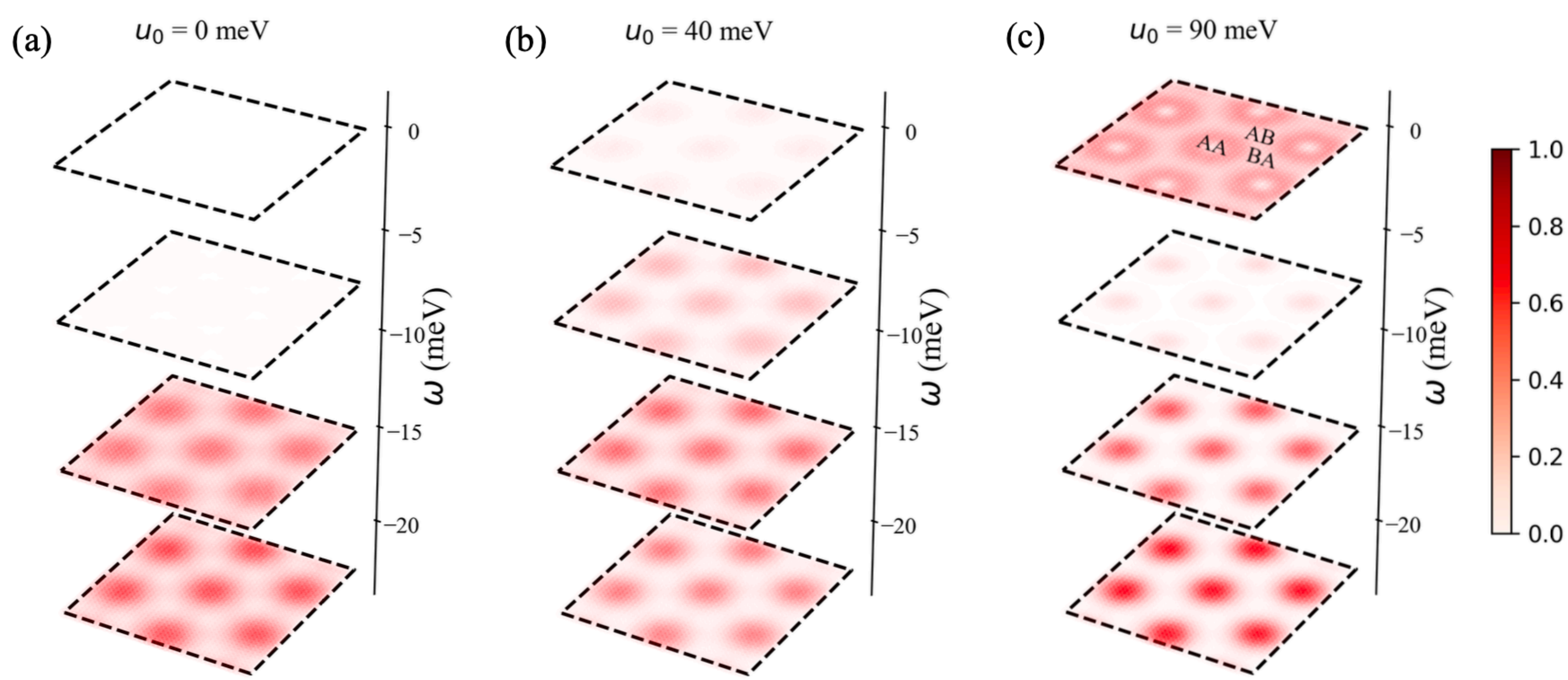


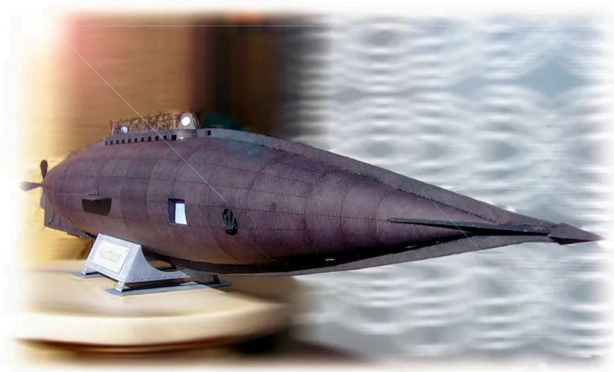


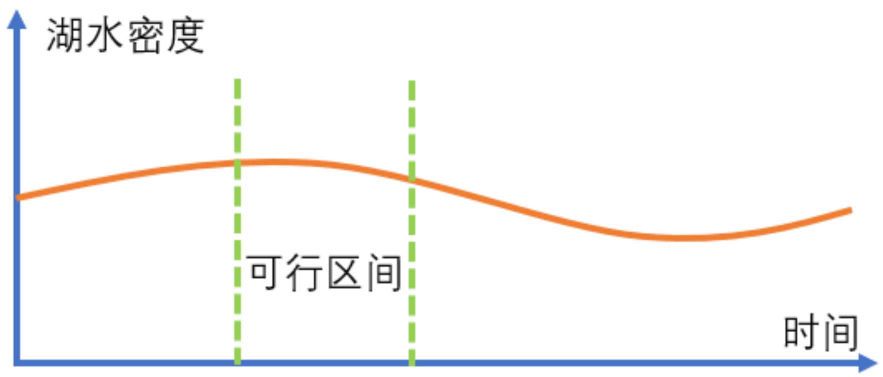
arXiv: 2304.14064



Xu Zhang

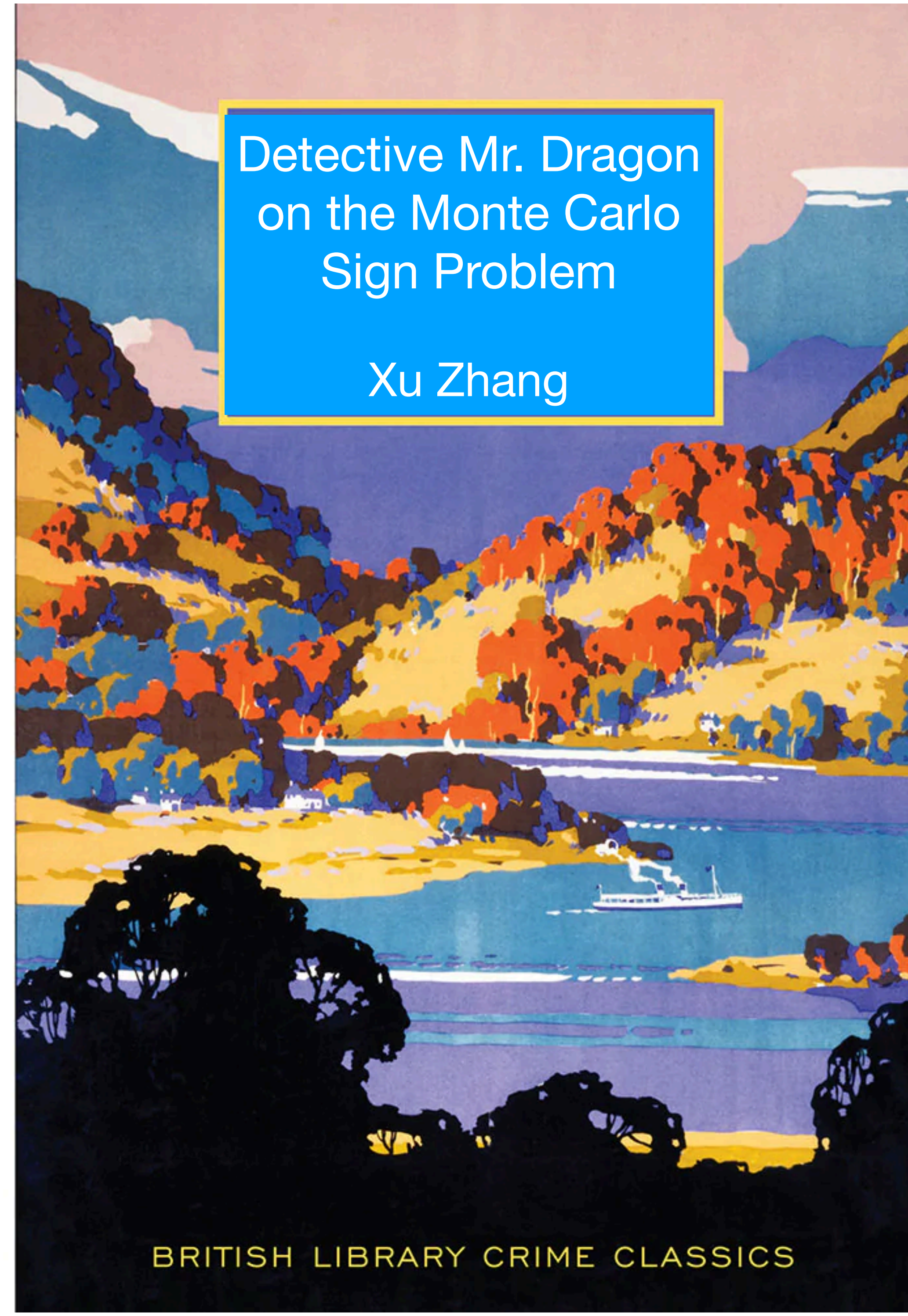
Caption Nemo and submarine Nautilus





$$\langle \rho \rangle_{V_i} = \frac{\sum_i V_i \rho_i}{\sum_i V_i} = \frac{\frac{\sum_i |V_i| (\pm \rho_i)}{\sum_i |V_i|}}{\frac{\sum_i |V_i| (\pm 1)}{\sum_i |V_i|}} = \frac{\langle \pm \rho_i \rangle_{|V_i|}}{\langle \pm 1 \rangle_{|V_i|}}$$

$\langle \pm 1 \rangle \sim e^{-N}$ **Sign problem and Sign bound**



- Twenty Thousand Leagues Under the Seas, Jules Verne
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- Xu Zhang et al., Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, PRB 107, L241105 (2023)