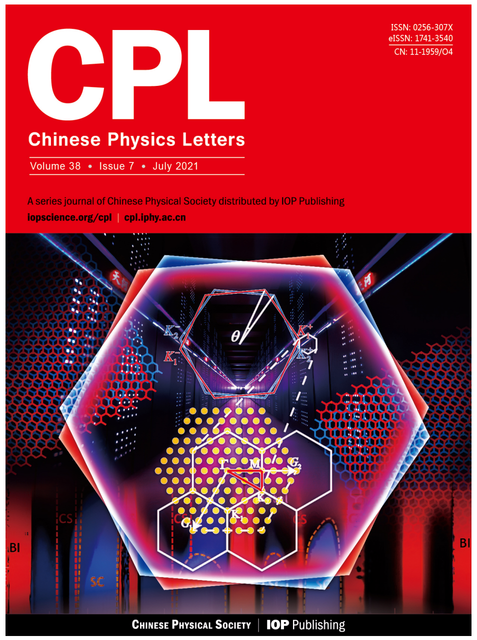
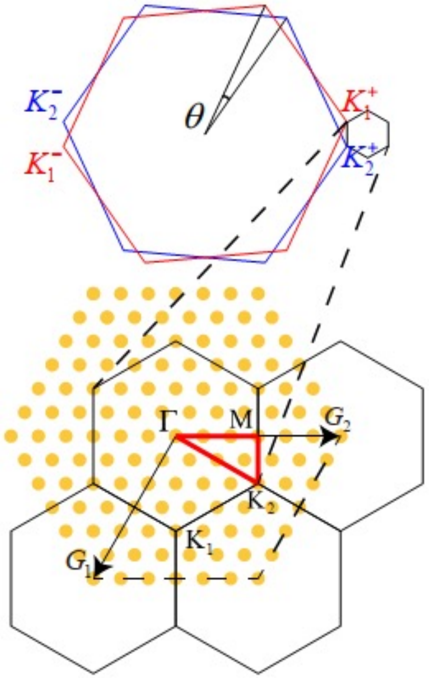
Projected Hamiltonians and their Global Update in QMC Simulations

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

Content

1. Momentum-space QMC for twisted bilayer graphene

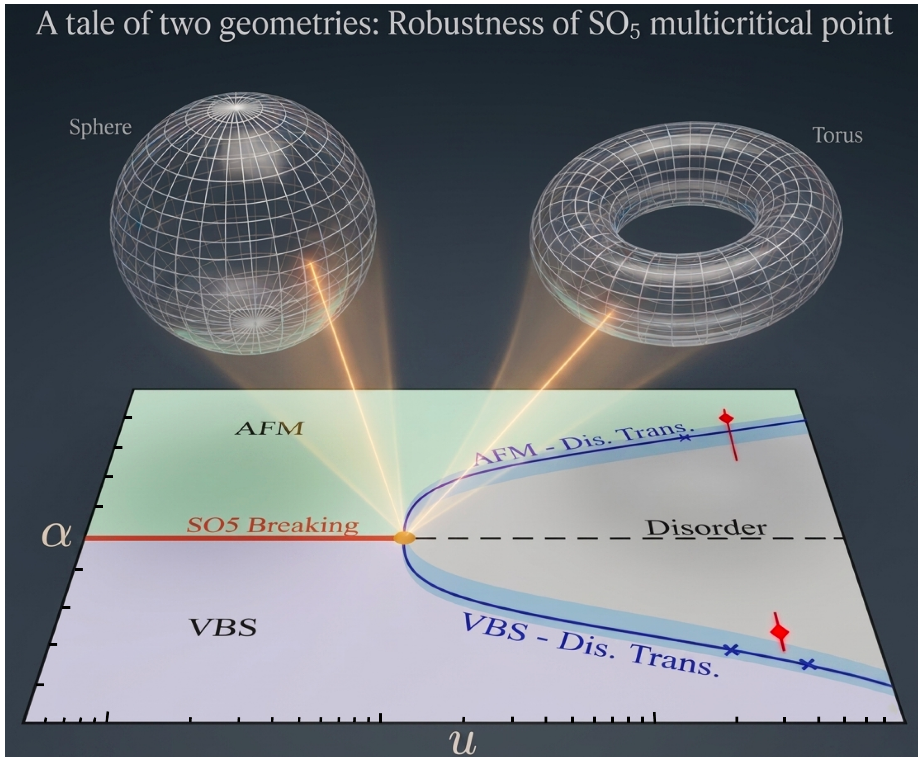




- CPL 38, 077305 (2021) [momentum-space QMC, 6 x 6]
- PRL 130, 016401 (2023) [Thermodynamic responses]
- PRB 107, L241105 (2023) [Polynomial sign problem]
- Nat. Comm. 16, 7176 (2025) [global update, 18 x 18]
- ......

2. (2+1)D SO(5) nonlinear sigma model with Wess-Zumino-Witten term

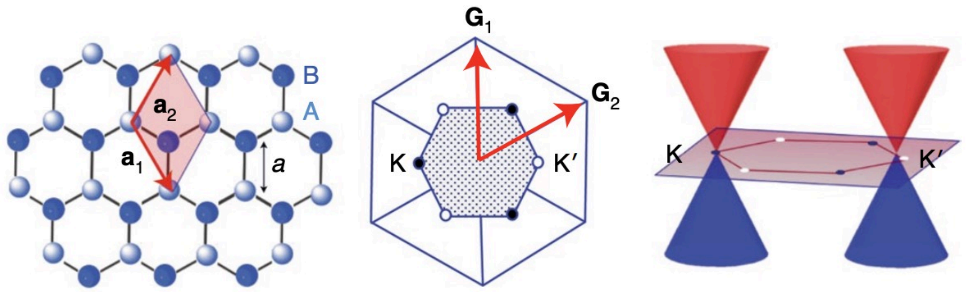
- PRL 132, 246503 (2023) [ED+DMRG, $N_\phi = 16$]
- arXiv: 2605.03700 (2026) [global update, $N_\phi = 160$]
- ......



3. Hybrid Monte Carlo for FQHs

- Rep. Prog. Phys. 10.1088/ae70a7 (2026) [global update, N = 1200]
- ......

TBG — Setting



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

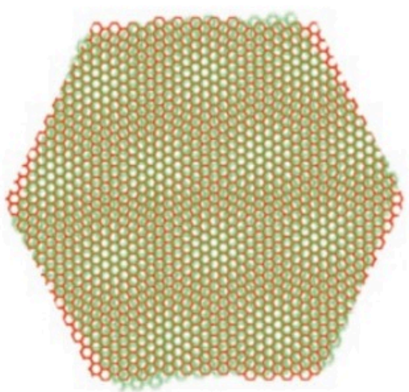
interlayer tunnelling produces avoided crossings

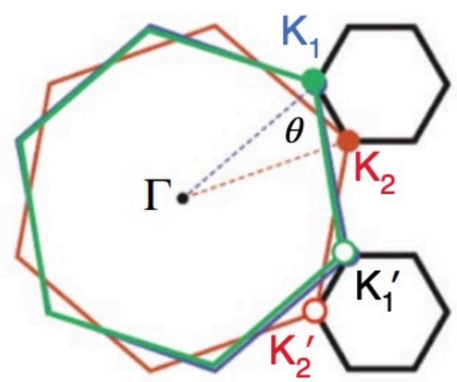
$\hbar v_F / a_0 = 2377.45$ meV

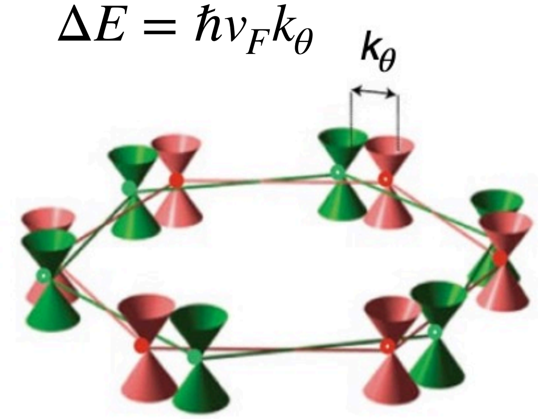
$\theta > 10^\circ$ $\Delta E > 1$ eV isolated graphene

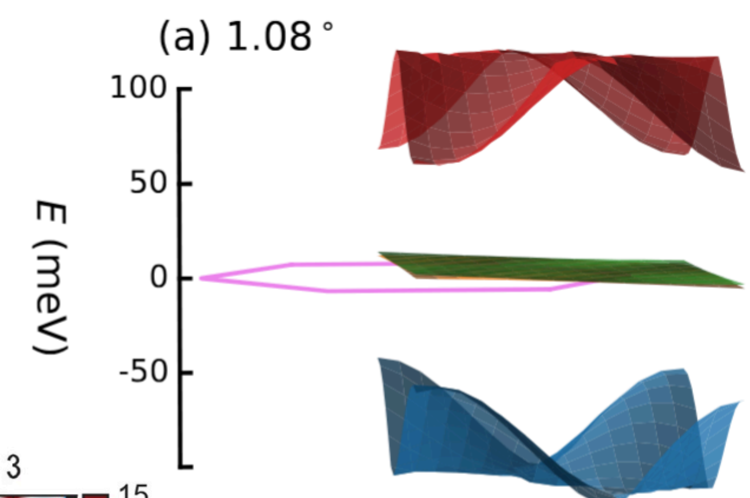
$\theta \sim 1^\circ$ layers hybridization
strong tunnelings couple Dirac cones
flat bands and strong correlation

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

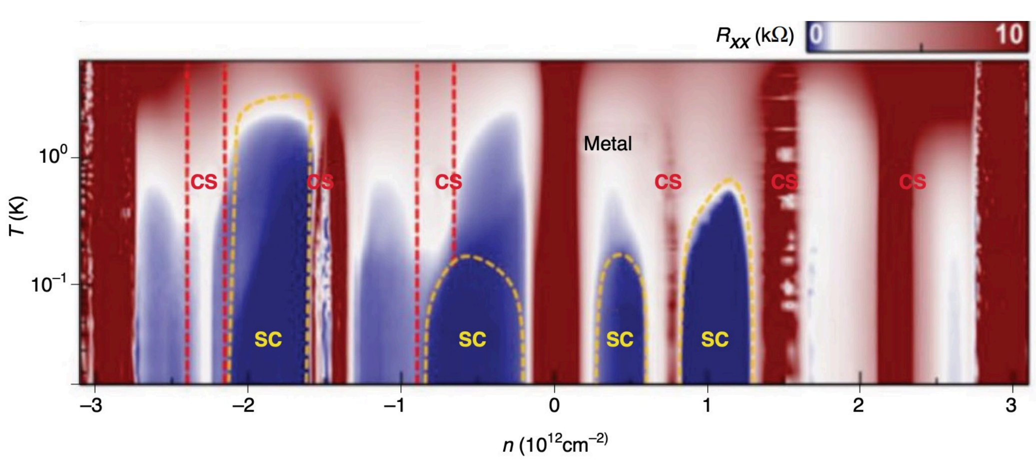


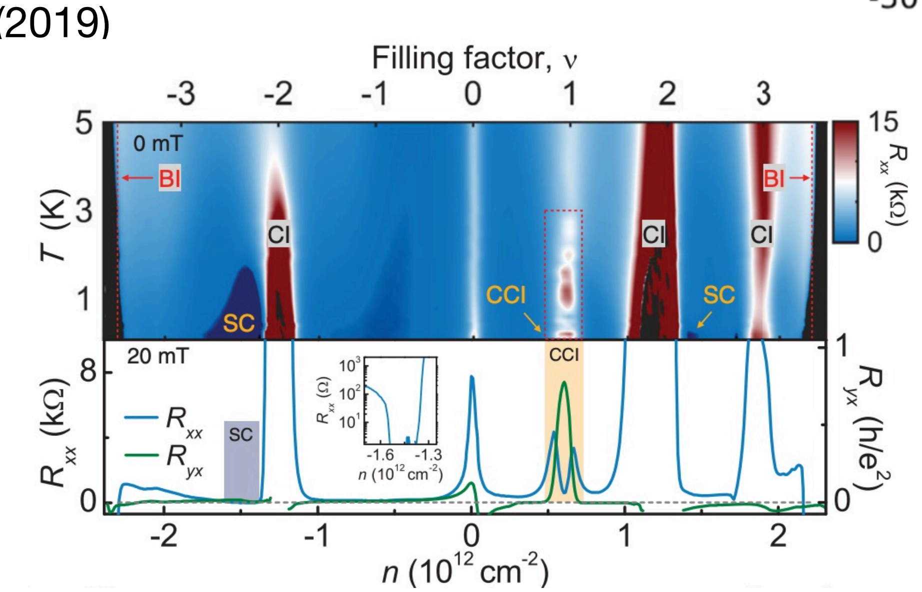






Lu, Stepanov, …, MacDonald, Efetov, Nature 574, 653 (2019)





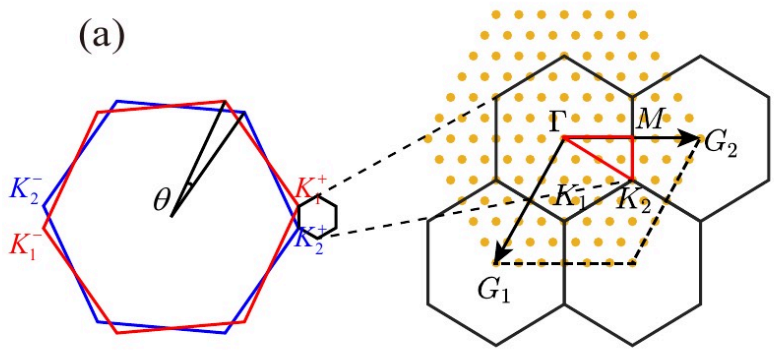
Stepanov, …, Bernevig, Efetov, PRL 127, 197701 (2021)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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

CPL 38, 077305 (2021)

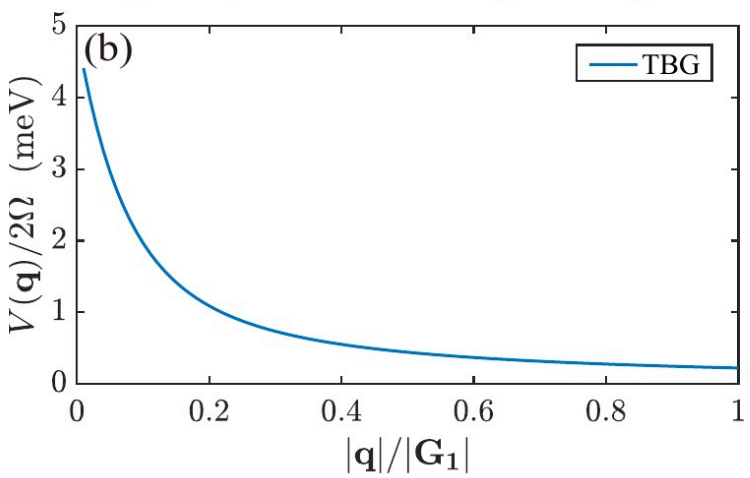
$$H = \underbrace{\sum_{s,\eta,\mathbf{k},m} \epsilon^{s,\eta}_{\mathbf{k},m} c^{\dagger}_{s,\eta,\mathbf{k},m} c_{s,\eta,\mathbf{k},m}}_{H_0} + \underbrace{\frac{1}{2\Omega} \sum_{\mathbf{q}\in mBZ,\mathbf{G}} V(\mathbf{q}+\mathbf{G})\delta\rho_{\mathbf{q}+\mathbf{G}}\delta\rho_{-\mathbf{q}-\mathbf{G}}}_{H_{int}}$$



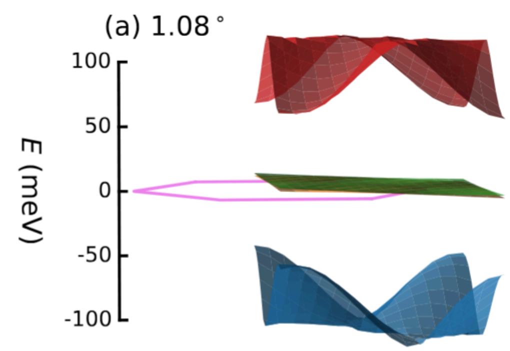
$$|\mathbf{G_1}|, |\mathbf{G_2}| = \frac{8\pi}{3a}\sin(\frac{\theta}{2})$$

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

Gate-screened Coulomb potential $V(\mathbf{Q}) = \frac{e^2}{2\epsilon|\mathbf{Q}|}(1 - e^{-|\mathbf{Q}|d})$



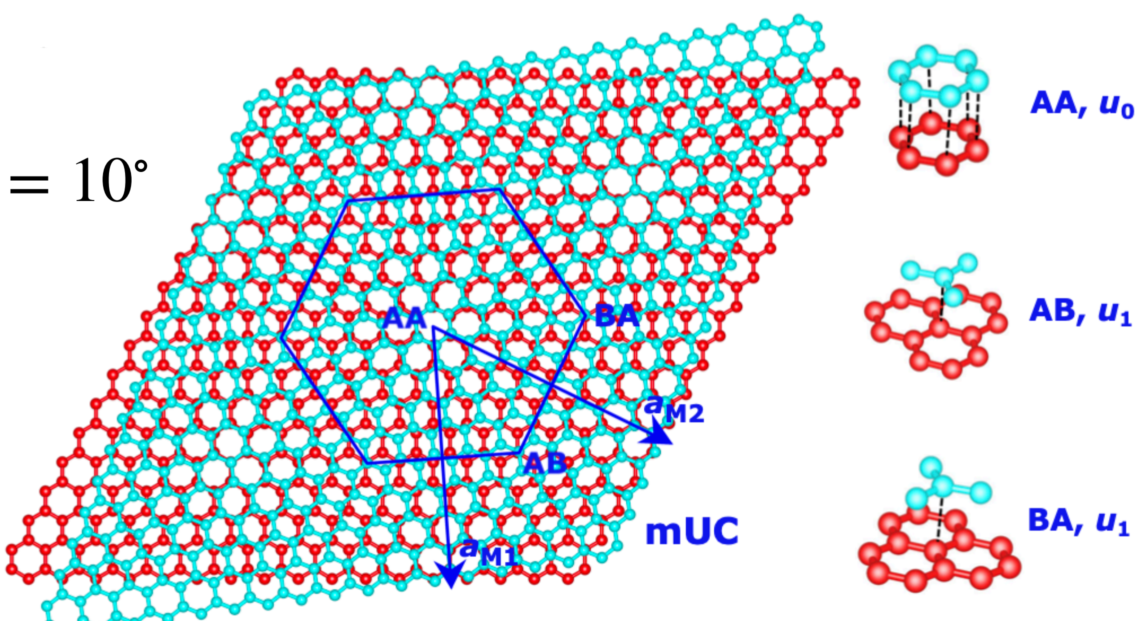
$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{s,\eta,\mathbf{k},m_1,m_2} \lambda^{s,\eta}_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})\left(c^{\dagger}_{s,\eta,\mathbf{k},m_1} c_{s,\eta,\mathbf{k}+\mathbf{q}+\mathbf{G},m_2} - \frac{\nu+4}{8}\delta_{\mathbf{q},0}\delta_{m_1,m_2}\right)$$

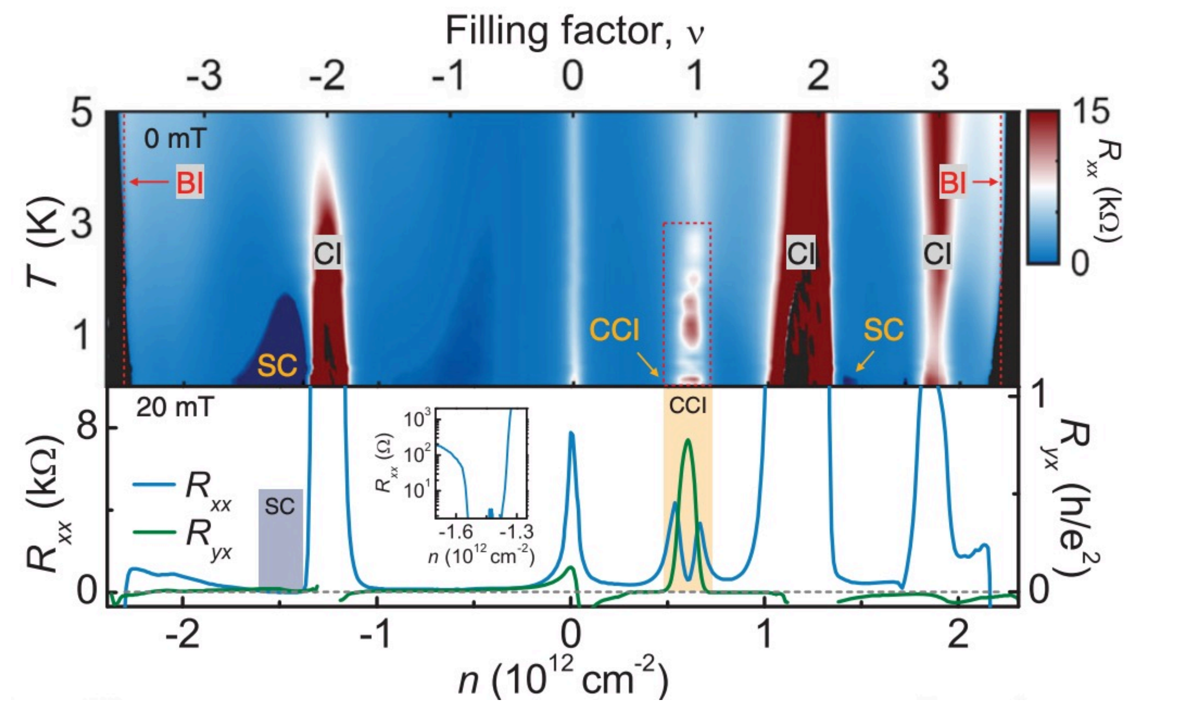


Form factors from Bloch WF

$$\lambda^{s,\eta}_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u^{s,\eta}_{\mathbf{k},m_1} | u^{s,\eta}_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$

$\theta = 10^{\circ}$

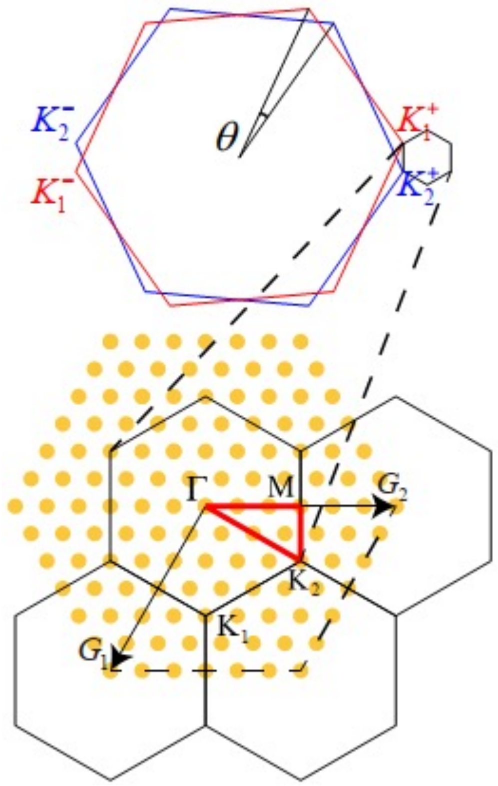




Stepanov … Efetov, PRL 127, 197701 (2021)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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



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

CPL 38, 077305 (2021)

Trambly de Laissardiere et al., Nano Lett. (2010)

Bistritzer & MacDonald, PNAS (2011)

$\eta = \pm$ valley

Pauli for sublattices

$\Lambda^\eta = (\eta\Lambda_x, \Lambda_y)$

$$H_O^{s,\eta}(\mathbf{k})_{\mathbf{G},\mathbf{G}'} = \delta_{\mathbf{G},\mathbf{G}'}\hbar v_F \begin{pmatrix} -(\mathbf{k}+\mathbf{G}-\mathbf{K}_1^\eta)\cdot\Lambda^\eta & 0 \\ 0 & -(\mathbf{k}+\mathbf{G}-\mathbf{K}_2^\eta)\cdot\Lambda^\eta \end{pmatrix} + \begin{pmatrix} 0 & T_1^\eta \\ T_2^{\eta\dagger} & 0 \end{pmatrix}$$

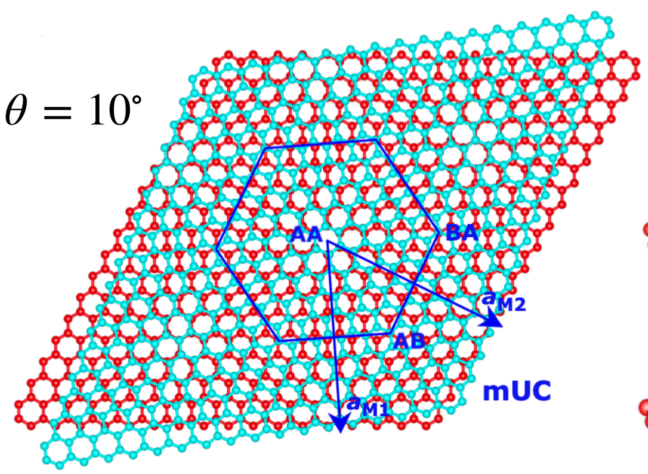
$$T_l^\eta = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}\delta_{\mathbf{G},\mathbf{G}'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}\eta} \\ u_1 e^{i\frac{2\pi}{3}\eta} & u_0 \end{pmatrix}\delta_{\mathbf{G},\mathbf{G}'+(-1)^l\eta\mathbf{G}_1} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}\eta} \\ u_1 e^{-i\frac{2\pi}{3}\eta} & u_0 \end{pmatrix}\delta_{\mathbf{G},\mathbf{G}'+(-1)^l\eta(\mathbf{G}_1+\mathbf{G}_2)}$$

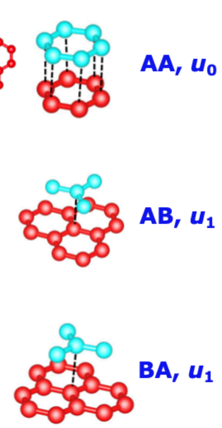
$$\mathbf{G},\mathbf{G}' \in \{n_1\mathbf{G}_1 + n_2\mathbf{G}_2\} \quad |\mathbf{G}|,|\mathbf{G}'| < 6|\mathbf{G}_1|$$

$$|\mathbf{G_1}|,|\mathbf{G_2}| = \frac{8\pi}{3a}\sin(\frac{\theta}{2})$$

$\hbar v_F/a = 2377.45$ meV

$\theta = 10^\circ$





interlayer, intrasublattice hopping

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

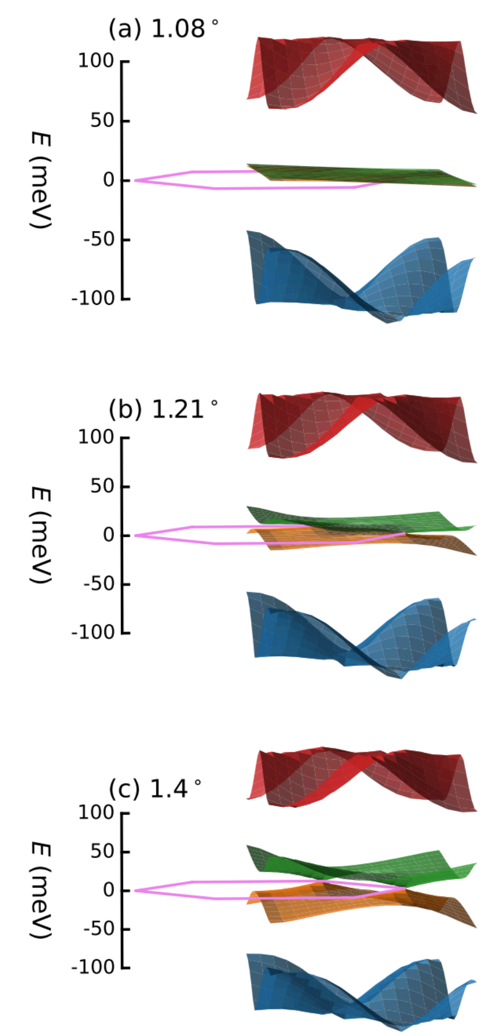
interlayer, intersublattice hopping

$\theta = 1.08^\circ$ 1st magic angle

$u_1 = 110$ meV

$u_0 = 0$ chiral limit

$u_0 \sim 60 - 90$ meV



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

$$H_0 = \sum_{s,\eta,\mathbf{k},m} \epsilon^{s,\eta}_{\mathbf{k},m} c^\dagger_{s,\eta,\mathbf{k},m} c_{s,\eta,\mathbf{k},m}$$

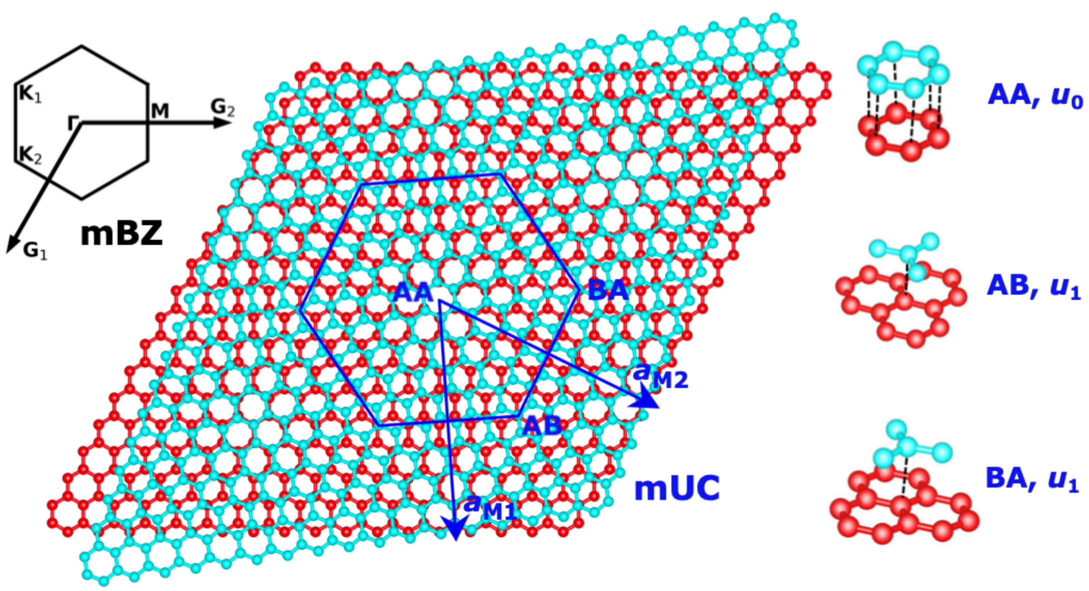
Intra-sublattice, interlayer hopping

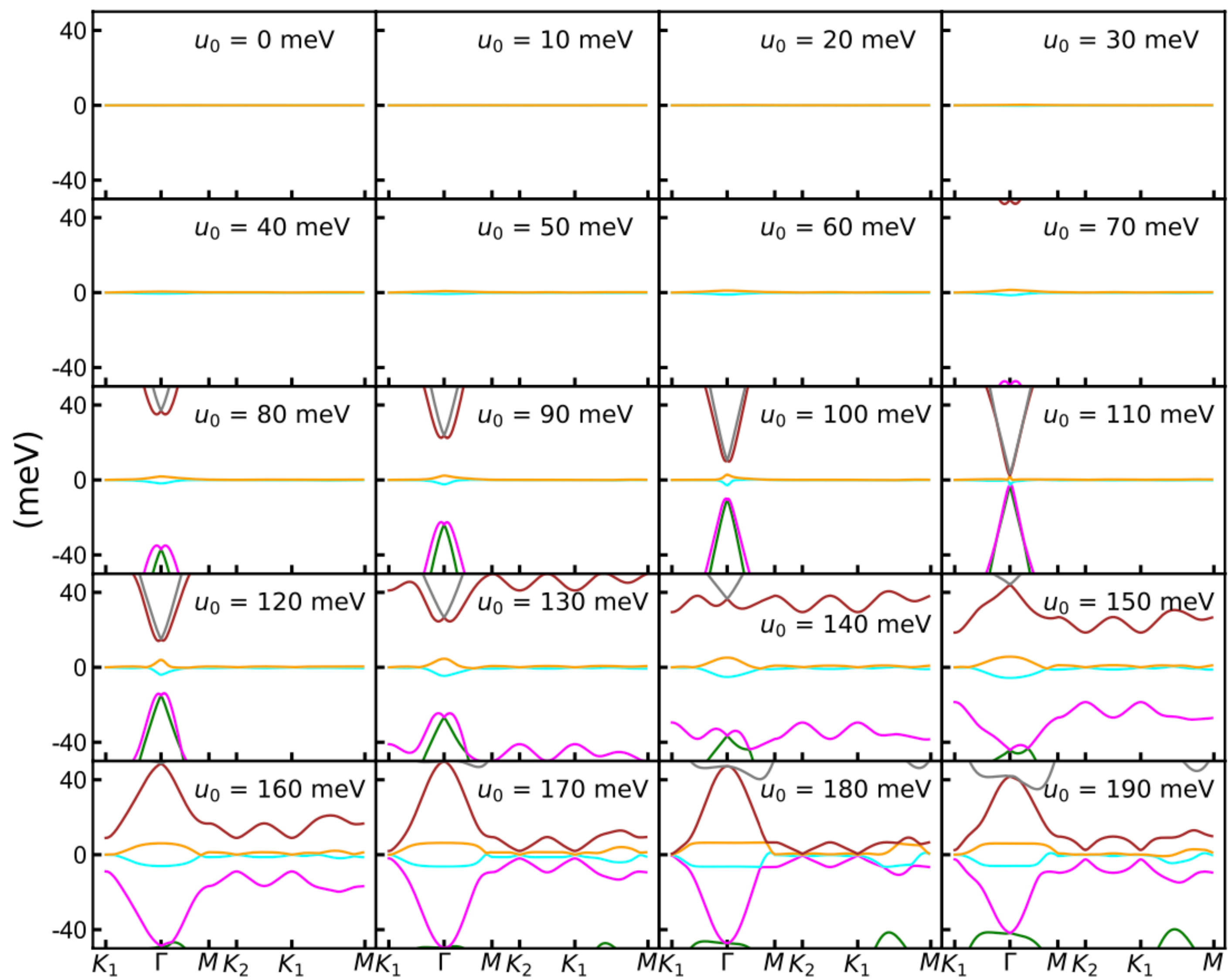
$$U_0 = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}$$

Inter-sublattice, interlayer hopping

Similar for matrices $U_1,\ U_2$

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



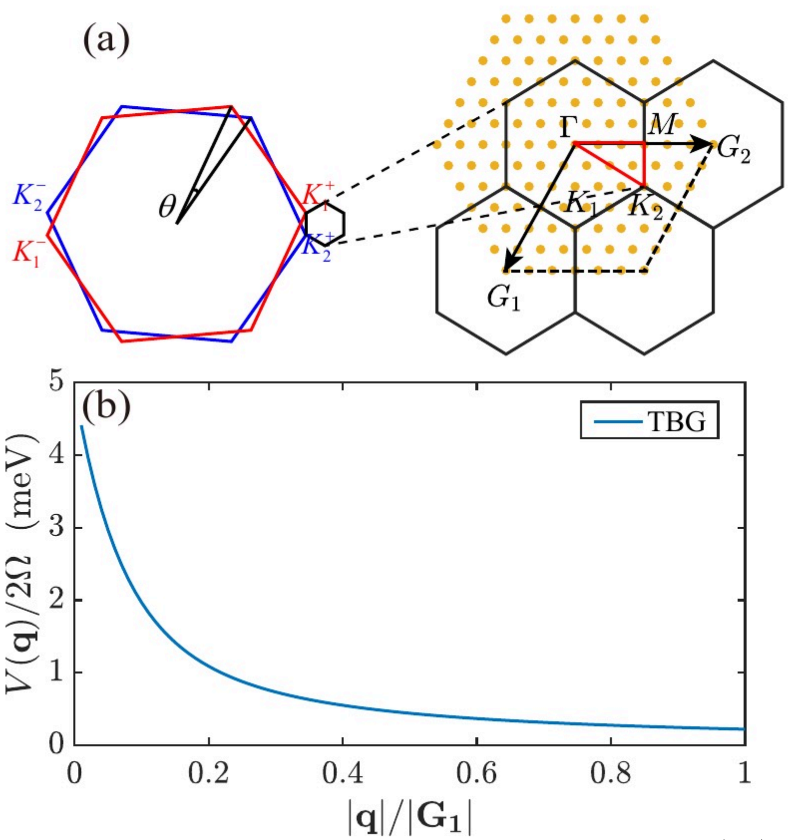


- Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in twisted bilayer graphene
  Cheng Huang, Xu Zhang, Gaopei Pan, Heqiu Li, Kai Sun, Xi Dai, Zi Yang Meng,
  Phys. Rev. B 109, 125404 (2024)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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

CPL 38, 077305 (2021)



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

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

$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{s,\eta,\mathbf{k},m_1,m_2} \lambda^{s,\eta}_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})\left(c^\dagger_{s,\eta,\mathbf{k},m_1} c_{s,\eta,\mathbf{k}+\mathbf{q}+\mathbf{G},m_2} - \frac{\nu+4}{8}\delta_{\mathbf{q},0}\delta_{m_1,m_2}\right)$$

$$\lambda^{s,\eta}_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u^{s,\eta}_{\mathbf{k},m_1} | u^{s,\eta}_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$

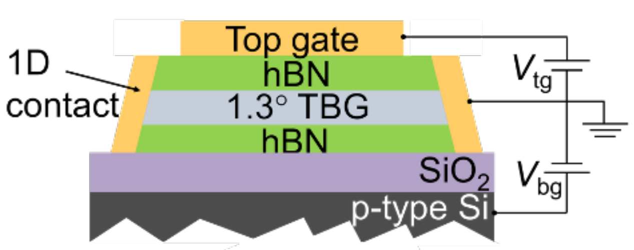
overlap of H_0 eigenstate

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

Single gate

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

$\varepsilon = 5,7,9\ \varepsilon_0$



$$\Omega = N_{\mathbf{k}}\frac{\sqrt{3}}{2}L_M^2 \quad N_{\mathbf{k}} = 6\times 6,\ 9\times 9,\ 12\times 12,\ 15\times 15, 18\times 18$$

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

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

CPL 38, 077305 (2021)

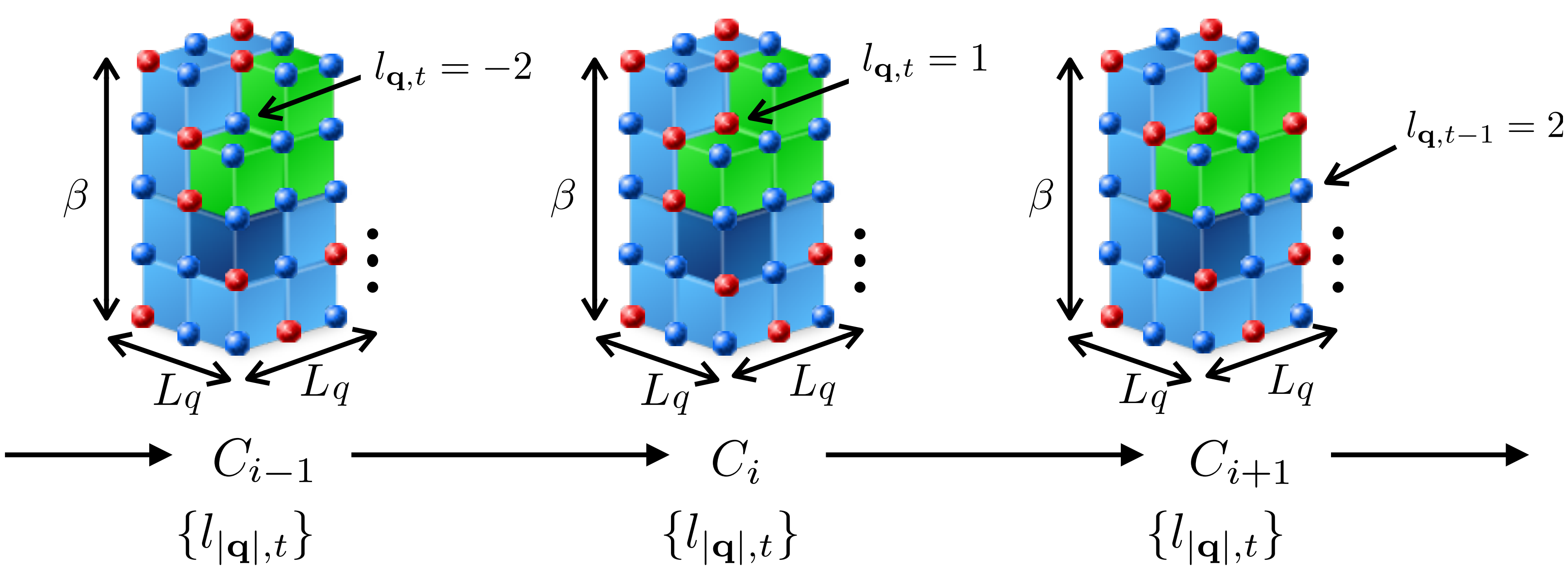
$$Z = \mathrm{Tr}\{\prod_{\tau} e^{-\Delta\tau\, H_{int}(\tau)}\} = \mathrm{Tr}\{\prod_{\tau} \exp\{-\frac{\Delta\tau}{4\Omega} \sum_{\mathbf{G},\mathbf{q}\in mBZ} V(\mathbf{q}+\mathbf{G}) \cdot [\underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}} + \delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{A_{\mathbf{Q}}} - \underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}} - \delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{B_{\mathbf{Q}}}]\}\}$$

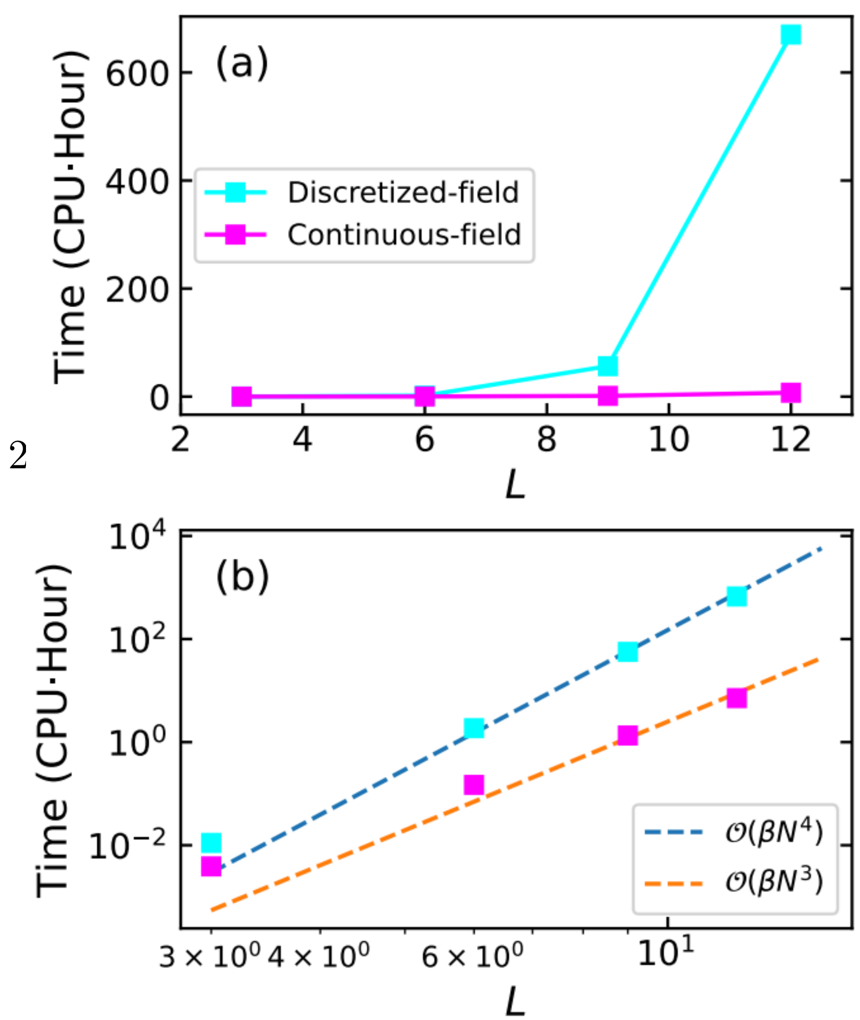
$$\exp(-\alpha_1(\mathbf{Q})A_{\mathbf{Q}}^2) = \frac{1}{4}\sum_{\{l_{\mathbf{Q},\tau,1}\}} \gamma(l_{\mathbf{Q},\tau,1})\ \exp(i\eta(l_{\mathbf{Q},\tau,1})\sqrt{\alpha_1(\mathbf{Q})}\ A_{\mathbf{Q}})) + O(\Delta\tau^4) \quad \{l_{\mathbf{Q},\tau,1}, l_{\mathbf{Q},\tau,2}\} \quad \alpha_1(\mathbf{Q}) = \frac{\Delta\tau V(\mathbf{Q})}{4\Omega}$$

$$Z = \mathrm{Tr}\{\prod_{\tau} e^{-\Delta\tau\, H_{int}(\tau)}\} = \sum_{\{\{l_{\mathbf{Q},\tau_1}\},\{l_{\mathbf{Q},\tau_2}\},\cdots\}} \det[\mathbf{1} + \mathbf{B}_{\tau_m}\mathbf{B}_{\tau_{m-1}}\cdots\mathbf{B}_{\tau_1}]$$

$$R = \det[\mathbb{1} + \Delta(\mathbb{1} - G_s(\tau))]$$

Δ circulant matrix





Update a single site and update the Green's function, entire space-time update

$O(N^3)$ $O(\beta N^4)$

Cheng Huang et al., Nat. Comm. 16, 7176 (2025)

Momentum-Space Quantum Monte Carlo

CPL 38, 077305 (2021)

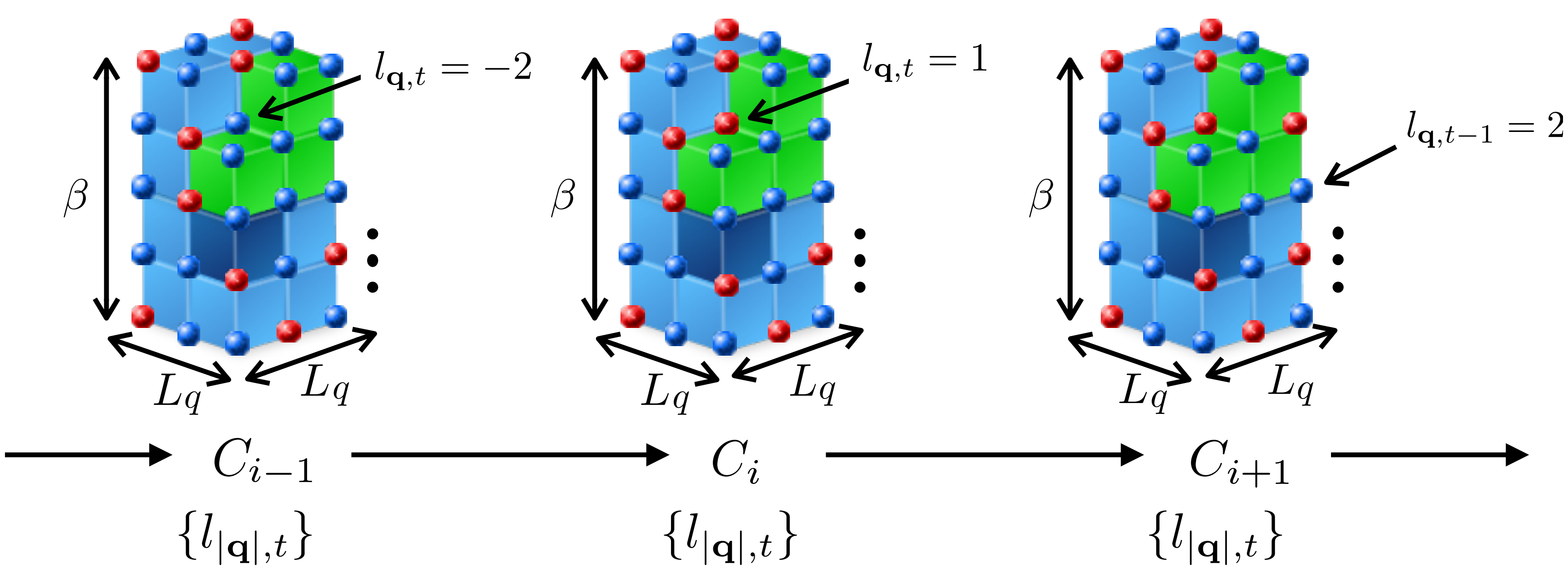
$$Z = \mathrm{Tr}\{\prod_\tau e^{-\Delta\tau\, H_{int}(\tau)}\} = \mathrm{Tr}\{\prod_\tau \exp\{-\frac{\Delta\tau}{4\Omega}\sum_{\mathbf{G},\mathbf{q}\in mBZ} V(\mathbf{q}+\mathbf{G})\cdot[\underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}}+\delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{A_\mathbf{Q}} - \underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}}-\delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{B_\mathbf{Q}}]\}\}$$

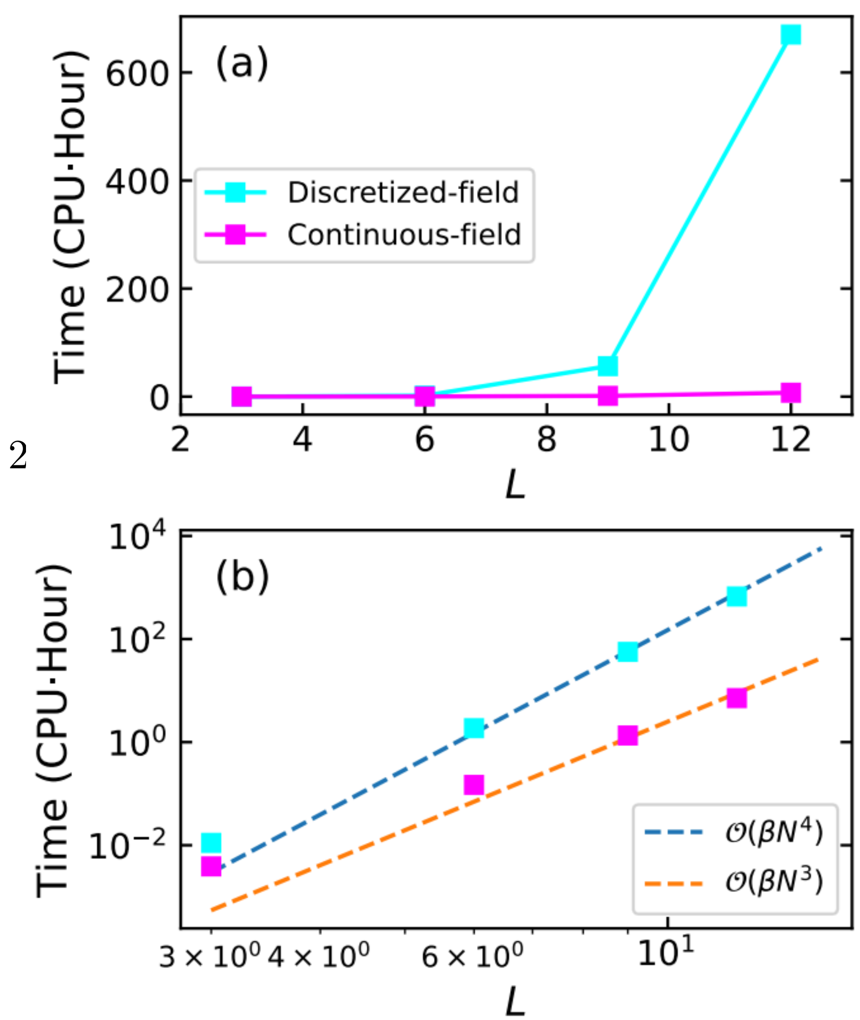
$$\exp(-\alpha_1(\mathbf{Q})A_\mathbf{Q}^2) = \frac{1}{4}\sum_{\{l_{\mathbf{Q},\tau,1}\}}\gamma(l_{\mathbf{Q},\tau,1})\ \exp(i\eta(l_{\mathbf{Q},\tau,1})\sqrt{\alpha_1(\mathbf{Q})}\ A_\mathbf{Q})) + O(\Delta\tau^4) \qquad \{l_{\mathbf{Q},\tau,1}, l_{\mathbf{Q},\tau,2}\} \qquad \alpha_1(\mathbf{Q}) = \frac{\Delta\tau V(\mathbf{Q})}{4\Omega}$$

$$Z = \mathrm{Tr}\{\prod_\tau e^{-\Delta\tau\, H_{int}(\tau)}\} = \sum_{\{\{l_{\mathbf{Q},\tau_1}\},\{l_{\mathbf{Q},\tau_2}\},\cdots\}} \det[\mathbf{1}+\mathbf{B}_{\tau_m}\mathbf{B}_{\tau_{m-1}}\cdots\mathbf{B}_{\tau_1}]$$

$$= \det[\mathbb{1} + \Delta(\mathbb{1} - G_s(\tau))]$$

Δ circulant matrix





Update a single site and update the Green's function, entire space-time update

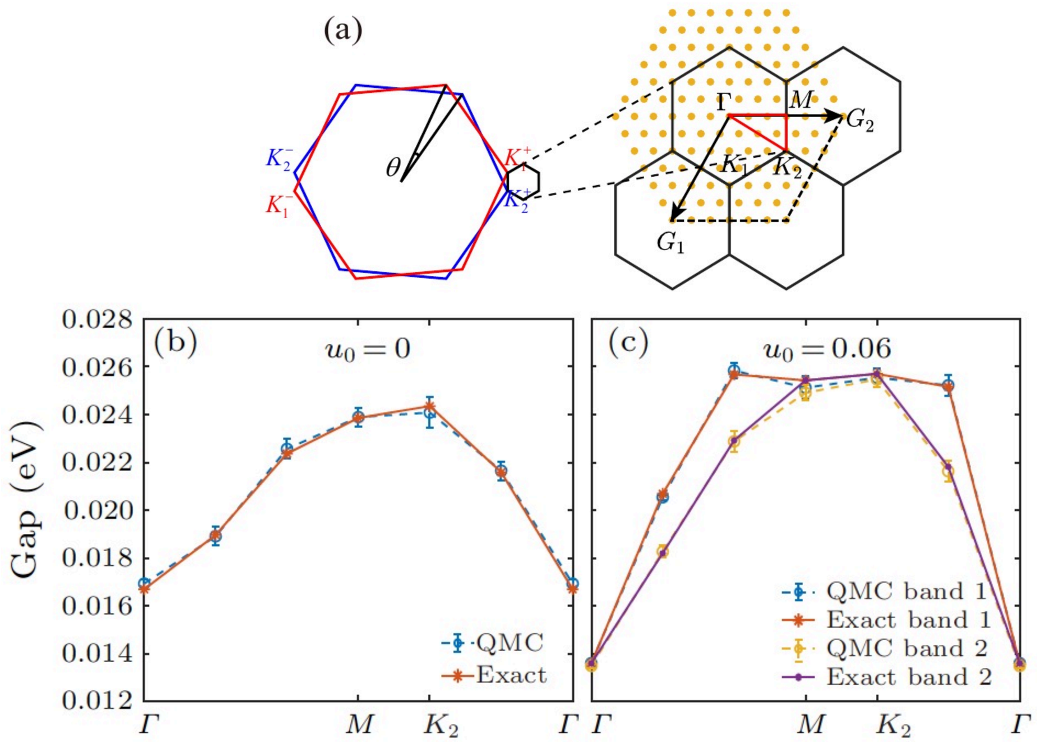
$O(N^3)$ $O(\beta N^4)$

Cheng Huang et al., Nat. Comm. 16, 7176 (2025)

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,†]

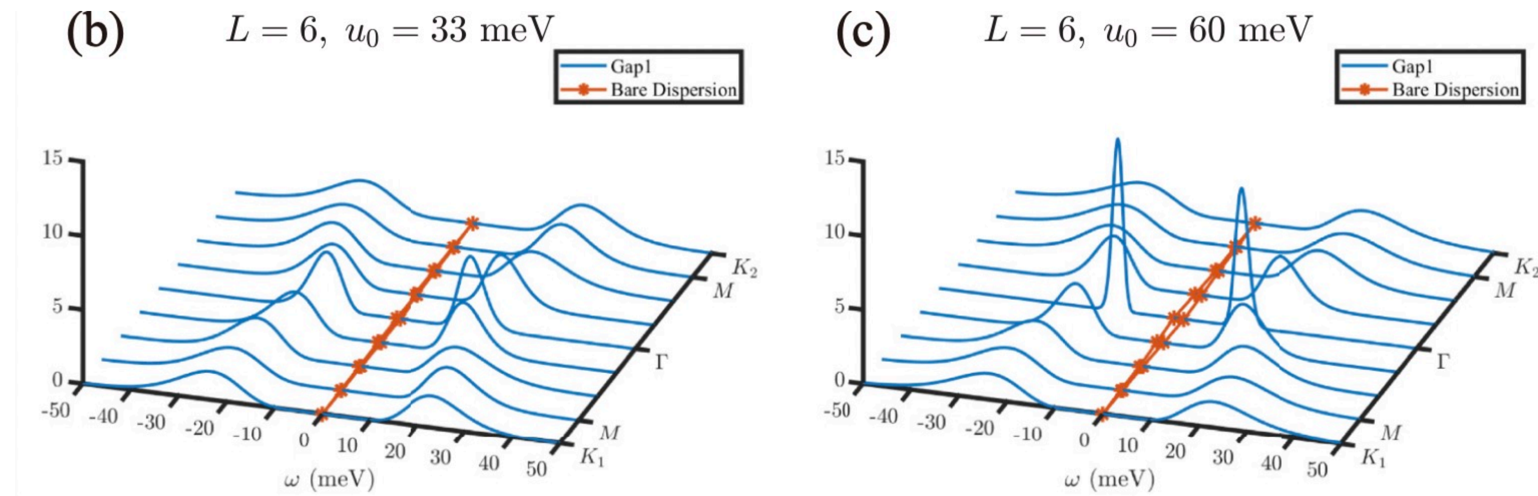
CPL 38, 077305 (2021)



single-particle excitations

PRB 105, L121110 (2022)

$T = 0.667$ meV



Bosonic collective excitations

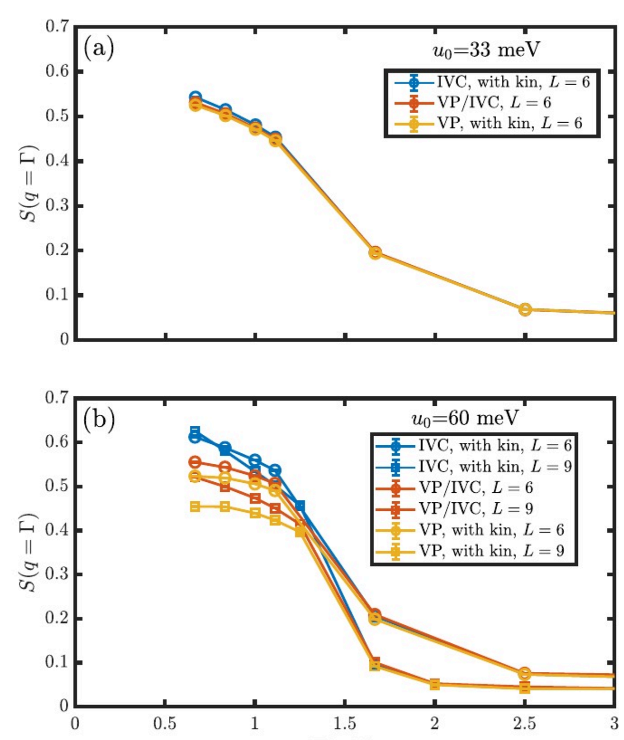
$$\mathcal{O}_a(\mathbf{q}) = \sum_{\mathbf{k}} d^\dagger_{\mathbf{k+q}} M_a d_{\mathbf{k}}$$

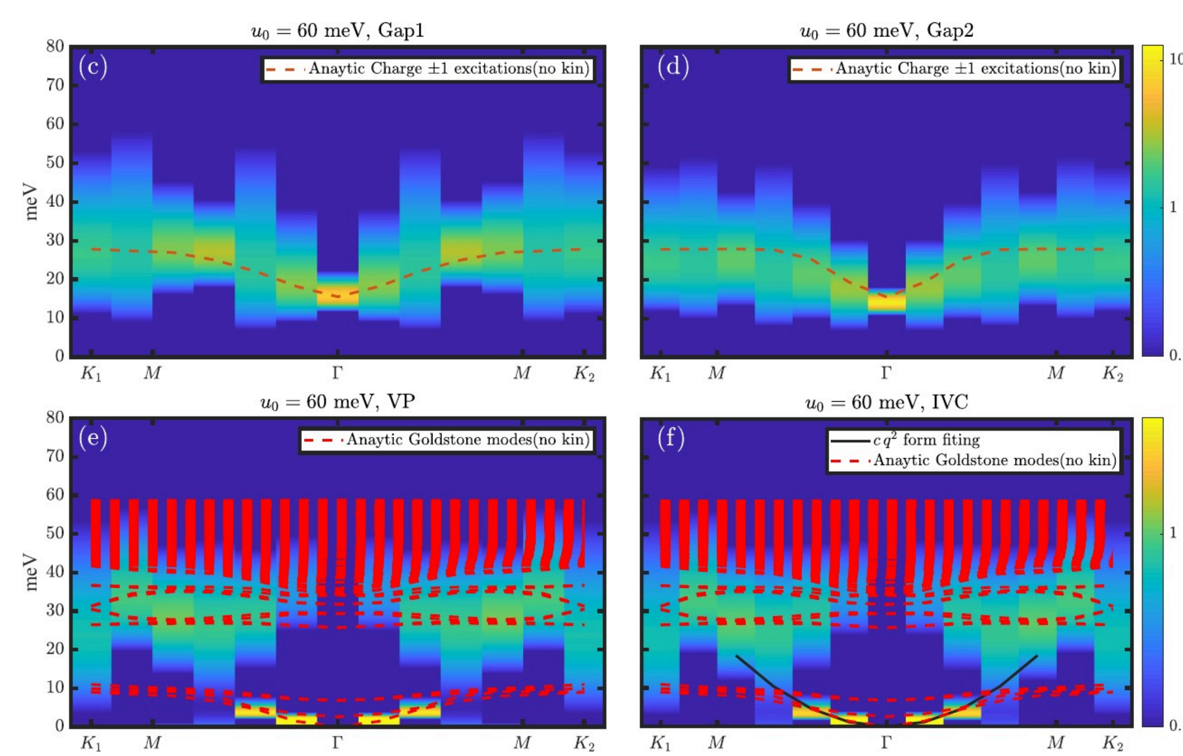
$$M_a = \tau_z \eta_0$$

for valley polarized state

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

for intervalley coherent state



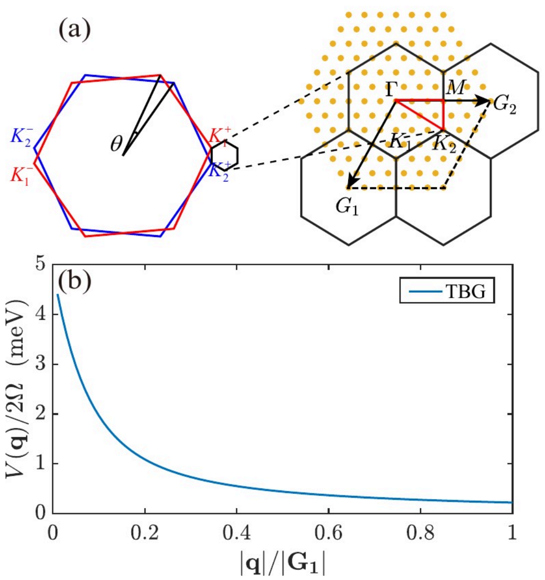


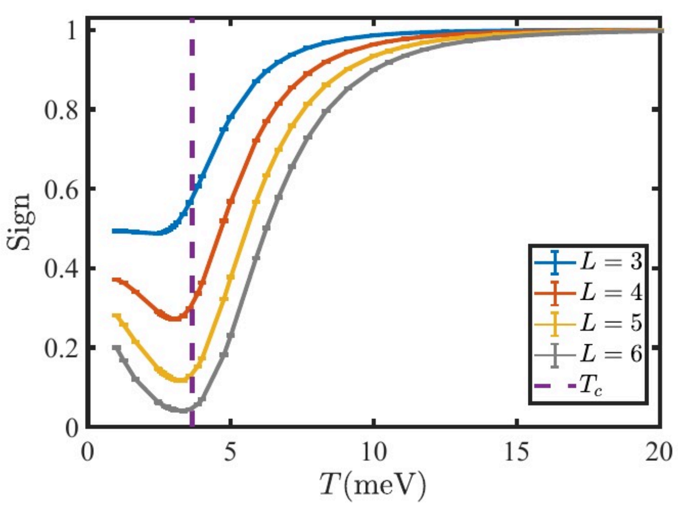
Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

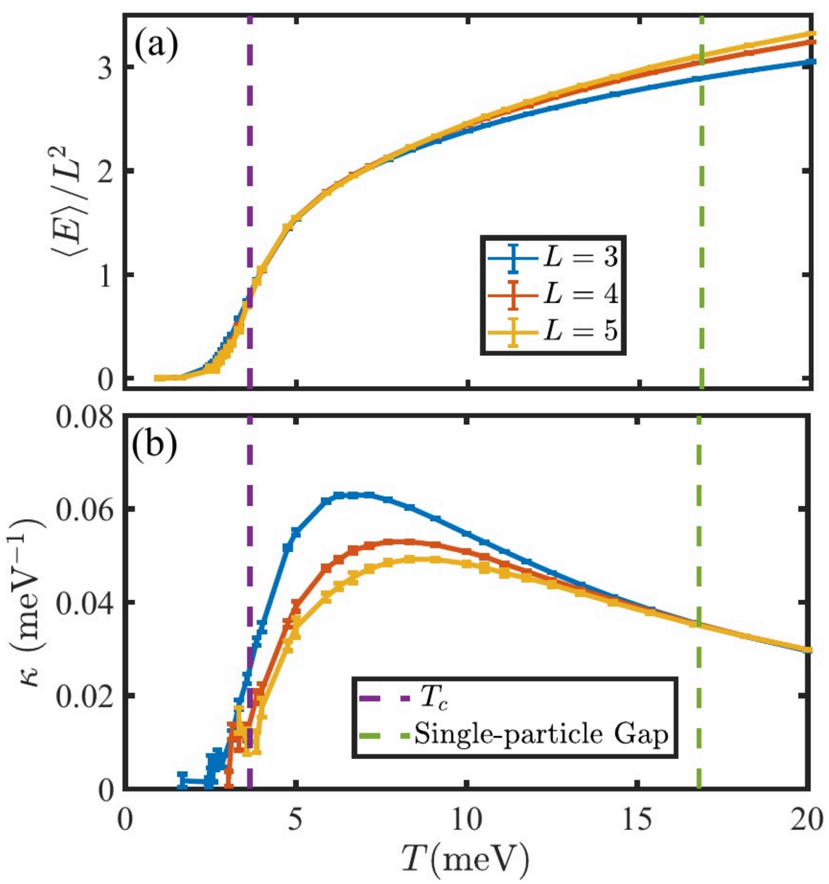
Gaopei Pan,[1,2] Xu Zhang,[3] Hongyu Lu,[3] Heqiu Li,[4] Bin-Bin Chen,[3] Kai Sun,[5,*] and Zi Yang Meng[3,†]

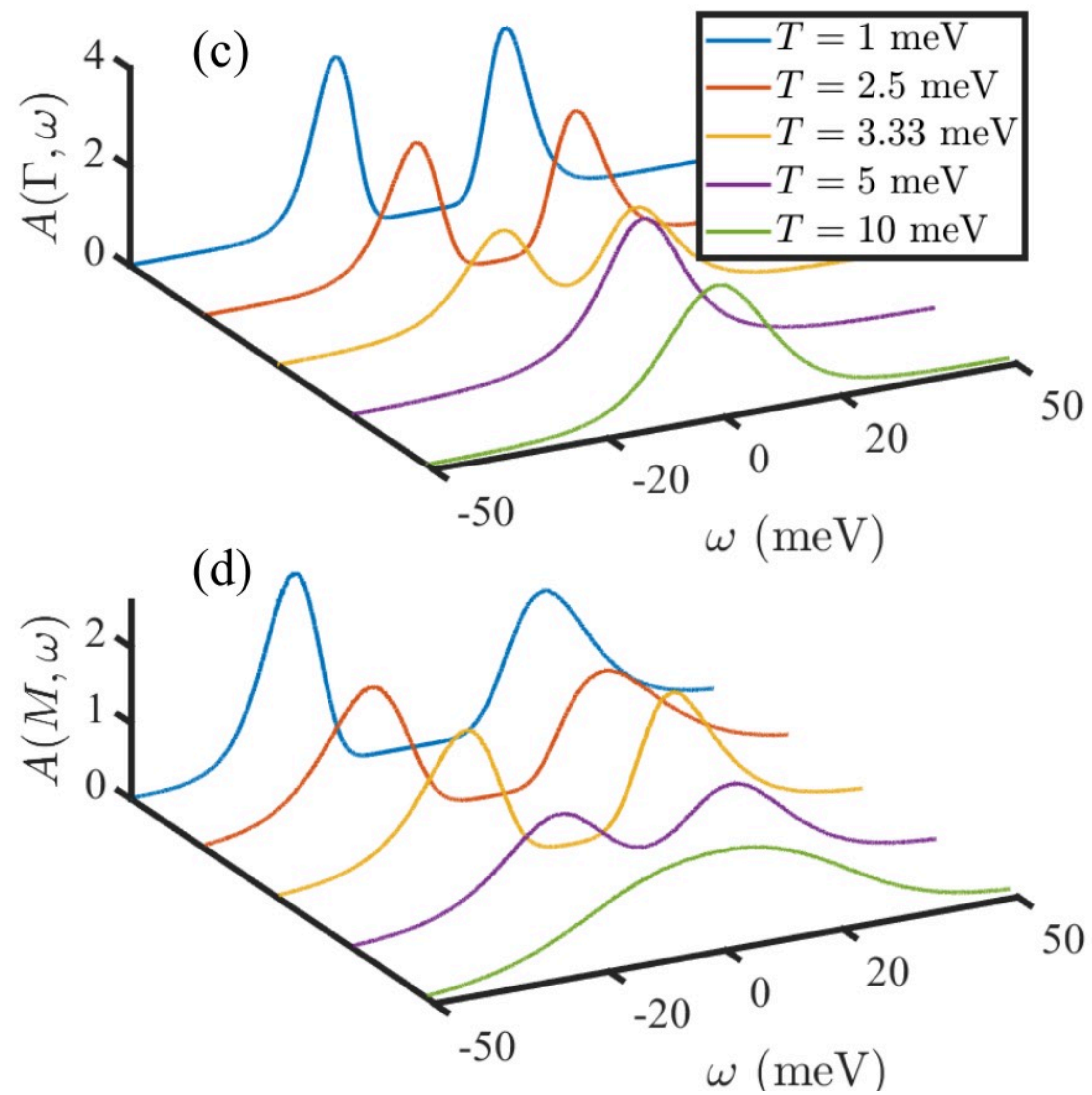
PRL 130, 016401 (2023)

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

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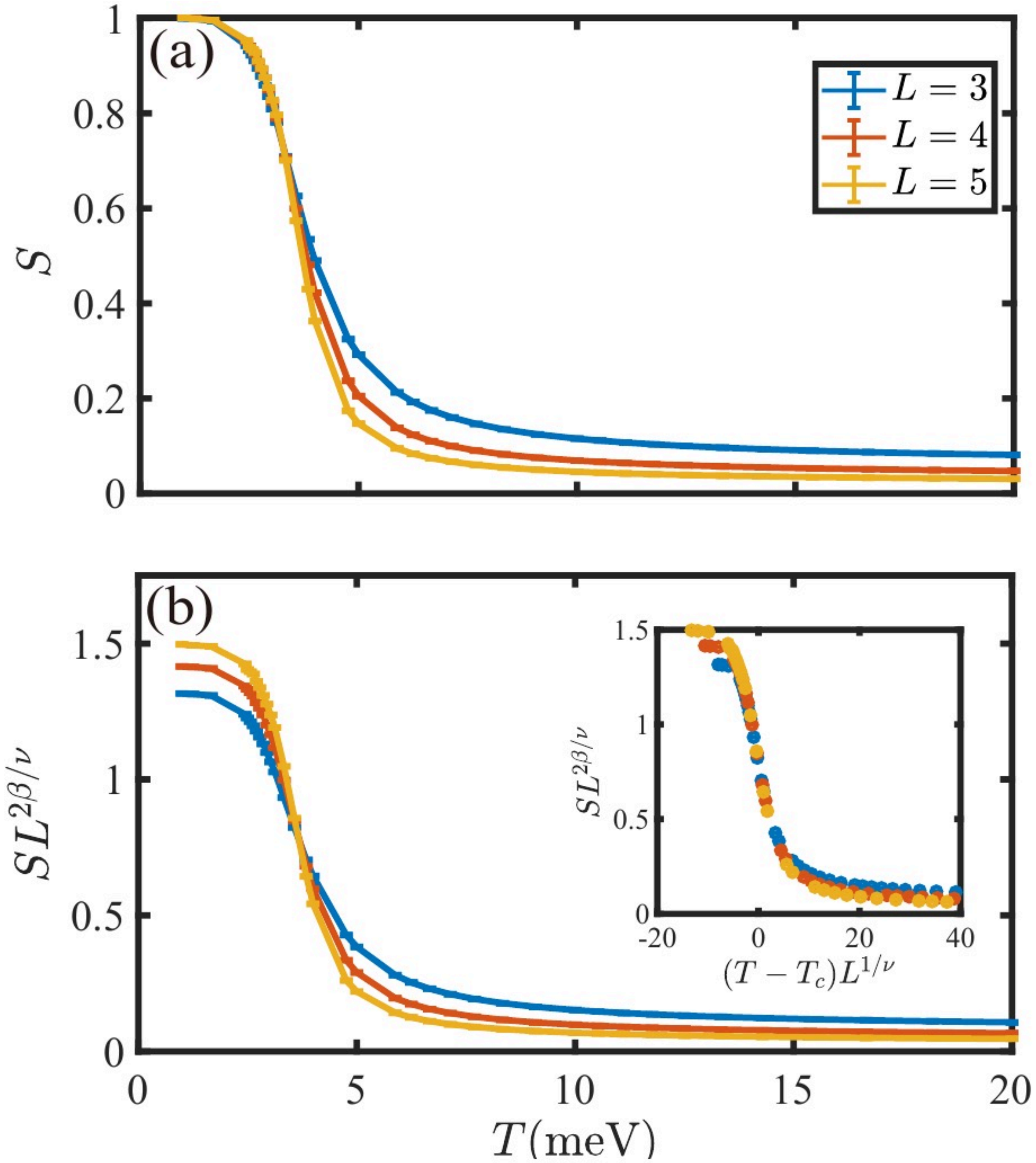
PRL 130, 016401 (2023)

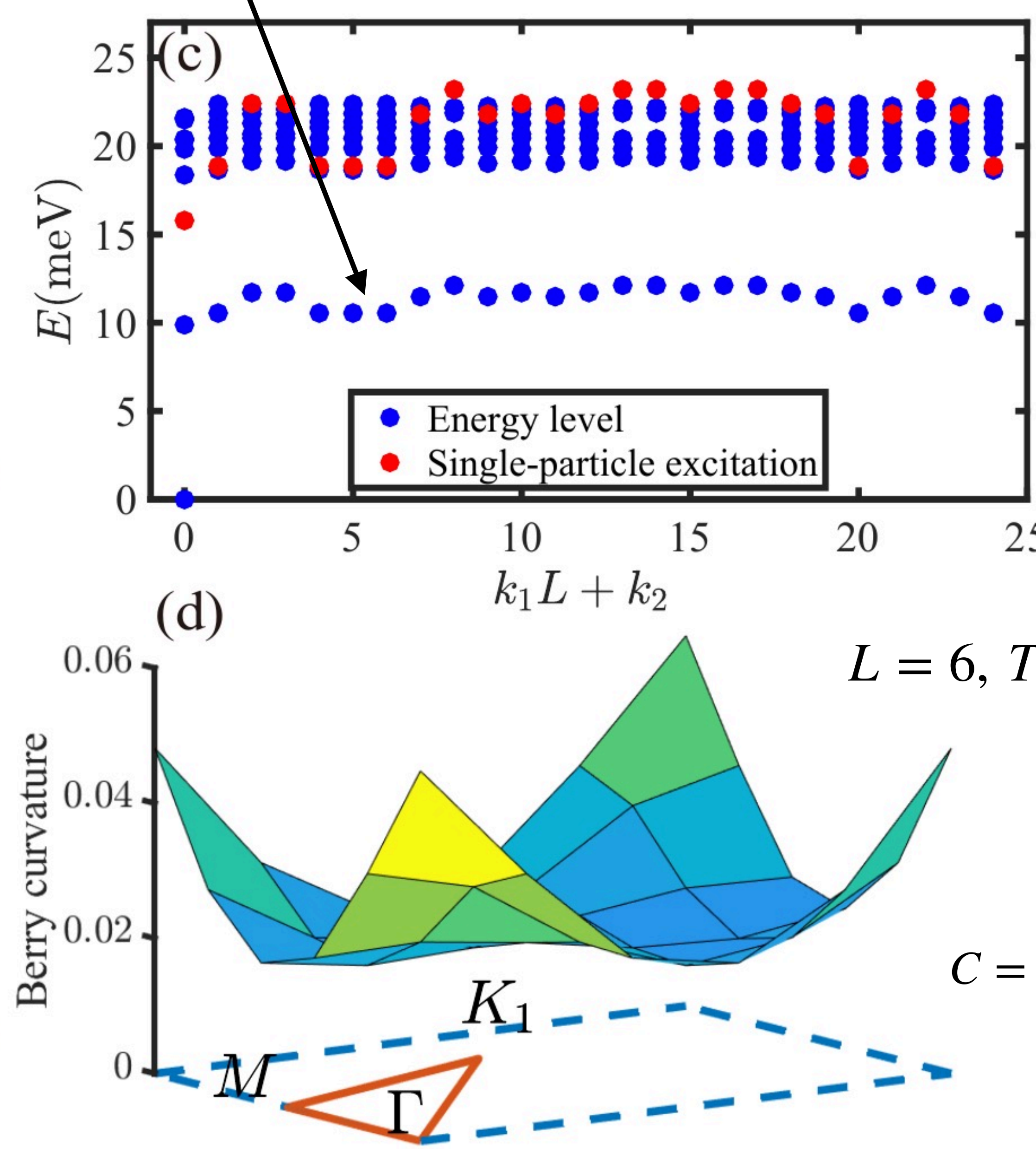
momentum-space QMC & exact diagonalization

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

Gapped excitons restore time-reversal

$L = 5$





$L = 6,\ T = 1.25$ meV

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

$T_c = 3.65(5)$ meV

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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

CPL 38, 077305 (2021)

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

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

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

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

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)

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

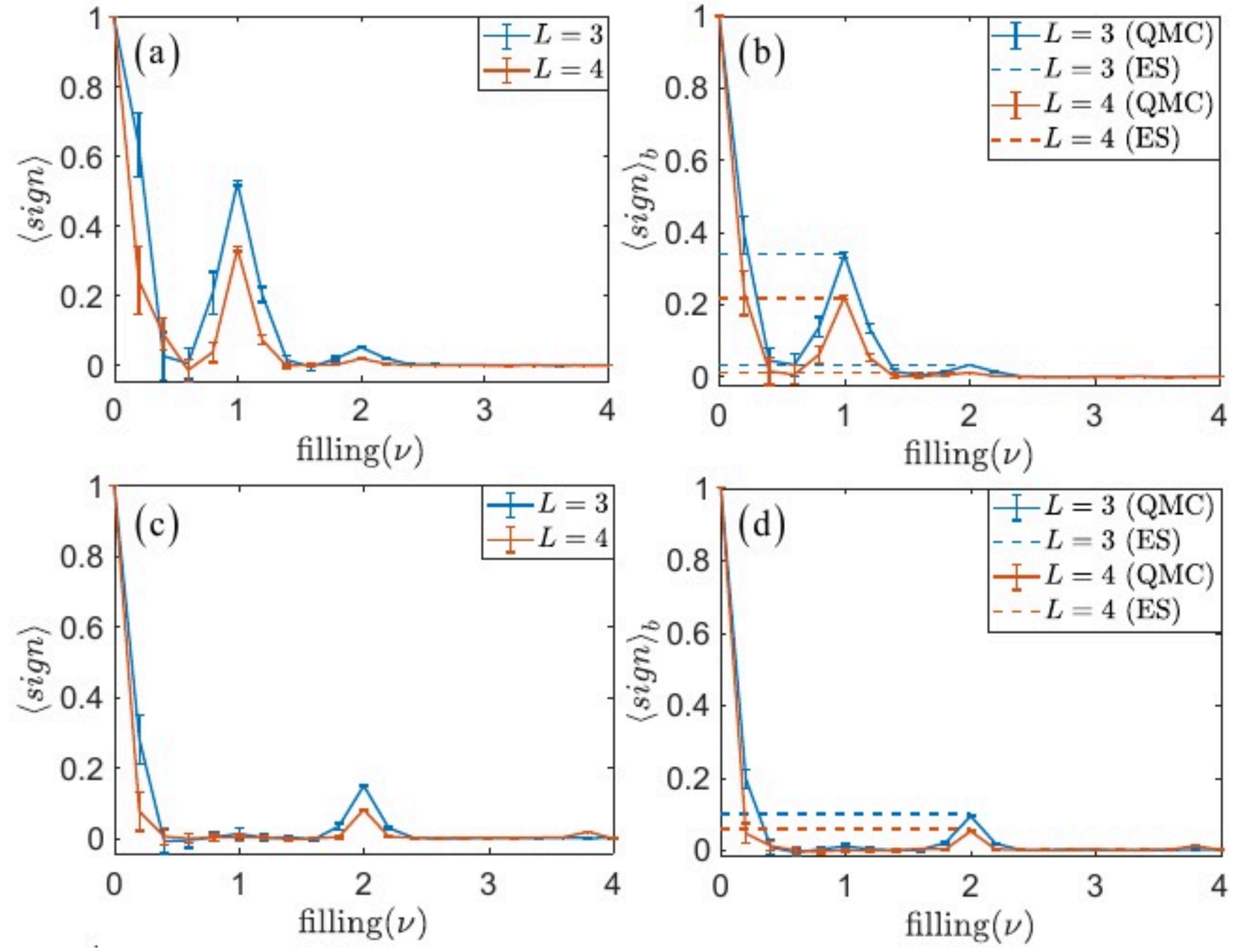
- Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)
- Xu Zhang et al., Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, PRB 107, L241105 (2023)

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}



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

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

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

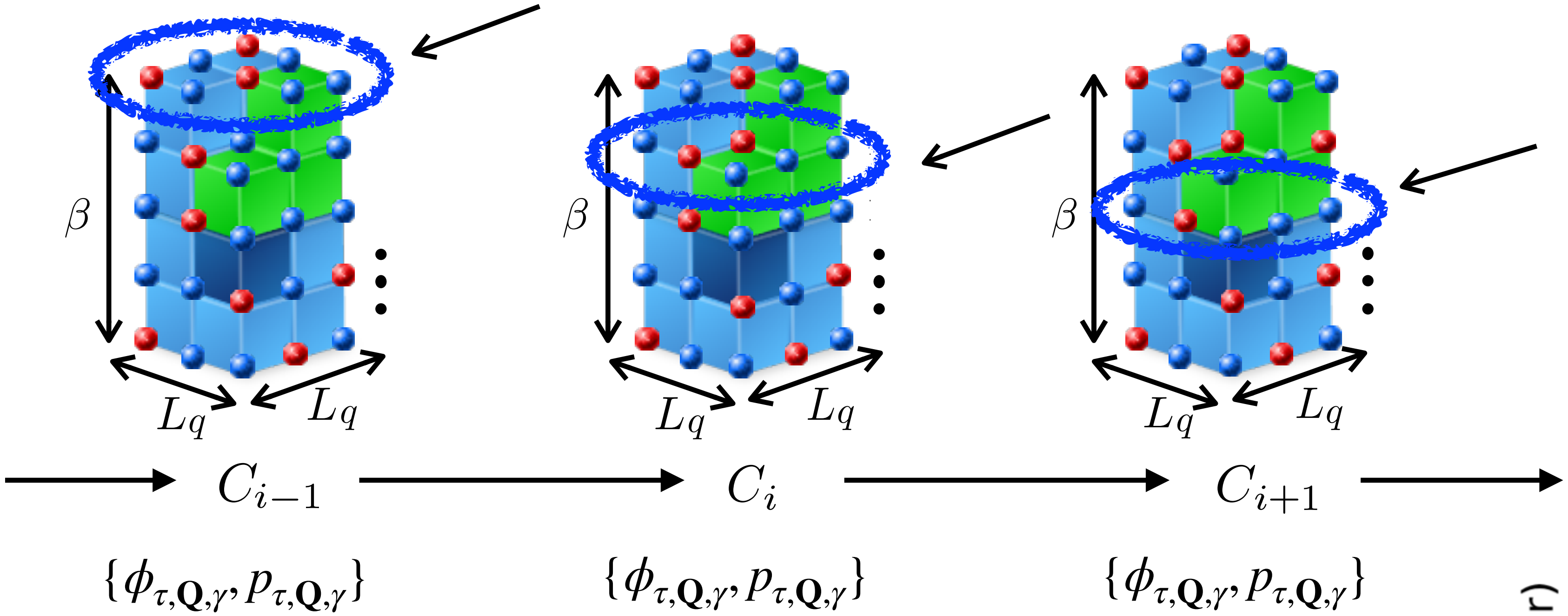
Continuous Field Momentum-Space QMC

Cheng Huang et al., Nat. Comm. 16, 7176 (2025)

$$Z = \int \prod_{\tau,\boldsymbol{Q}} d\phi_{\tau,\boldsymbol{Q},1} d\phi_{\tau,\boldsymbol{Q},2} \mathrm{e}^{-\frac{1}{2}\sum_{\tau,Q}\left(\phi^2_{\tau,\boldsymbol{Q},1}+\phi^2_{\tau,\boldsymbol{Q},2}\right)} \times \mathrm{Tr}\left(\prod_{\tau} \mathrm{e}^{-\Delta\tau H_0} \mathrm{e}^{\mathrm{i}\sum_{\boldsymbol{Q}}\left(-\phi_{\tau,\boldsymbol{Q},1}\sqrt{\alpha_2(\boldsymbol{Q})}A_{\boldsymbol{Q}}+\mathrm{i}\phi_{\tau,\boldsymbol{Q},2}\sqrt{\alpha_2(\boldsymbol{Q})}B_{\boldsymbol{Q}}\right)}\right)$$

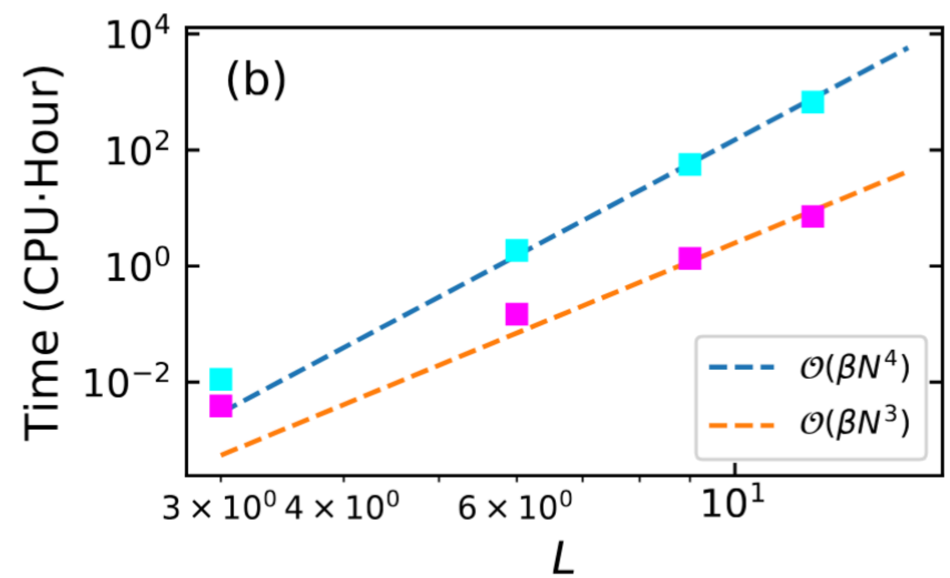
$$= \int \prod_{\tau,\mathbf{Q},\gamma} d\phi_{\tau,\mathbf{Q},\gamma}\, dp_{\tau,\mathbf{Q},\gamma}\, \exp\Bigg(- \underbrace{\Big(\frac{1}{2}\sum_{\tau,\mathbf{Q},\gamma}(p^2_{\tau,\mathbf{Q},\gamma}+\phi^2_{\tau,\mathbf{Q},\gamma}) - \ln(\det(M)\Big)}_{\mathscr{H}}\Bigg)$$

$$M = \begin{pmatrix} \mathbf{1} & 0 & 0 & \cdots & 0 & B_{N_\tau} \\ -B_1 & \mathbf{1} & 0 & \cdots & 0 & 0 \\ 0 & -B_2 & \mathbf{1} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{1} & 0 \\ 0 & 0 & 0 & \cdots & -B_{N_\tau-1} & \mathbf{1} \end{pmatrix}$$



$$\begin{cases} \dfrac{dp_{\tau,\mathbf{Q},\gamma}}{dt} = -\dfrac{\partial \mathscr{H}}{\partial \phi_{\tau,\mathbf{Q},\gamma}} = -\phi_{\tau,\mathbf{Q},\gamma} + \mathrm{Tr}\left(M^{-1}\dfrac{\partial M}{\partial \phi_{\tau,\mathbf{Q},\gamma}}\right) \\ \dfrac{d\phi_{\tau,\mathbf{Q},\gamma}}{dt} = \dfrac{\partial \mathscr{H}}{\partial p_{\tau,\mathbf{Q},\gamma}} = p_{\tau,\mathbf{Q},\gamma} \end{cases}$$

sparse matrix
O(N^2)



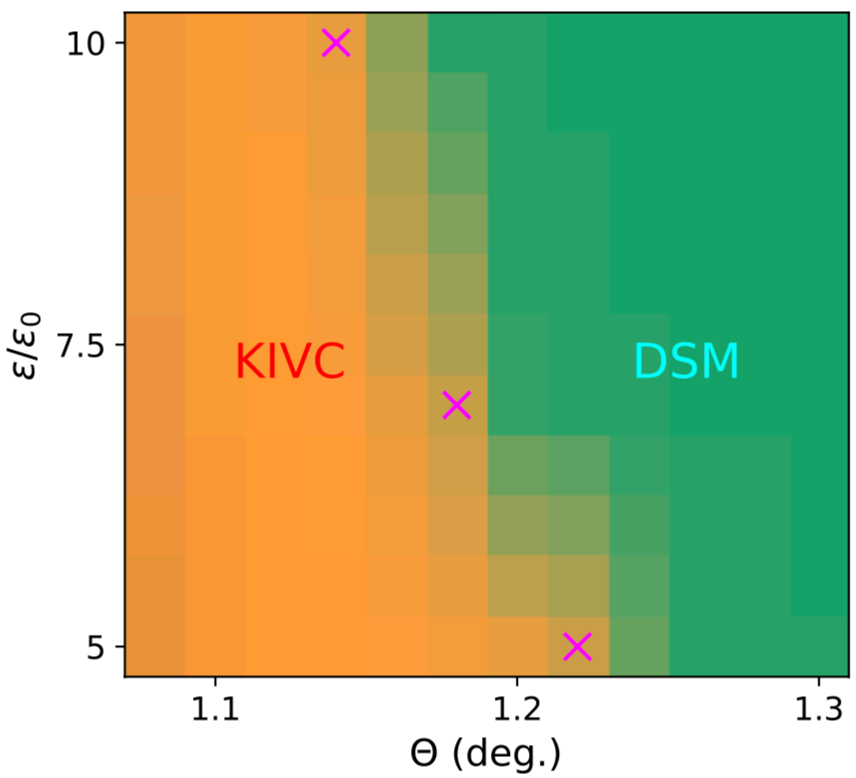
Update the entire time slice and update the Green's function

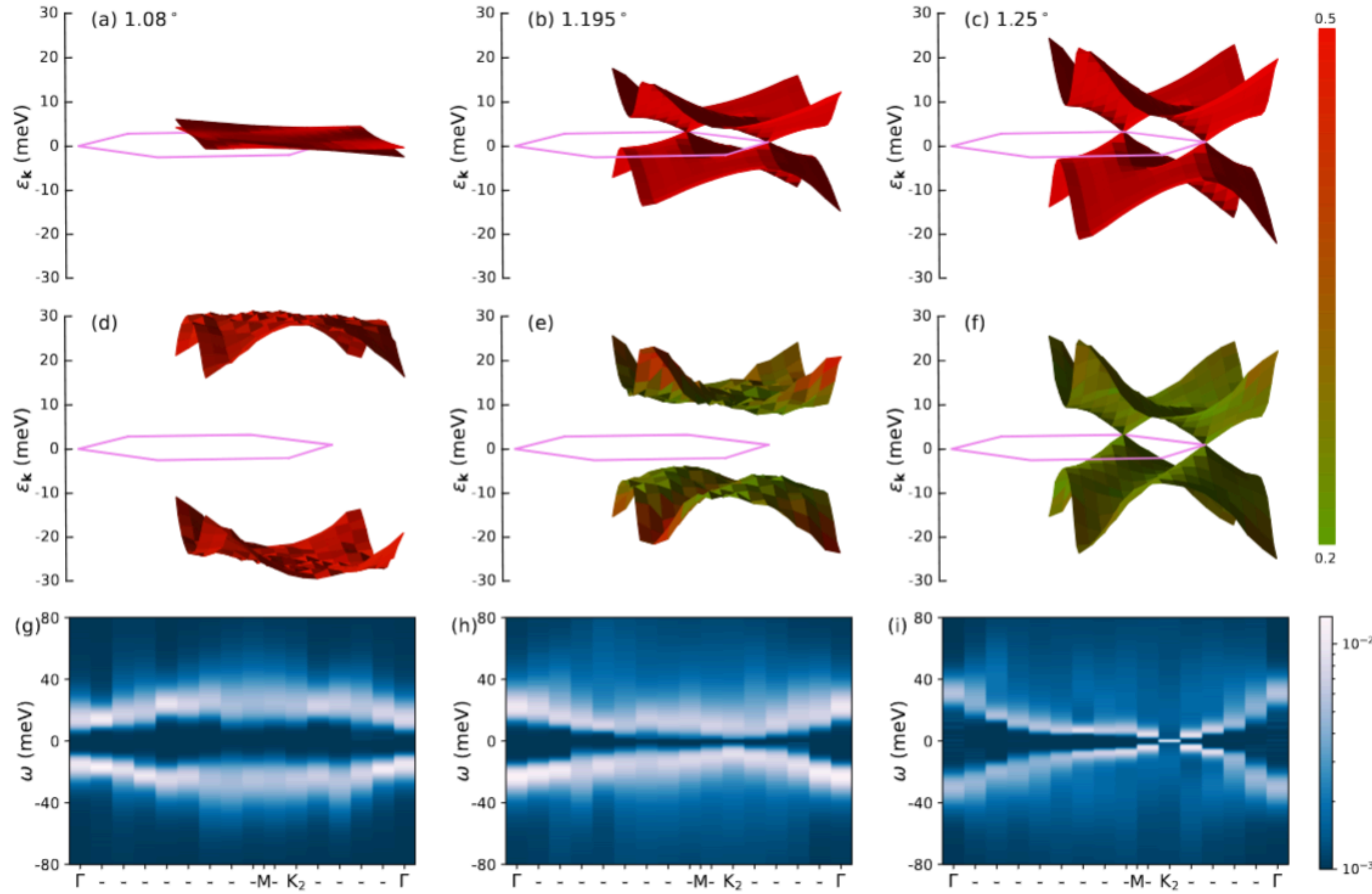
$O(N^2)$ $O(N^3)$

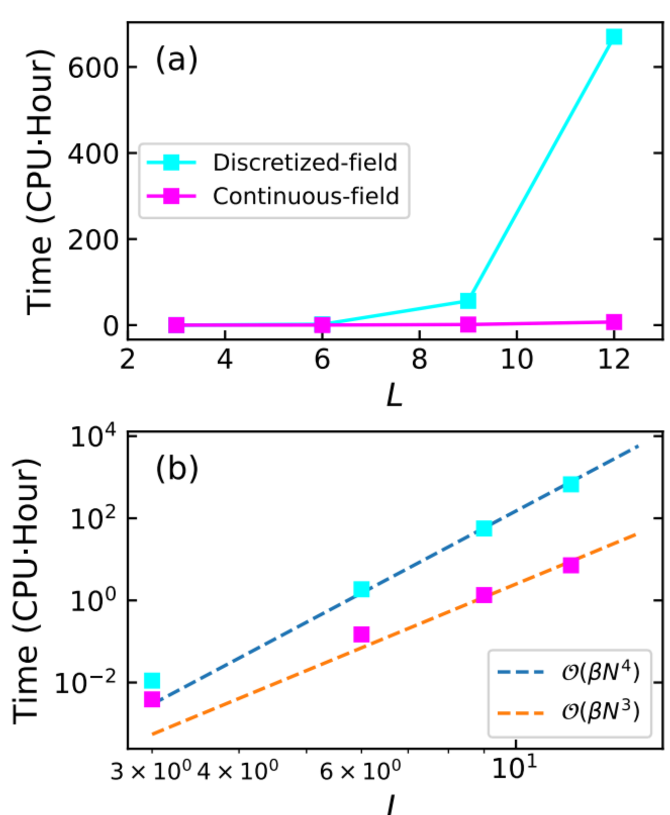
Angle-Tuned Gross-Neveu Quantum Criticality in Twisted Bilayer Graphene: A Quantum Monte Carlo Study

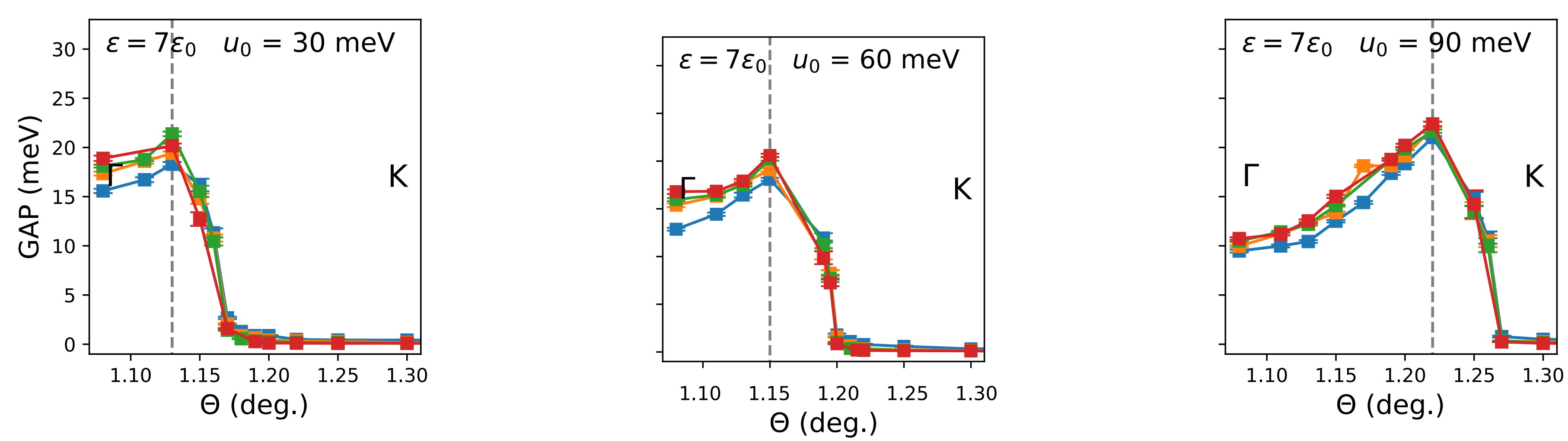
Cheng Huang,[1] Nikolaos Parthenios,[2,3] Maksim Ulybyshev,[4] Xu Zhang,[1,5] Fakher F. Assaad,[4,6] Laura Classen,[2,3,*] and Zi Yang Meng[1,†]

Nat. Comm. 16, 7176 (2025)









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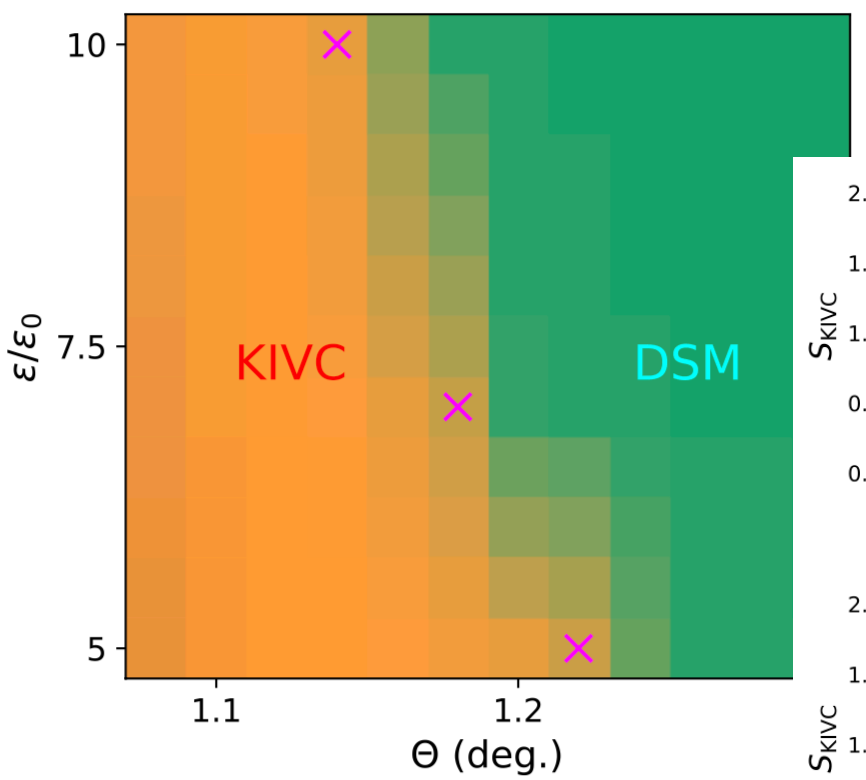
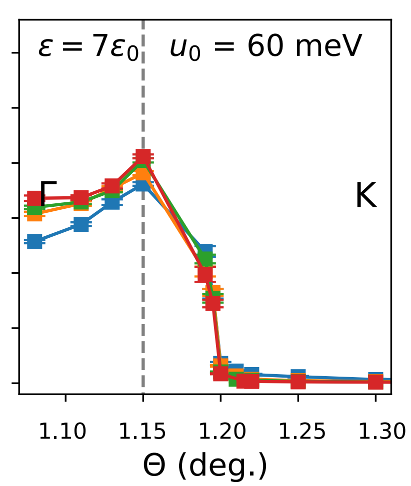
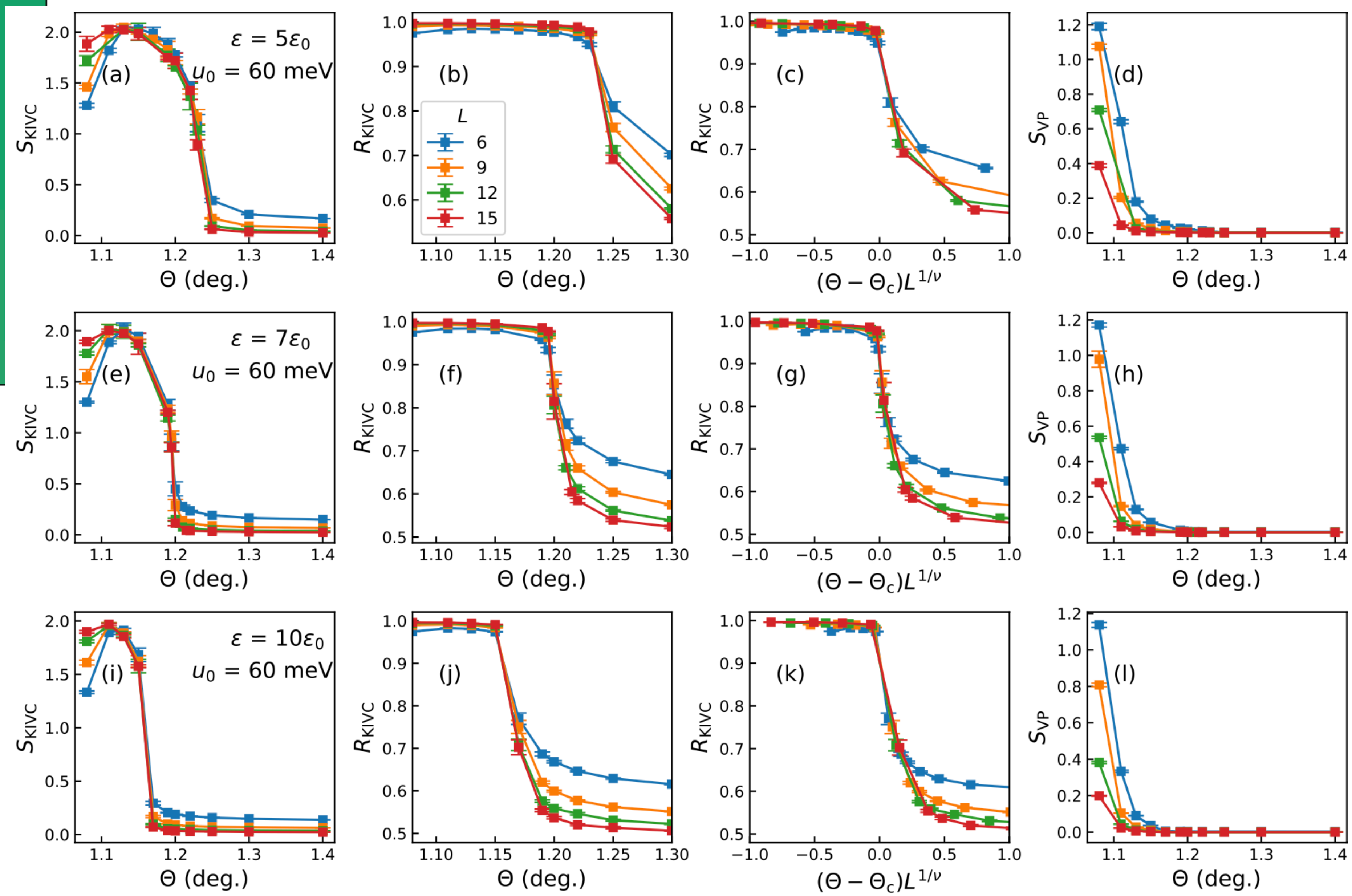
Nat. Comm. 16, 7176 (2025)



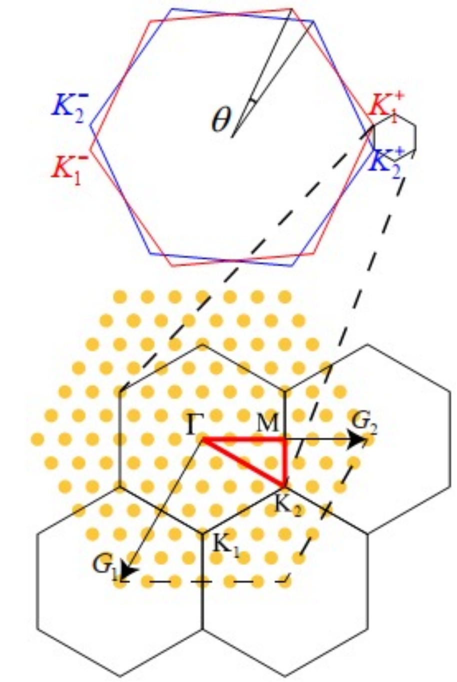




Content

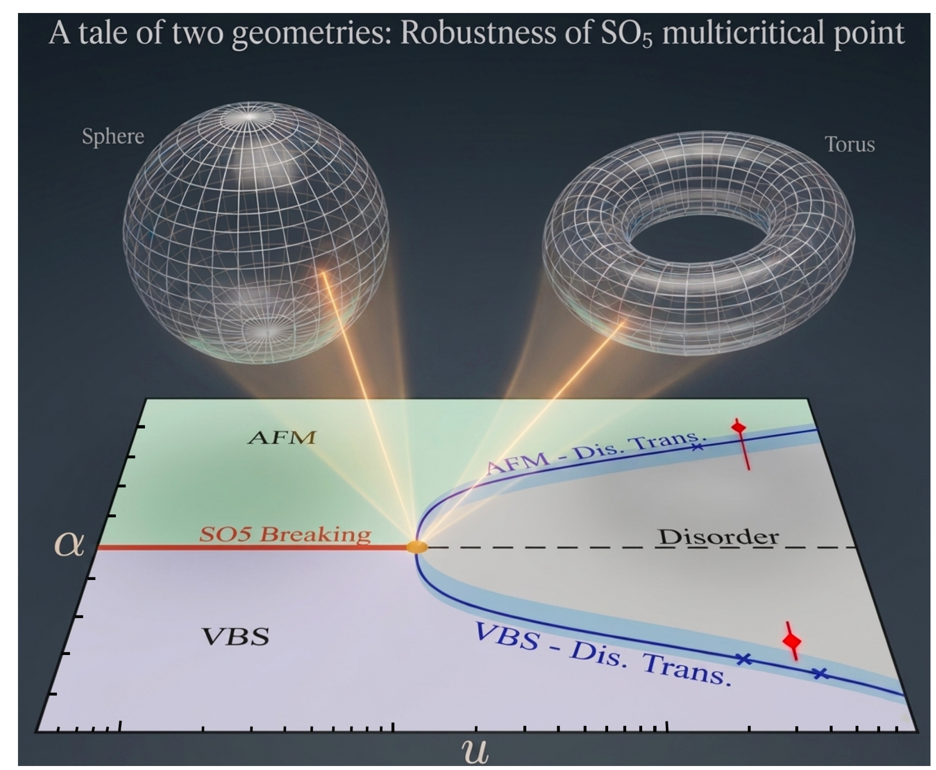
1. Momentum-space QMC for twisted bilayer graphene

- CPL 38, 077305 (2021) [momentum-space QMC, 6 x 6]
- PRL 130, 016401 (2023) [Thermodynamic responses]
- PRB 107, L241105 (2023) [Polynomial sign problem]
- Nat. Comm. 16, 7176 (2025) [global update, 18 x 18]
- ......



2. (2+1)D SO(5) nonlinear sigma model with Wess-Zumino-Witten term

- PRL 132, 246503 (2023) [ED+DMRG, $N_\phi = 16$]
- arXiv: 2605.03700 (2026) [global update, $N_\phi = 160$]
- ......



3. Hybrid Monte Carlo for FQHs

- Rep. Prog. Phys. 10.1088/ae70a7 (2026) [global update, N = 1200]
- ......

Phases of (2+1)D SO(5) non-linear sigma model with a topological term on a sphere: multicritical point and disorder phase

Bin-Bin Chen,[1] Xu Zhang,[1] Yuxuan Wang,[2,*] Kai Sun,[3,†] and Zi Yang Meng[1,‡]

PRL 132, 246503 (2023) [ED+DMRG]

Wess-Zumino-Witten Terms in Graphene Landau Levels

Junhyun Lee and Subir Sachdev
Phys. Rev. Lett. **114**, 226801 – Published 1 June 2015

$$S=\frac{1}{g}\int d^3x(\nabla\hat{\boldsymbol{\varphi}})^2+S_{\mathrm{WZW}}+\cdots$$

$$H=\frac{1}{2}\int d\Omega\{U_0[\psi^\dagger(\Omega)\psi(\Omega)-2]^2-\sum_{i=1}^{5}u_i[\psi^\dagger(\Omega)\Gamma^i\psi(\Omega)]^2\}$$

$\psi_{\tau\sigma}(\Omega)$ $\quad\Gamma^i=\{\tau_x\otimes\mathbb{I},\tau_y\otimes\mathbb{I},\tau_z\otimes\sigma_x,\tau_z\otimes\sigma_y,\tau_z\otimes\sigma_z\}$

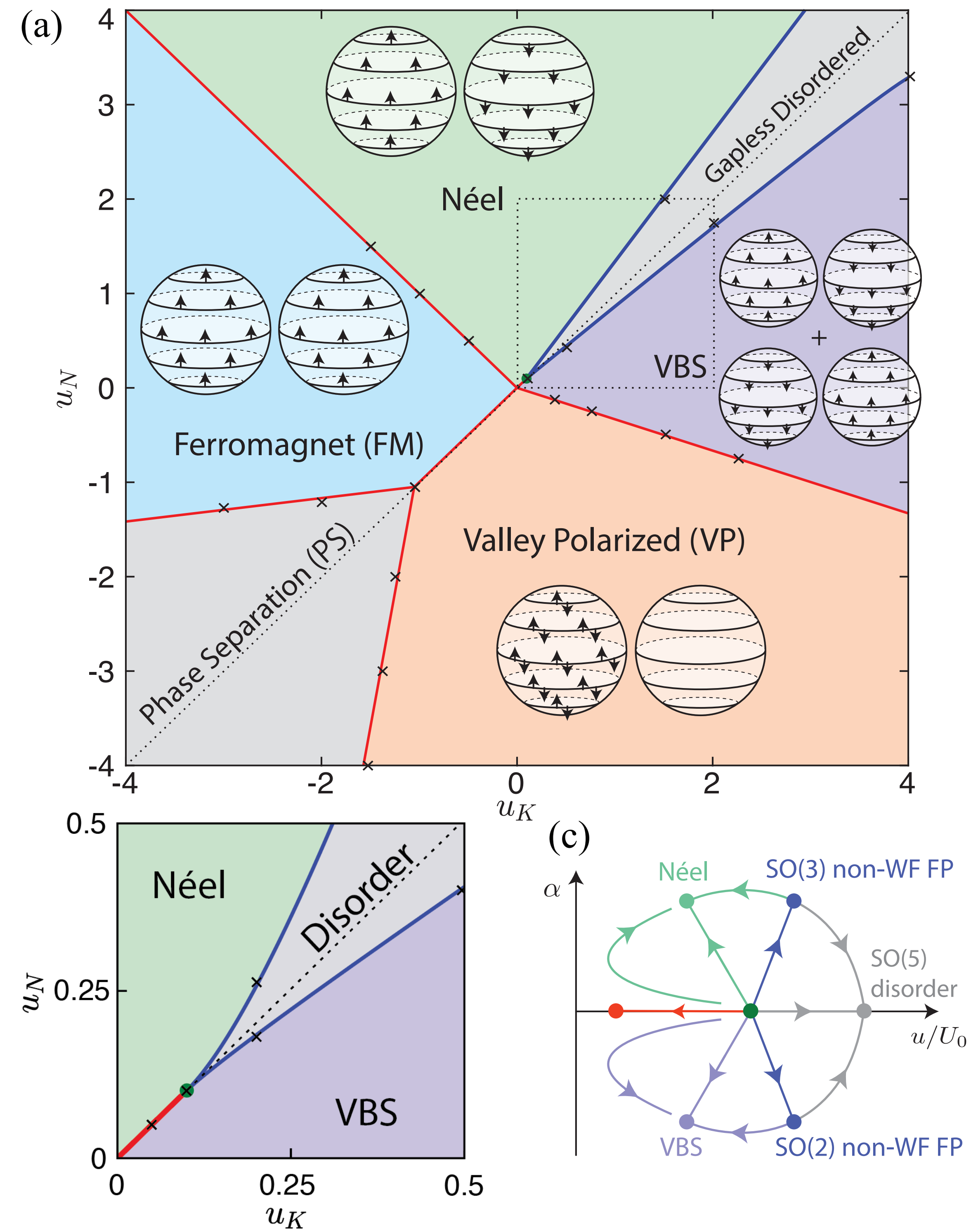
magnet monople inside a sphere $\quad 4\pi s$

Projected to the LLL with degeneracy $\quad N_\phi=2s+1$

$$\psi(\Omega)=\sum_{m=-s}^{s}\Phi_m(\Omega)c_m \qquad \Phi_m(\Omega)\propto e^{im\phi}\cos^{s+m}(\frac{\theta}{2})\sin^{s-m}(\frac{\theta}{2})$$

- M. Ippoliti, R. Mong, F. Assaad, M. Zaletel, PRB 98, 235108 (2018)
- Z. Wang, M. Zaletel, R. Mong, F. Assaad, PRL 126, 045701 (2021)
- Z. Zhou, L. Hu, W. Zhu, and Y.-C. He, PRX 14, 021044 (2024)

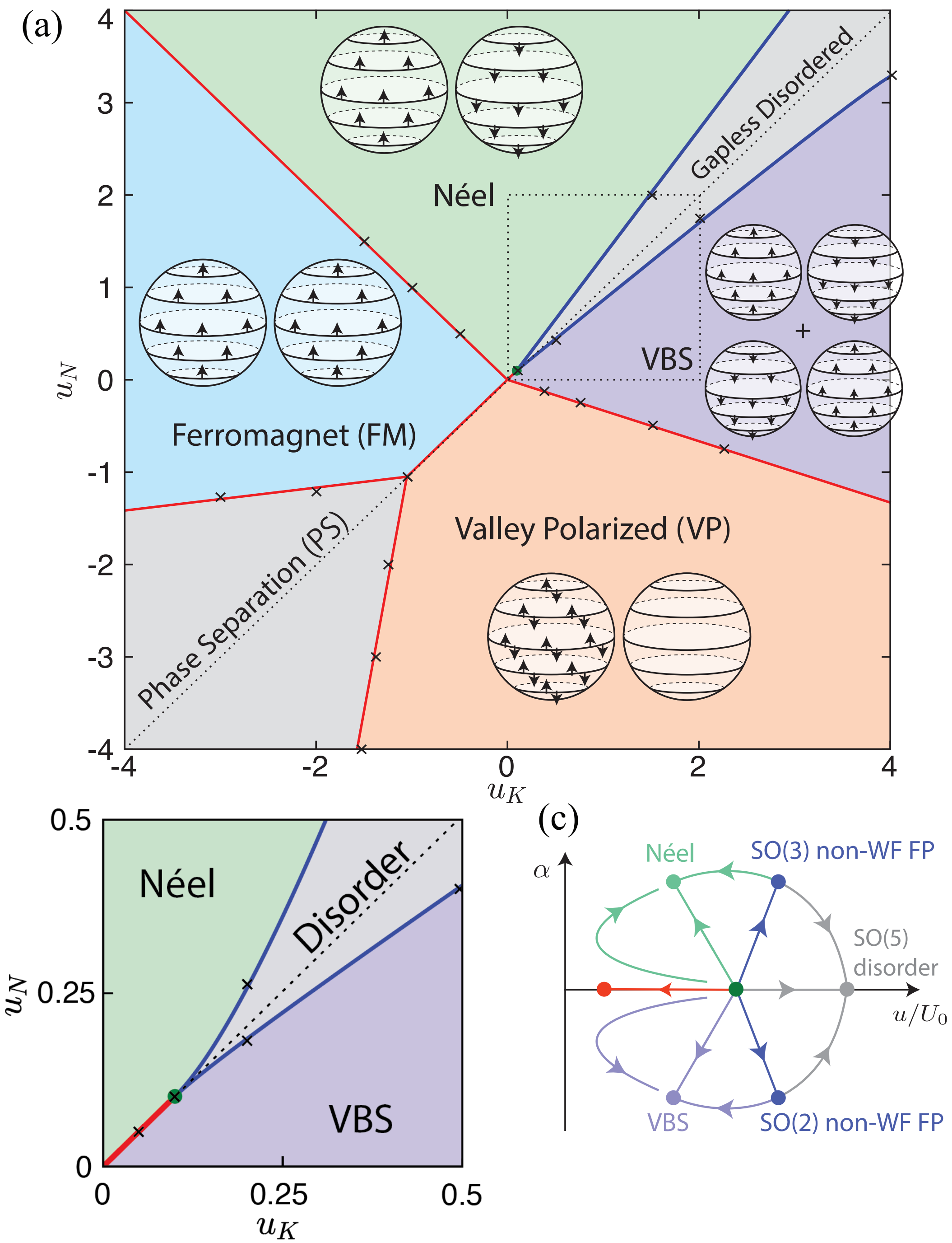
$N_\phi\sim 10$



Phases of (2+1)D SO(5) non-linear sigma model with a topological term on a sphere: multicritical point and disorder phase

Bin-Bin Chen,[1] Xu Zhang,[1] Yuxuan Wang,[2,*] Kai Sun,[3,†] and Zi Yang Meng[1,‡]

PRL 132, 246503 (2023) [ED+DMRG]

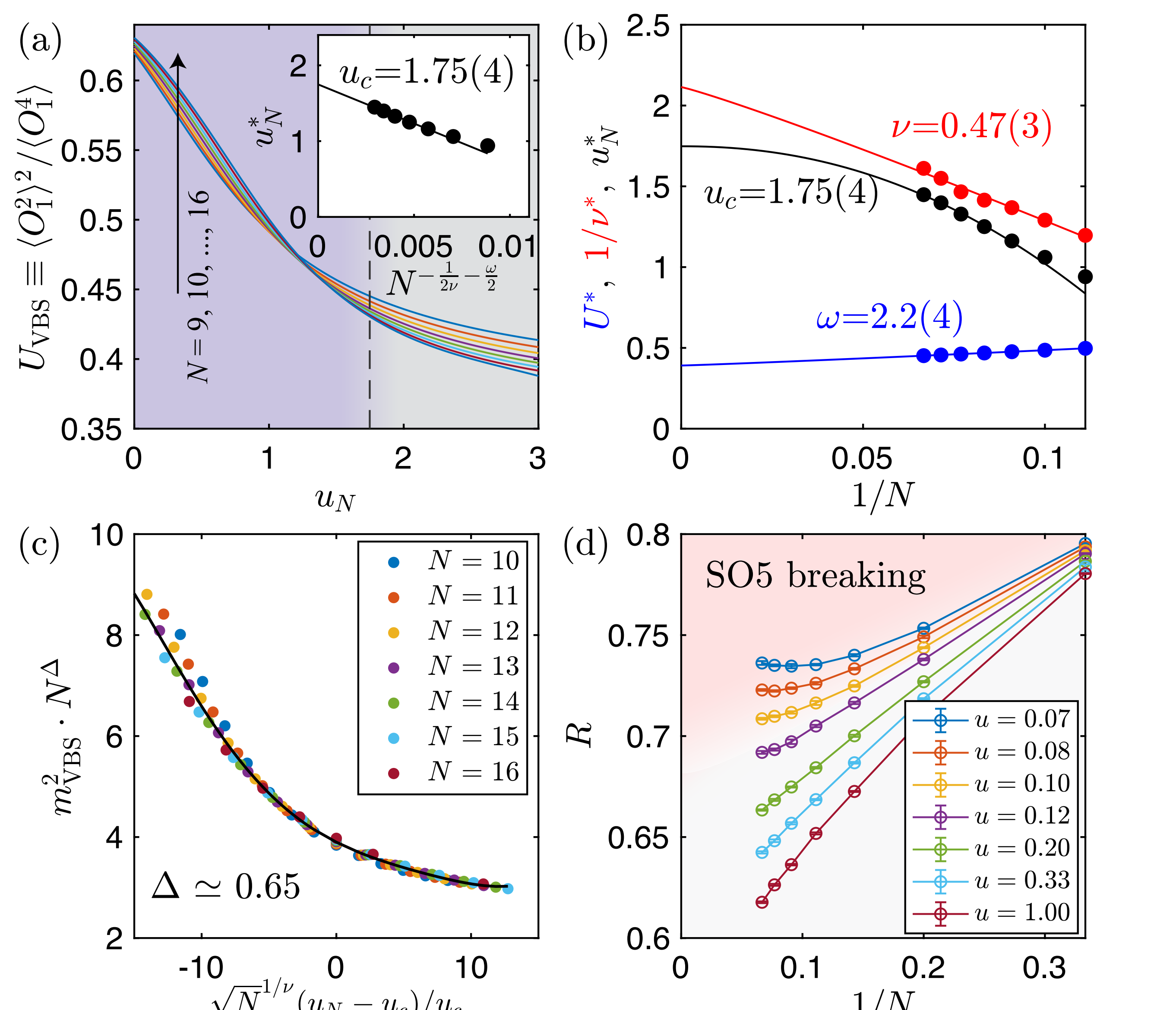


$$U_0 = 1,\ u_1 = u_2 = u_K, u_3 = u_4 = u_5 = u_N$$

$$\langle O_i \rangle = \int d\Omega \psi^\dagger(\Omega)\Gamma^i\psi(\Omega) = \sum_{m=-s}^{s} c_m^\dagger \Gamma^i c_m$$

$$m_{VBS}^2 = \frac{1}{2N^2}\langle (O_1^2 + O_2^2)\rangle \qquad m_{Neel}^2 = \frac{1}{3N^2}\langle (O_3^2 + O_4^2 + O_5^2)\rangle$$

$u_K = 2$



Phases of (2+1)D SO(5) non-linear sigma model with a topological term on a sphere: multicritical point and disorder phase

Bin-Bin Chen,[1] Xu Zhang,[1] Yuxuan Wang,[2,*] Kai Sun,[3,†] and Zi Yang Meng[1,‡]

PRL 132, 246503 (2023) [ED+DMRG]

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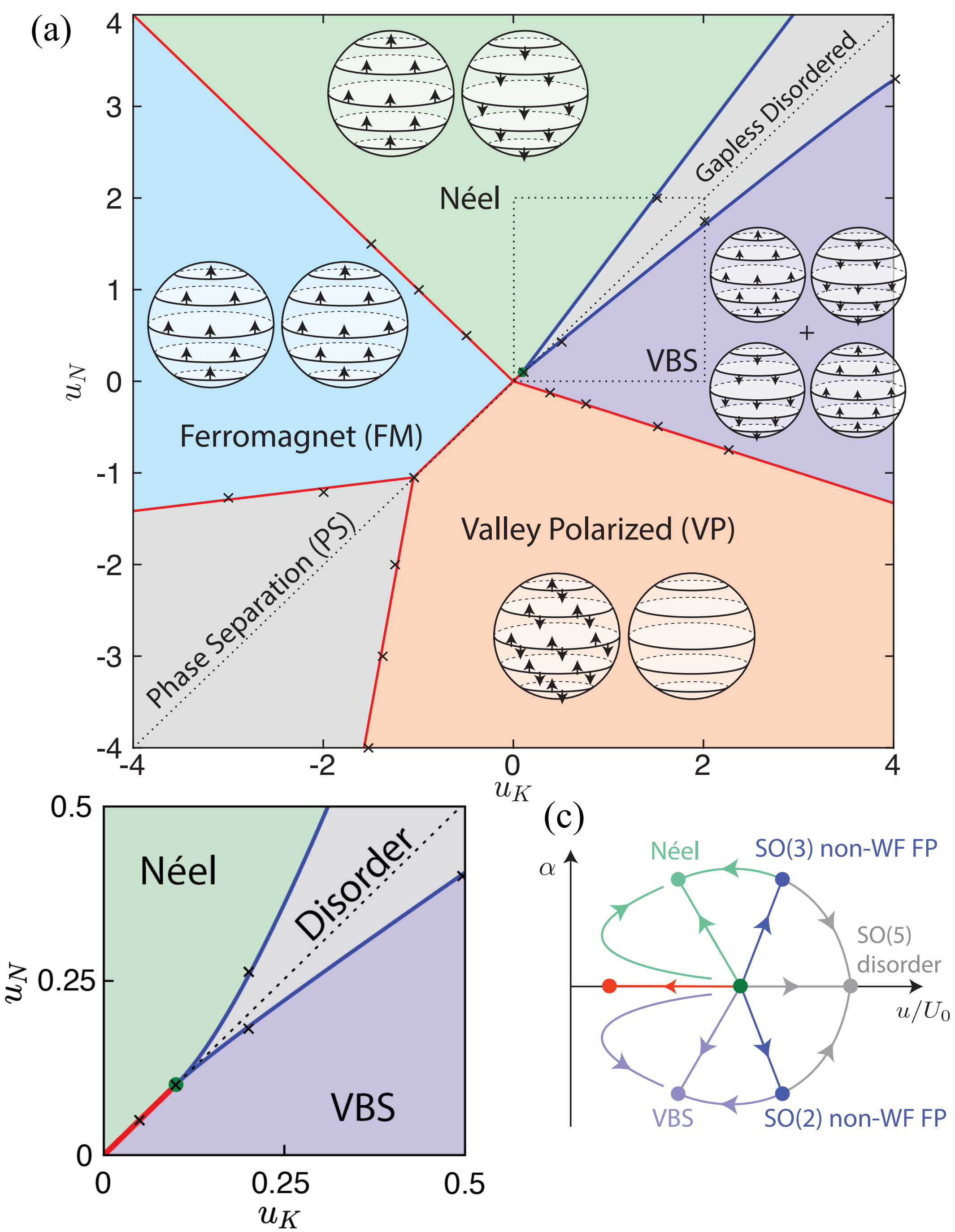
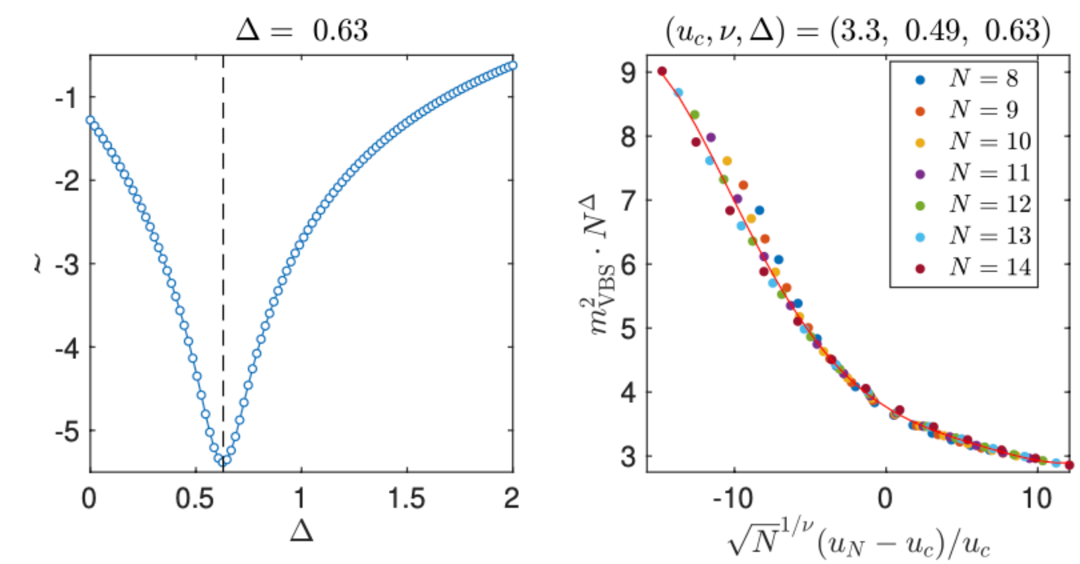
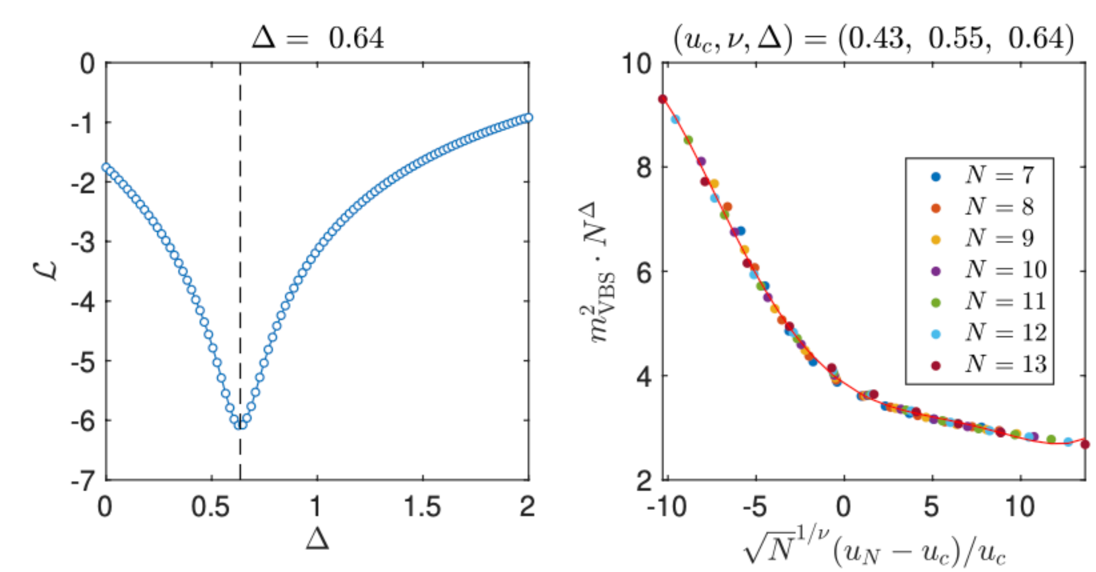
$$m^2_{VBS} = \frac{1}{2N^2}\langle (O_1^2 + O_2^2)\rangle \qquad m^2_{Neel} = \frac{1}{3N^2}\langle (O_3^2 + O_4^2 + O_5^2)\rangle$$



$u_K = 4$



$u_K = 0.5$



Numerical evidence of a critical point in the (2+1)D SO(5) nonlinear sigma model with Wess-Zumino-Witten term

Yuan Da Liao [1,2] Bin-Bin Chen,[3] Fakher F. Assaad [4,5] Lukas Janssen [6] and Zi Yang Meng [1,2]

arXiv: 2605.03700 (2026) [global update]

$$\mathcal{H} = U_0\mathcal{H}_0 - \sum_{i=1}^{5} U_i\mathcal{H}_i, \quad \mathcal{H}_i = \sum_{\mathbf{q}}^{N_\mathbf{q}} n_\mathbf{q}^{\Gamma^i} n_{-\mathbf{q}}^{\Gamma^i}$$

$$n_\mathbf{q}^{\Gamma^i} = \int d\boldsymbol{r}\, e^{i\mathbf{q}\cdot\boldsymbol{r}}\hat{\boldsymbol{\psi}}_{\boldsymbol{r}}^\dagger\Gamma^i\hat{\boldsymbol{\psi}}_{\boldsymbol{r}} \qquad \hat{\psi}_{\boldsymbol{r}} = \sum_{k=1}^{N_\phi}\phi_k(\boldsymbol{r})\mathbf{c}_k$$

$$k = 1,2,\cdots,N_\phi$$

Toric regularisation

$$\phi_k(\boldsymbol{r}) = \frac{1}{\sqrt{L_y l_B\sqrt{\pi}}} e^{-\left(r_x/l_B - l_B 2\pi k/L_y\right)^2/2} e^{i2\pi k r_y/L_y} \qquad l_B = \sqrt{\frac{\phi_0}{2\pi B}} = 1 \qquad N_\phi = BL_xL_y/\phi_0$$

$$n_\mathbf{q}^{\Gamma^i} = \frac{e^{-\frac{2\pi}{4N_\phi}\left(q_x^2+q_y^2\right)}}{4\pi\sqrt{N_\phi}} \sum_{k=1}^{N_\phi}\sum_{a,b=1}^{4} e^{\frac{i}{2}(2k-q_y)q_x(2\pi/N_\phi)}\left(c_{k,a}^\dagger\Gamma_{a,b}^i c_{k-q_y,b} - 2\delta_{q_y,0}\delta_{i,0}\right)$$

momentum

$$\mathbf{q} = \left(q_x\sqrt{\frac{2\pi}{N_\phi}}, q_y\sqrt{\frac{2\pi}{N_\phi}}\right)$$

$$N_\mathbf{q} \propto N_\phi$$

Spherical regularisation

$$\phi_k(\boldsymbol{r}) = N_{m_k} e^{im_k\phi}\cos^{s+m_k}\left(\frac{\theta}{2}\right)\sin^{s-m_k}\left(\frac{\theta}{2}\right) \qquad N_\phi = 2s+1$$

$$m_k = k-1-s$$

$$n_{l,m}^{\Gamma^i} = \sum_{k=1}^{N_\phi}\sum_{a,b=1}^{4}(-1)^{s+k+m}\frac{(2s+1)\sqrt{2l+1}}{2}\begin{pmatrix} s & l & s \\ -k & -m & k+m\end{pmatrix}\begin{pmatrix} s & l & s \\ -s & 0 & s\end{pmatrix}\left(c_{k,a}^\dagger\Gamma_{a,b}^i c_{k+m,b} - 2\delta_{m,0}\delta_{i,0}\right)$$

angular momentum $\quad (l,m) \quad l \in (0,1,2,\cdots,2s) \quad m \in (-l,-l+1,\cdots,l-1,l) \qquad N_\mathbf{q} \propto (N_\phi+1)^2$

Numerical evidence of a critical point in the (2+1)D SO(5) nonlinear sigma model with Wess-Zumino-Witten term

Yuan Da Liao [1,2] Bin-Bin Chen,[3] Fakher F. Assaad [4,5] Lukas Janssen [6] and Zi Yang Meng [1,2]

$\Gamma^i = \{\tau_x \otimes \mathbb{I}_2, \tau_y \otimes \mathbb{I}_2, \tau_z \otimes \sigma_x, \tau_z \otimes \sigma_y, \tau_z \otimes \sigma_z\}$ ⟶ $O^i = \{\mathbb{I}_2 \otimes \mathbb{I}_2, \tau_x \otimes \mathbb{I}_2, \tau_y \otimes \mathbb{I}_2, \tau_z \otimes \mathbb{I}_2\}$ arXiv: 2605.03700 (2026) [global update]

Fierz identity

$$H_i = \sum_{\mathbf{q}} \frac{1}{2}\left[(n^{O^i}_{\mathbf{q}} + n^{O^i}_{-\mathbf{q}})^2 - (n^{O^i}_{\mathbf{q}} - n^{O^i}_{-\mathbf{q}})^2\right] = \sum_{q=1}^{2N_q} \frac{(Q^i_q)^2}{2}$$

$$e^{-\frac{\Delta\tau g_i}{2}(Q^i_q)^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\phi^i_q e^{-\phi^{i2}_q/2} e^{\alpha\phi^i_q Q^i_q},$$

$$Z = \int \mathcal{D}\phi\, e^{-S_0[\phi]} \det\left[1 + B(\beta, 0; \phi)\right],$$

$$G(\tau,\tau;\phi) = (1 + B(\tau,0;\phi)B(\beta,\tau;\phi))^{-1},$$

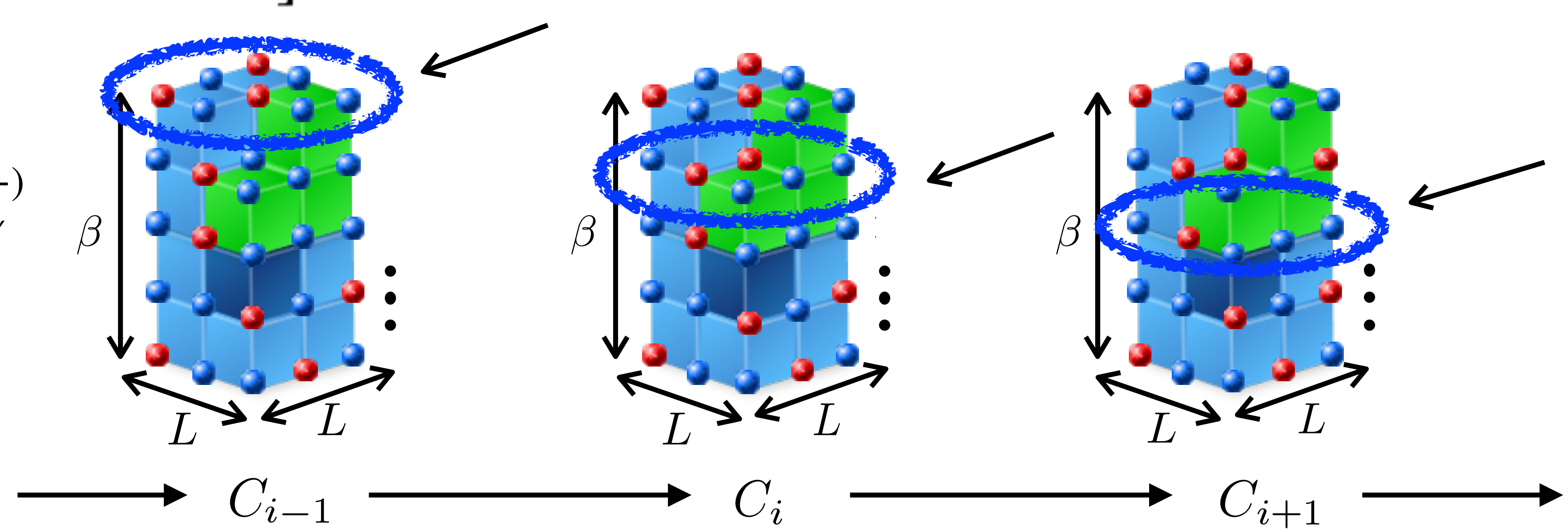
$$\phi^{i\,\prime}_{\tau,q} = \phi^i_{\tau,q} + \frac{\epsilon^2}{2}\nabla_{\phi^i_{\tau,q}} S[\phi] + \epsilon\mathcal{N}(0,1),$$

$$S[\phi] = S_0[\phi] - \ln\det\left[1 + B(\beta,0;\phi)\right]$$

$$\nabla_{\phi^i_{\tau,q}} S[\phi] = \phi^i_{\tau,q} - \mathrm{Tr}\left[G(\tau,\tau;\phi)\frac{\partial B(\tau,0;\phi)}{\partial\phi^i_{\tau,q}}\right]$$

$$S_0[\phi] = \tfrac{1}{2}\textstyle\sum_{\tau,i,q}(\phi^i_{\tau,q})^2$$

$$\begin{cases} \dfrac{dp_{\tau,\mathbf{Q},\gamma}}{dt} = -\dfrac{\partial\mathcal{H}}{\partial\phi_{\tau,\mathbf{Q},\gamma}} = -\phi_{\tau,\mathbf{Q},\gamma} + \mathrm{Tr}\left(M^{-1}\dfrac{\partial M}{\partial\phi_{\tau,\mathbf{Q},\gamma}}\right) \\ \dfrac{d\phi_{\tau,\mathbf{Q},\gamma}}{dt} = \dfrac{\partial\mathcal{H}}{\partial p_{\tau,\mathbf{Q},\gamma}} = p_{\tau,\mathbf{Q},\gamma} \end{cases}$$

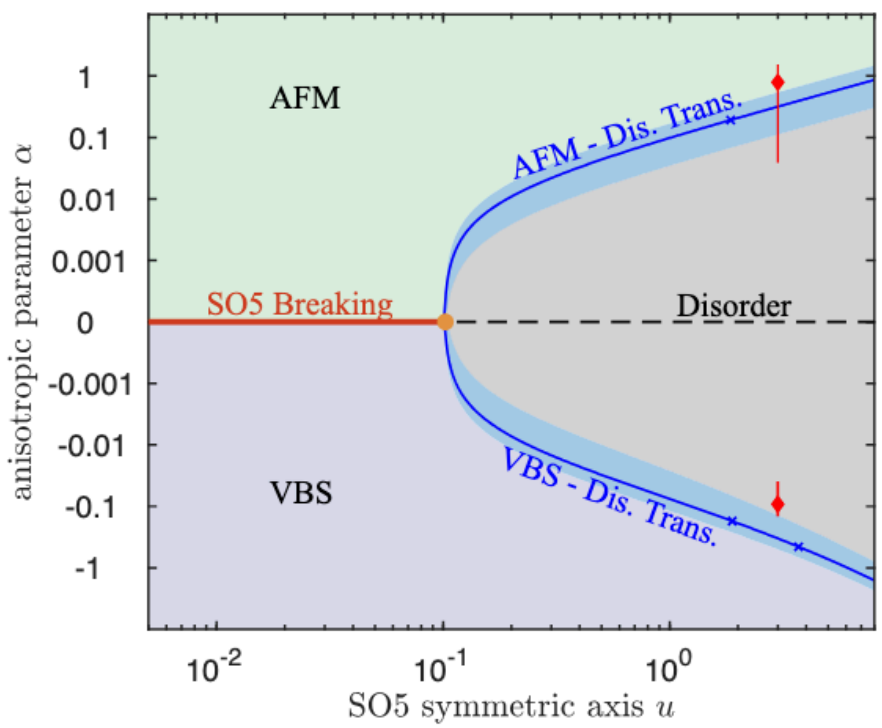


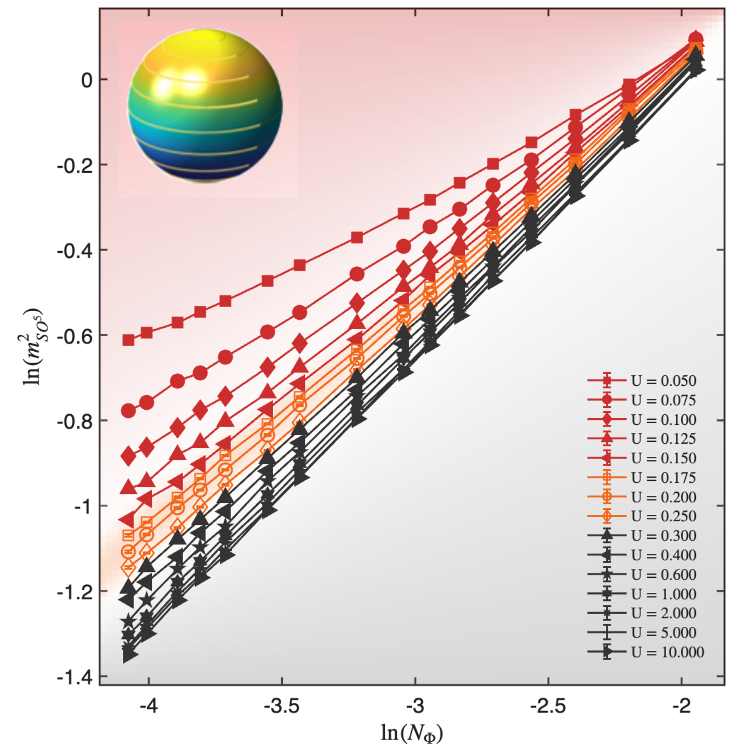
Update the entire time slice $O(N^2)$ and update the Green's function $O(N^3)$

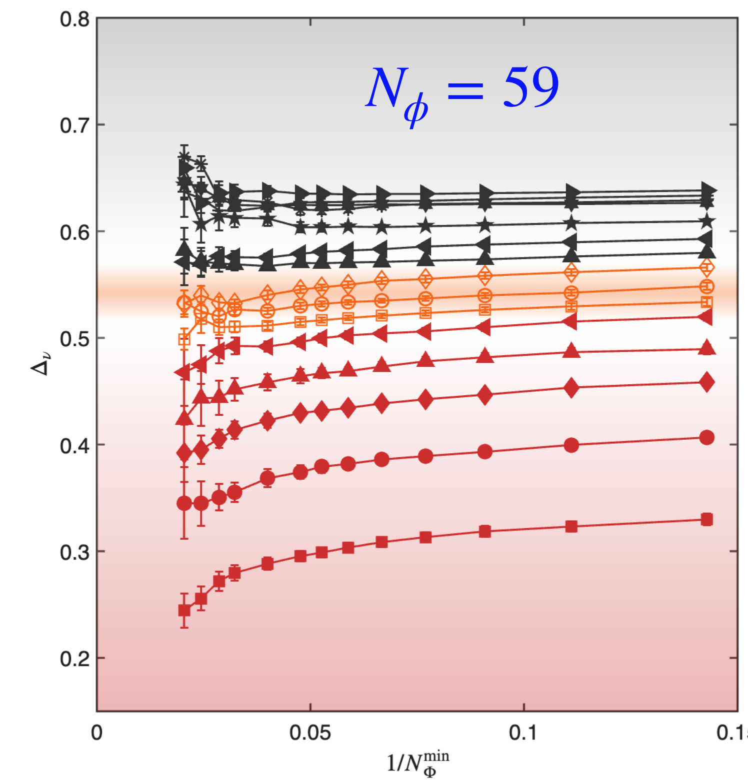
Numerical evidence of a critical point in the (2+1)D SO(5) nonlinear sigma model with Wess-Zumino-Witten term

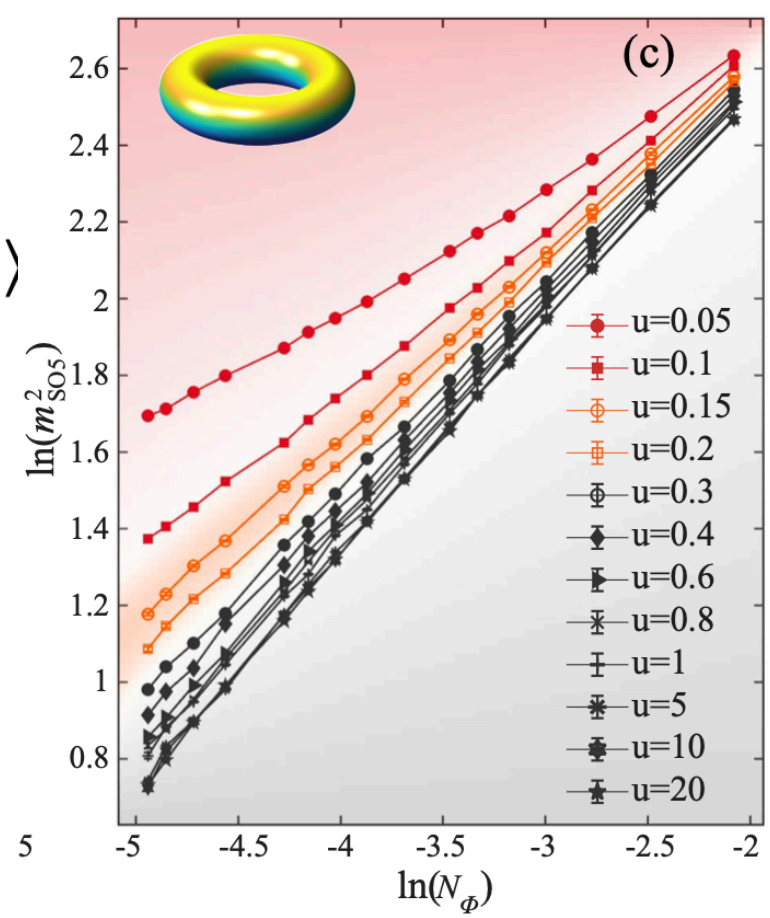
Yuan Da Liao [1,2] Bin-Bin Chen,[3] Fakher F. Assaad [4,5] Lukas Janssen [6] and Zi Yang Meng [1,2]

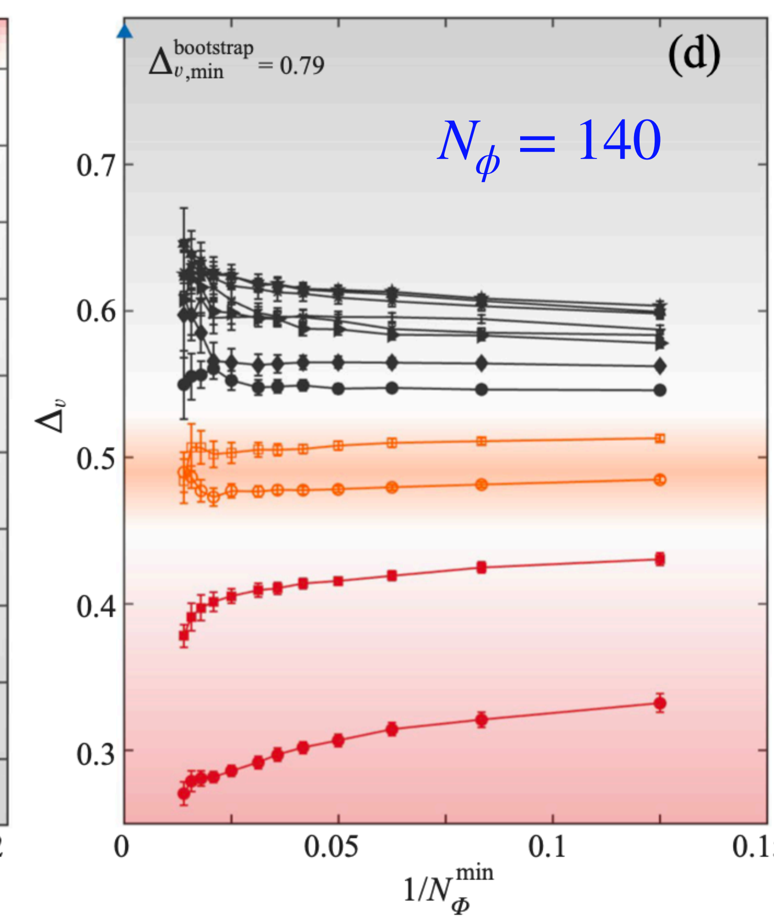
arXiv: 2605.03700 (2026) [global update]











$$m^2_{\mathrm{SO(5)}} = \frac{1}{5N_\phi^2}\sum_{i=1}^{5} S^i_{\mathbf{q}=0}, \quad S^i_{\mathbf{q}} = \langle n^{\Gamma^i}_{\mathbf{q}} n^{\Gamma^i}_{-\mathbf{q}} \rangle$$

$$m^2_{SO(5)} \sim \frac{1}{N_\phi^{\Delta_v}}$$

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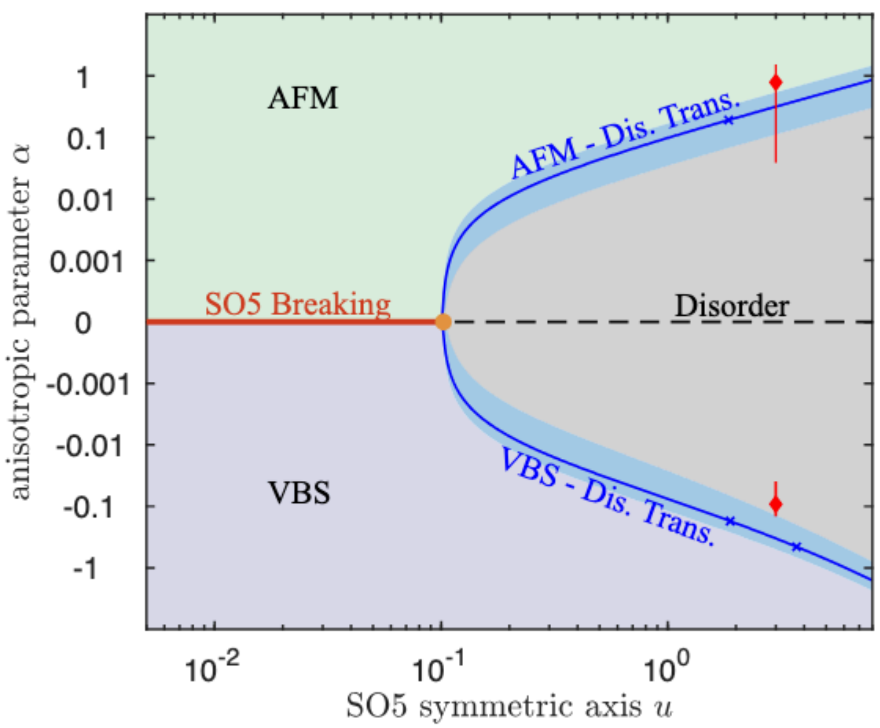
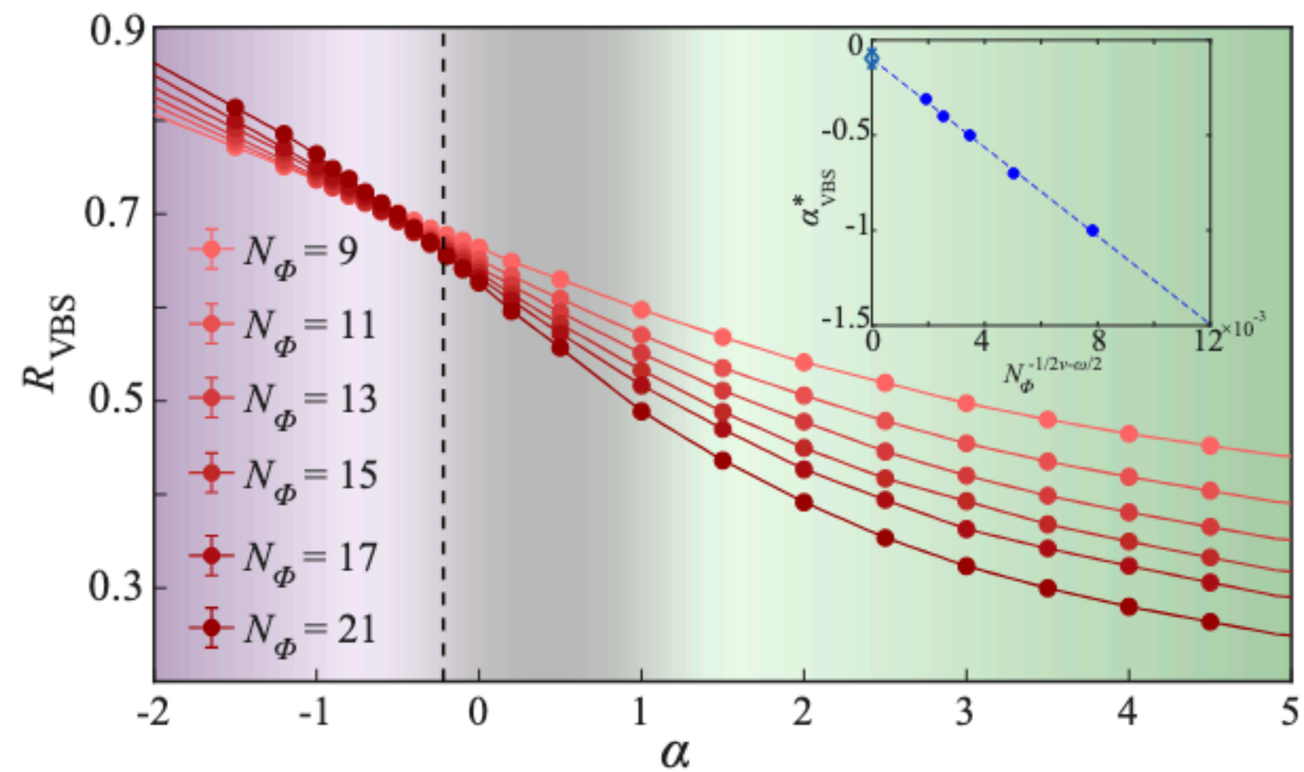
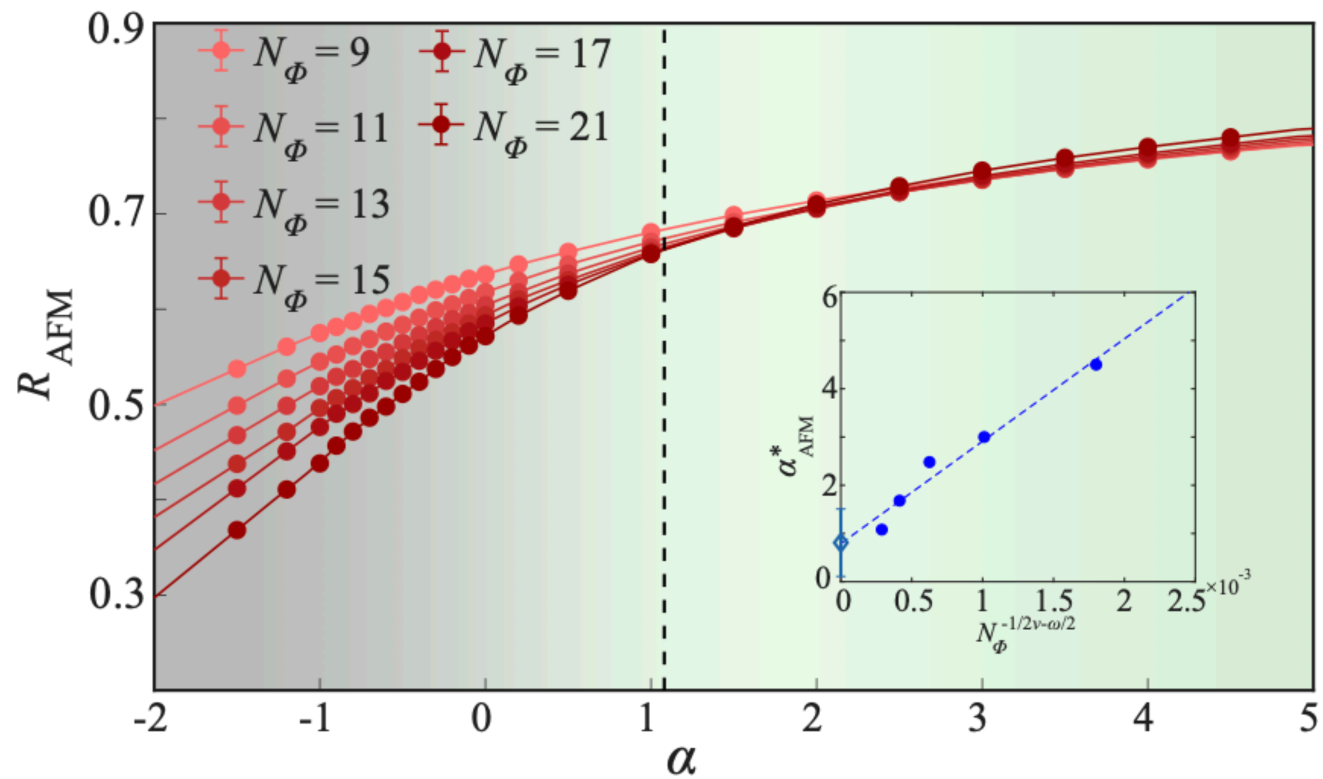




$$m^2_{\rm SO(5)} = \frac{1}{5N_\phi^2}\sum_{i=1}^{5} S^i_{\mathbf{q}=0}, \quad S^i_{\mathbf{q}} = \langle n^{\Gamma^i}_{\mathbf{q}} n^{\Gamma^i}_{-\mathbf{q}} \rangle$$

$$m^2_{SO(5)} \sim \frac{1}{N_\phi^{\Delta_v}}$$

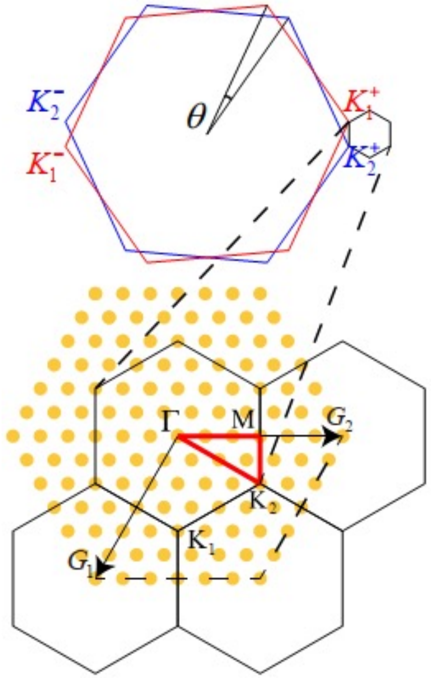
$$R = 1 - \frac{S(\mathbf{Q}+\Delta\mathbf{q})}{S(\mathbf{Q})}$$



Content

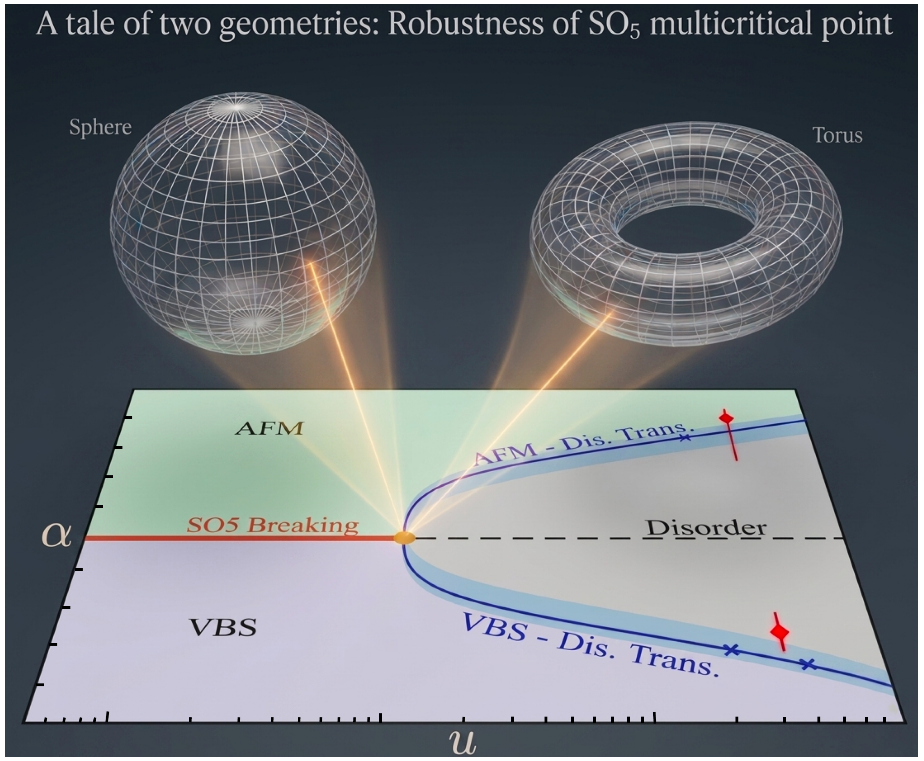
1. Momentum-space QMC for twisted bilayer graphene

- CPL 38, 077305 (2021) [momentum-space QMC, 6 x 6]
- PRL 130, 016401 (2023) [Thermodynamic responses]
- PRB 107, L241105 (2023) [Polynomial sign problem]
- Nat. Comm. 16, 7176 (2025) [global update, 18 x 18]
- ......



2. (2+1)D SO(5) nonlinear sigma model with Wess-Zumino-Witten term

- PRL 132, 246503 (2023) [ED+DMRG, $N_\phi = 16$]
- arXiv: 2605.03700 (2026) [global update, $N_\phi = 160$]
- ......



3. Hybrid Monte Carlo for FQHs

- Rep. Prog. Phys. 10.1088/ae70a7 (2026) [global update, N = 1200]
- ......

Hybrid Monte Carlo for Fractional Quantum Hall States

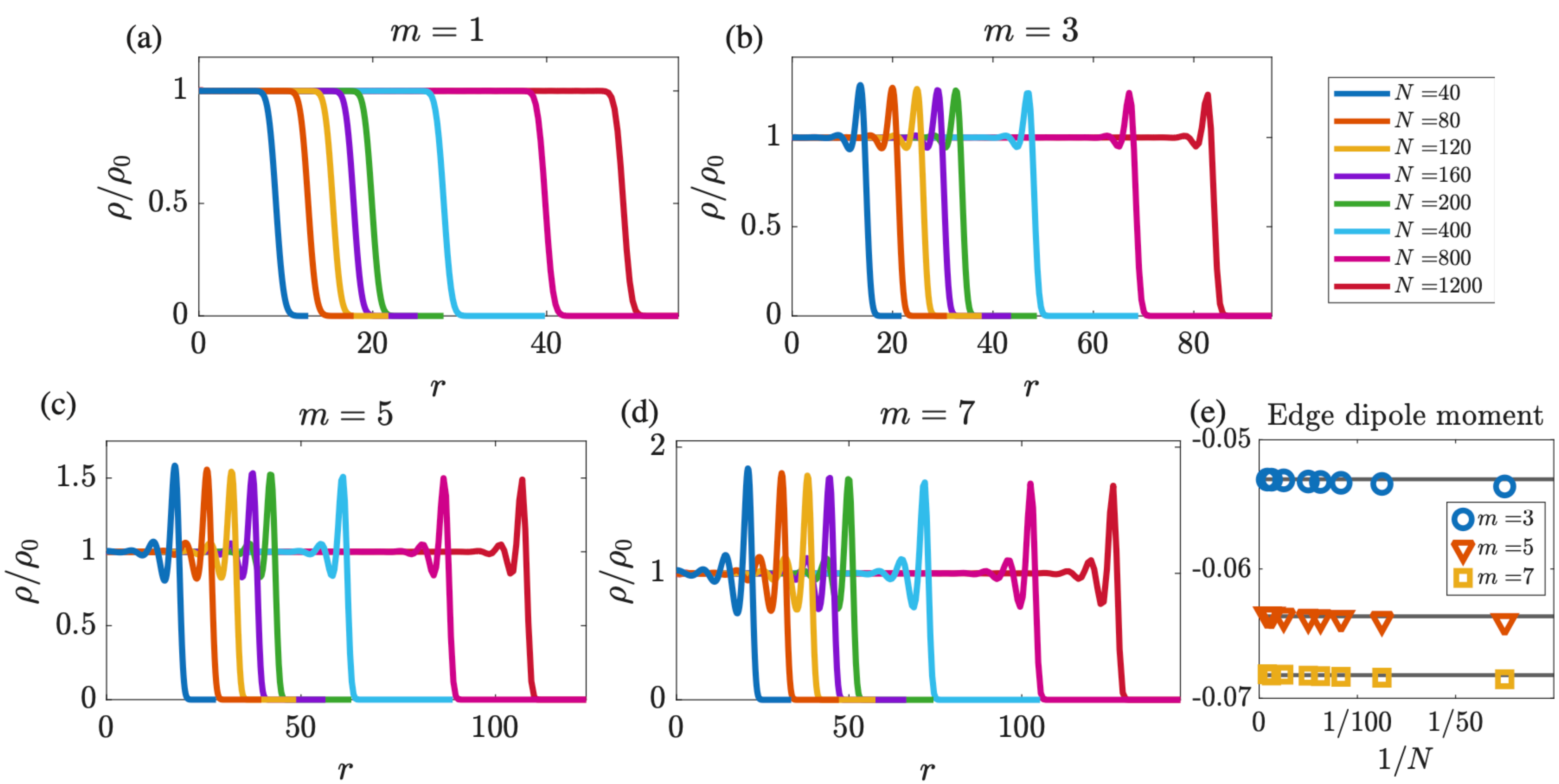
Ting-Tung Wang,[1,2] Ha Quang Trung,[3] Qianhui Xu,[3] Min Long,[1,2] Bo Yang,[3,*] and Zi Yang Meng[1,2,†]

Rep. Prog. Phys. 10.1088/ae70a7 (2026)

$$\Psi_m(\{z_j\}) = \prod_{i<j}^{N}(z_i - z_j)^m \exp\left(-\sum_k |z_k|^2/4\right), \qquad \langle \hat{O} \rangle = \frac{\int \prod_j d^2 z_j \, |\Psi_m(\{z_j\})|^2 \, O(\{z_j\})}{\int \prod_j d^2 z_j \, |\Psi_m(\{z_j\})|^2},$$

$$|\Psi_m(\{z_j\})|^2 = e^{-V(\{z_j\})}, \qquad V(\{z_j\}) := -2m \sum_{i<j}^{N} \log|z_i - z_j| + \frac{1}{2}\sum_k |z_k|^2$$

$$Z = \int \prod_j d^2 z_j \, e^{-V(\{z_j\})} = \int \prod_j d^2 z_j \int \prod_j d^2 p_j e^{-V(\{z_j\}) - \frac{1}{2}\sum_j |p_j|^2} \qquad \begin{cases} \frac{\mathrm{d}z_j}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial p_j} = p_j \\ \frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial V}{\partial z_j} = 2m \sum_{i \neq j} \frac{z_i - z_j}{|z_i - z_j|^2} - z_i \end{cases}$$



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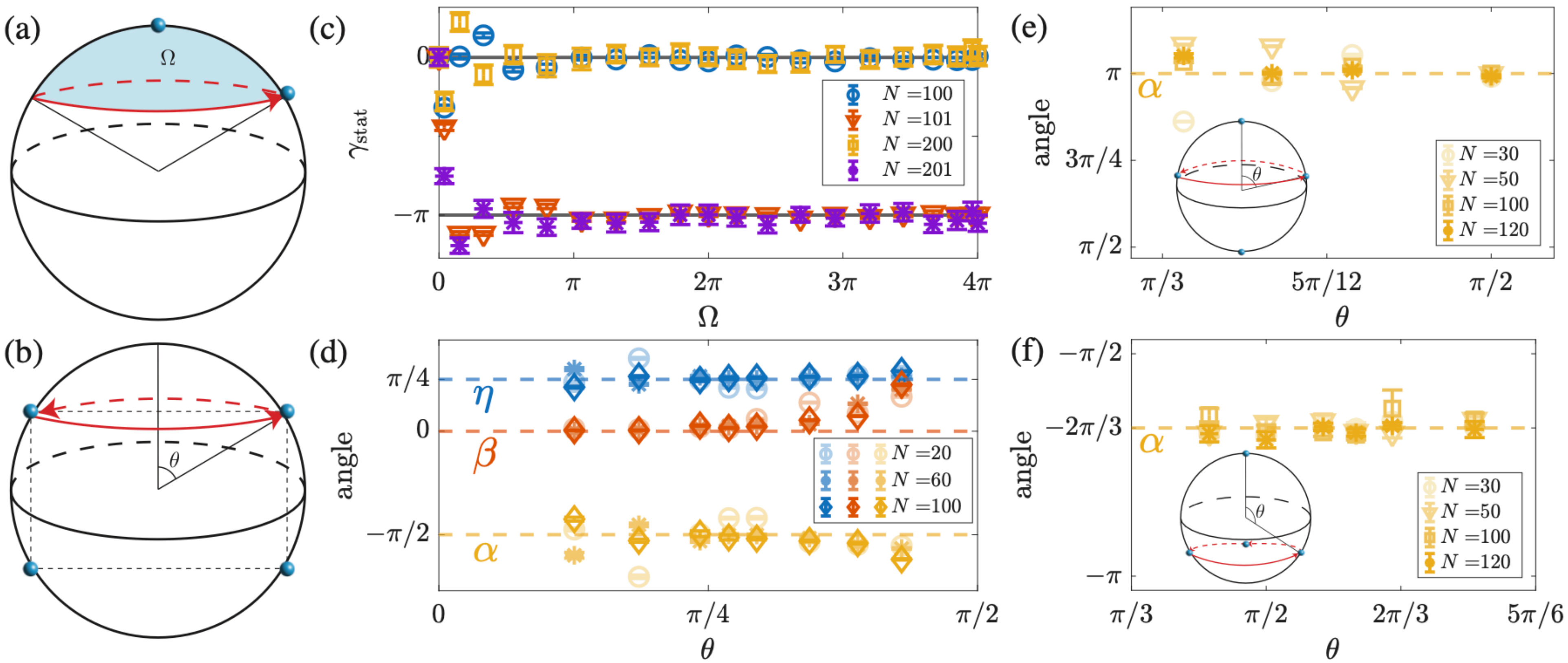
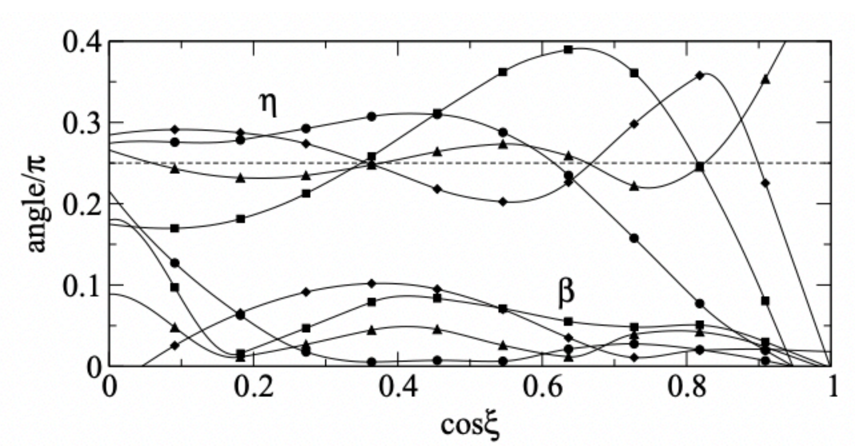
Rep. Prog. Phys. 10.1088/ae70a7 (2026)

$$\Psi_{\mathrm{MR}}(\{z_j\}) = \mathrm{Pf}\left(\frac{1}{z_i - z_j}\right)\prod_{i<j}^{N}(z_i - z_j)^2 \exp\left(-\sum_k |z_k|^2/4\right),$$

$$\Psi_{\mathrm{MR}}(\{z_i\};\{\eta_j\}) = \mathrm{Pf}\left[\frac{(z_i-\eta_1)(z_i-\eta_2)(z_j-\eta_3)(z_j-\eta_4) + (i \leftrightarrow j)}{z_i - z_j}\right]\prod_{i<j}(z_i - z_j)^2 \exp\left(\sum_i |z_i|^2/4\right)$$





$$U = e^{i\chi}\begin{pmatrix} e^{i\eta}\cos\beta/2 & ie^{-i\epsilon/2}\sin\beta/2 \\ ie^{i\epsilon/2}\sin\beta/2 & e^{-i\eta}\cos\beta/2 \end{pmatrix}$$

Monte Carlo Evaluation of Non-Abelian Statistics,
Yaroslav Tserkovnyak, Steven H. Simon, PRL 90, 016802 (2003)