Computation in projected Hamiltonian & quantum Fisher information

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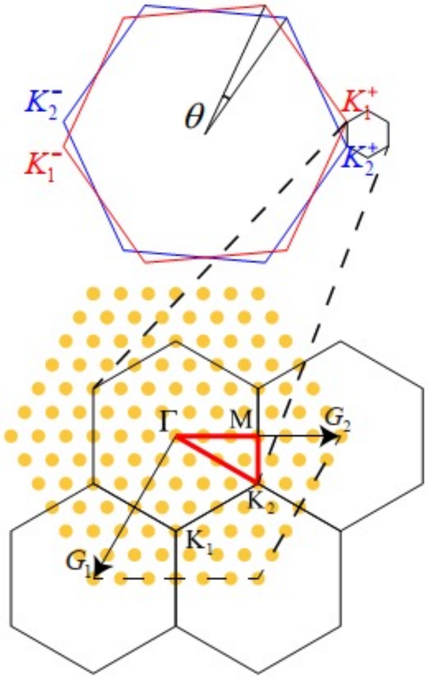

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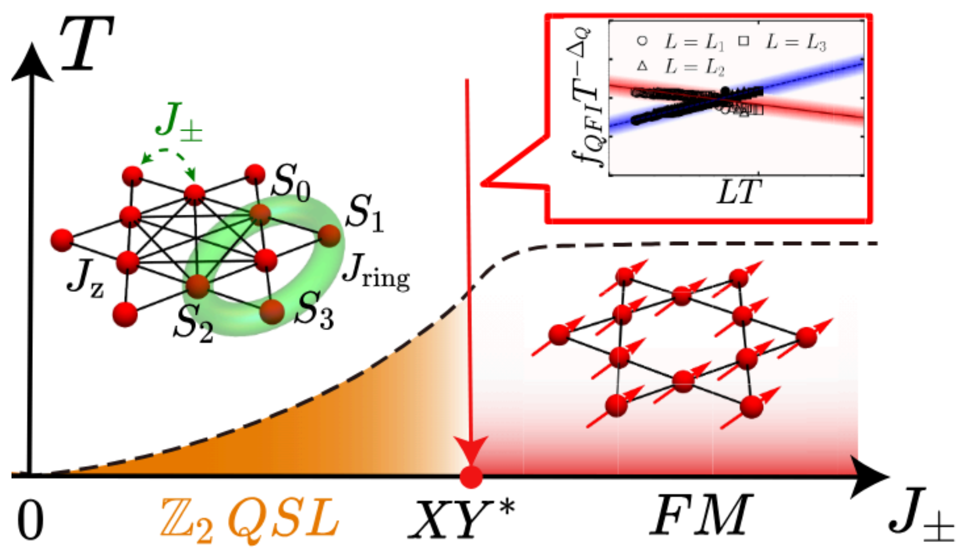
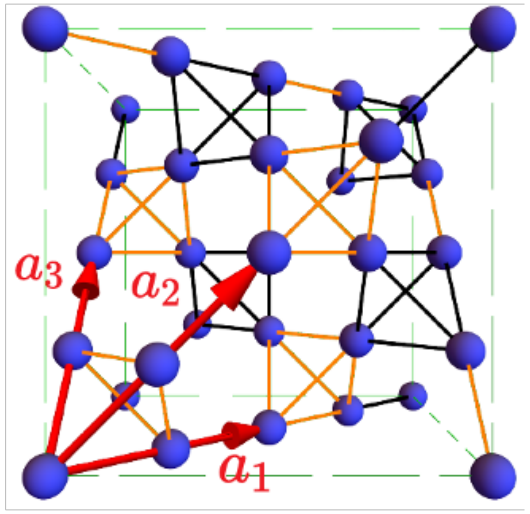
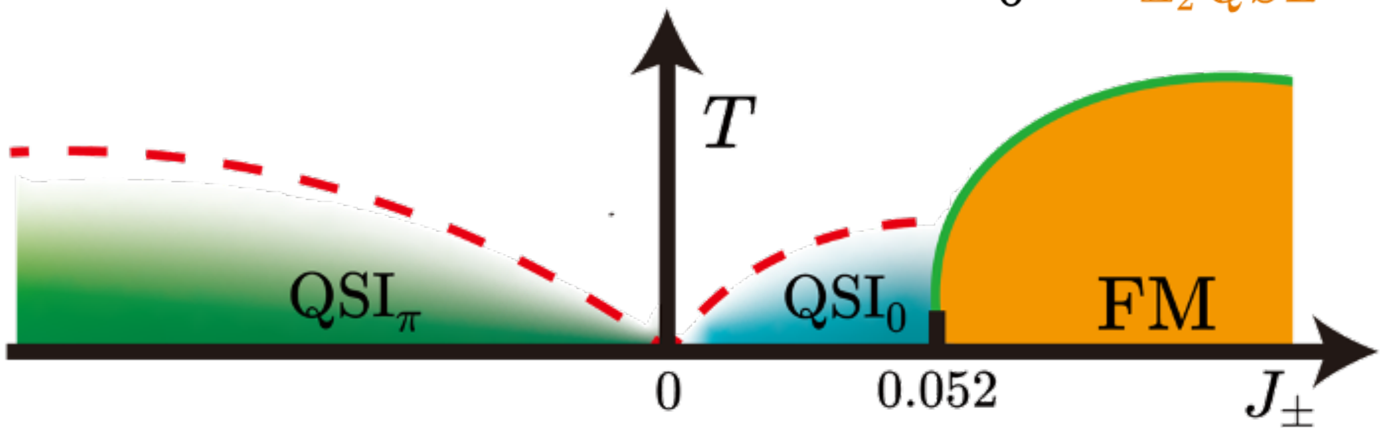


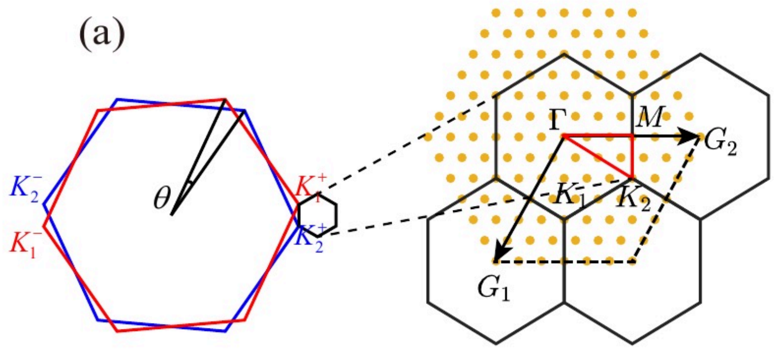




Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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)



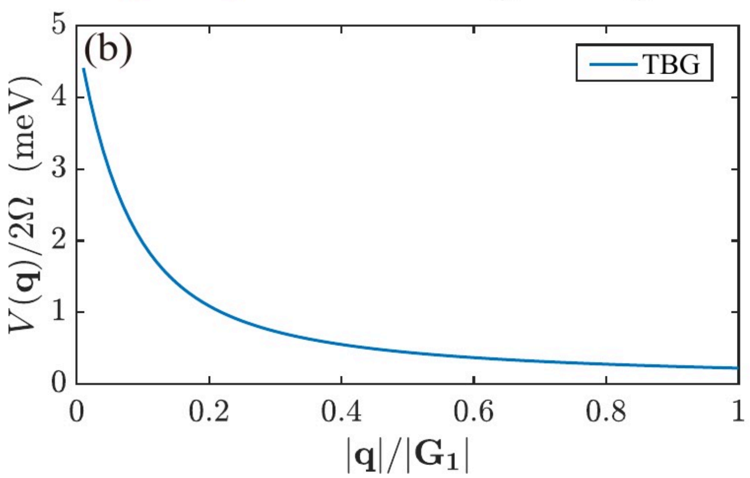
$$H = \underbrace{\sum_{s,\eta,\mathbf{k},m} \epsilon^{s,\eta}_{\mathbf{k},m} c^{\dagger}_{s,\eta,\mathbf{k},m} c_{s,\eta,\mathbf{k},m}}_{H_0} + \underbrace{\frac{1}{2\Omega} \sum_{\mathbf{q}\in mBZ,\mathbf{G}} V(\mathbf{q}+\mathbf{G}) \delta\rho_{\mathbf{q}+\mathbf{G}} \delta\rho_{-\mathbf{q}-\mathbf{G}}}_{H_{int}}$$

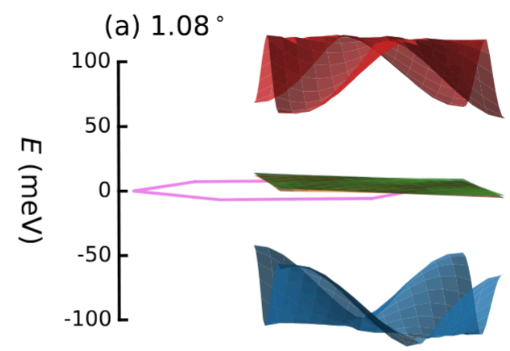
$$|\mathbf{G_1}|, |\mathbf{G_2}| = \frac{8\pi}{3a}\sin(\frac{\theta}{2})$$

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

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

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

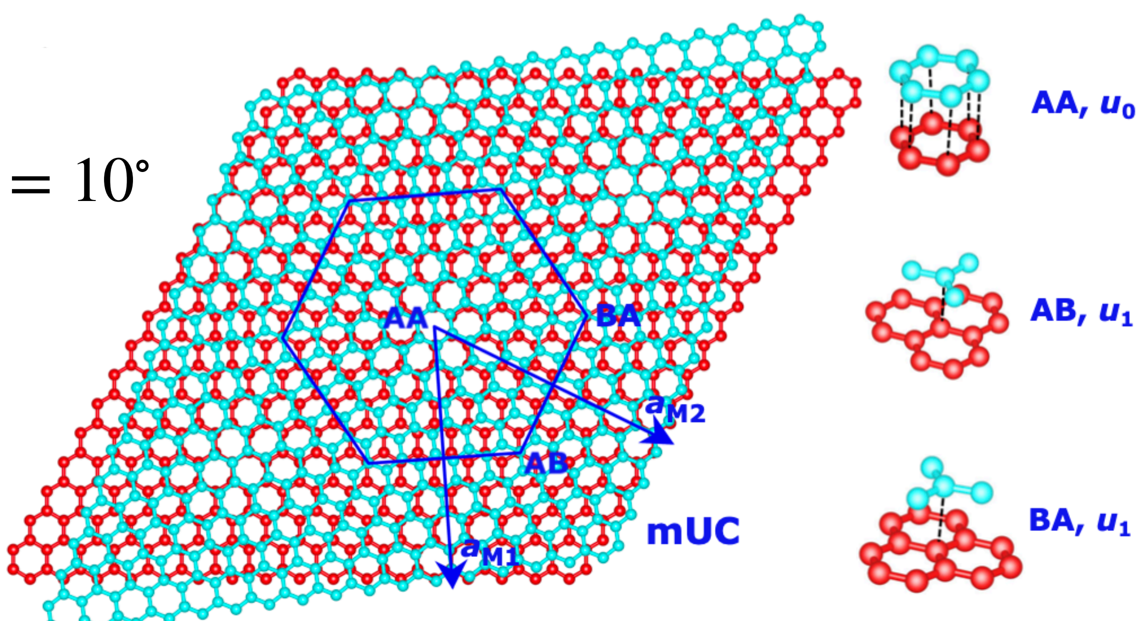


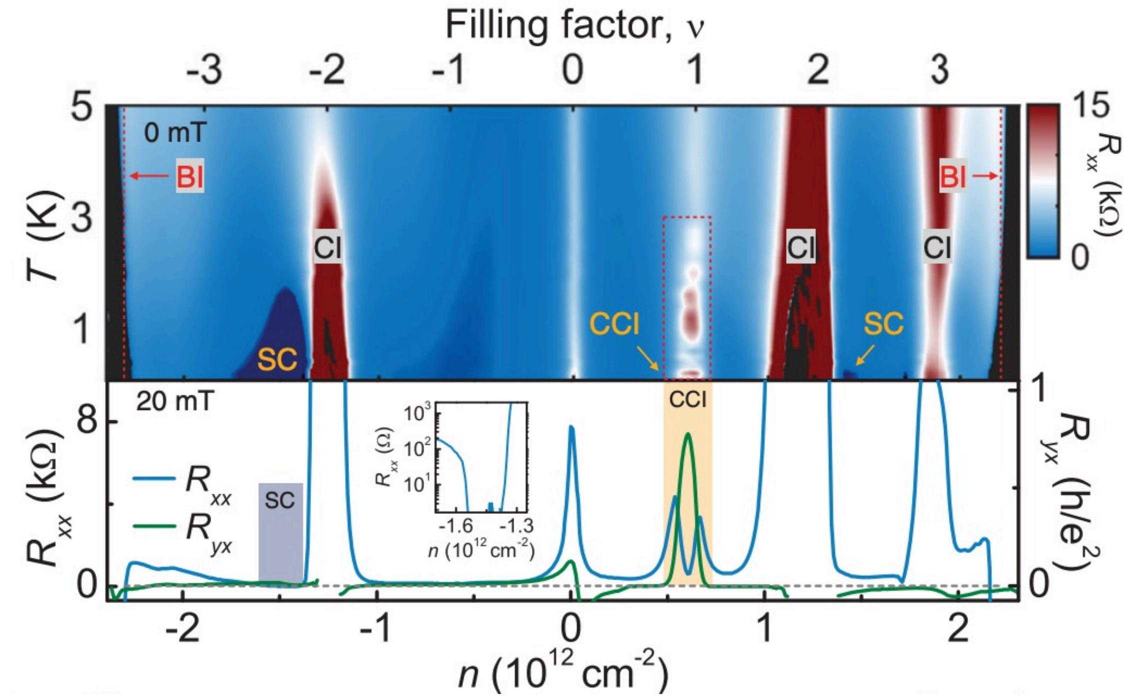


Form factors from Bloch WF

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

$\theta = 10^\circ$





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],
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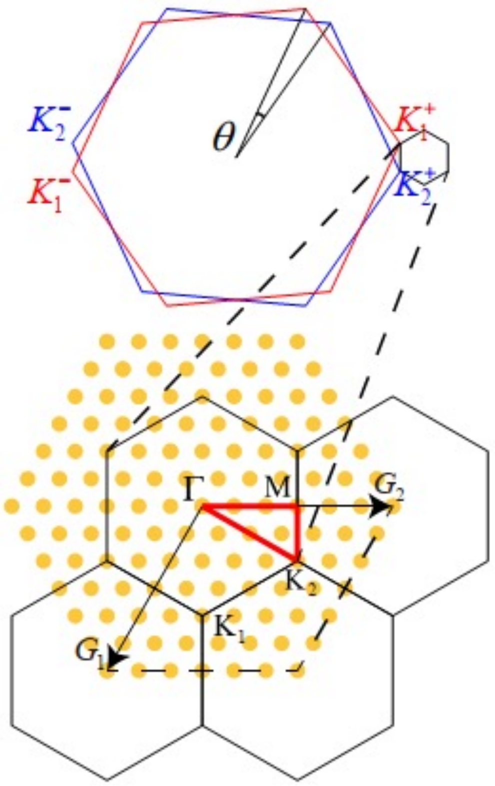


$$H = H_0 + H_{int}$$

CPL 38, 077305 (2021)

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

Bistritzer & MacDonald, PNAS (2011)

$\eta = \pm$ valley

Pauli for sublattices

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

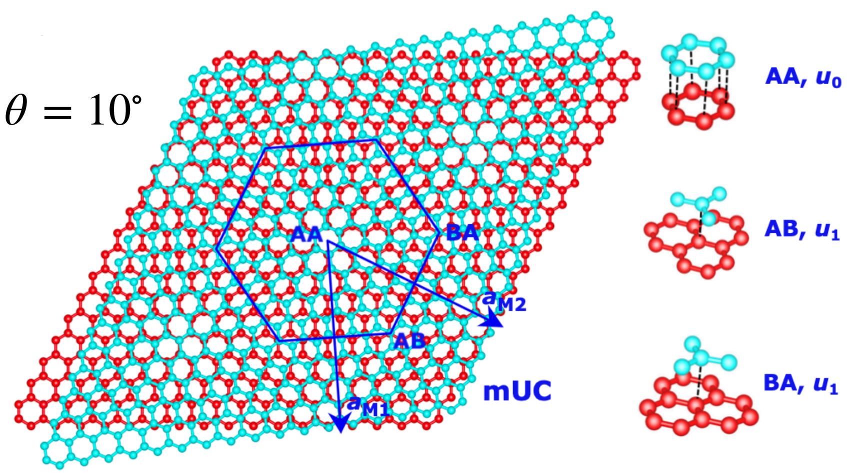
$$H_O^{s,\eta}(\mathbf{k})_{\mathbf{G},\mathbf{G}'} = \delta_{\mathbf{G},\mathbf{G}'}\hbar v_F \begin{pmatrix} -(\mathbf{k}+\mathbf{G}-\mathbf{K}_1^\eta)\cdot\Lambda^\eta & 0 \\ 0 & -(\mathbf{k}+\mathbf{G}-\mathbf{K}_2^\eta)\cdot\Lambda^\eta \end{pmatrix} + \begin{pmatrix} 0 & T_1^\eta \\ T_2^{\eta\dagger}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

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

$$|\mathbf{G}|, |\mathbf{G}'| < 6|\mathbf{G}_1|$$

$\hbar v_F/a = 2377.45$ meV

$\theta = 10^\circ$



interlayer, intrasublattice hopping

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

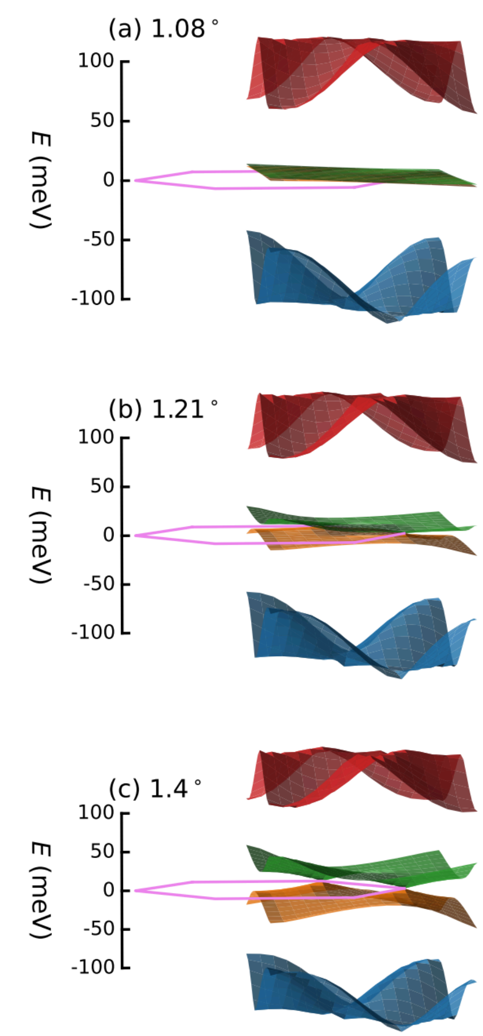
interlayer, intersublattice hopping

$\theta = 1.08^\circ$ 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

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

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

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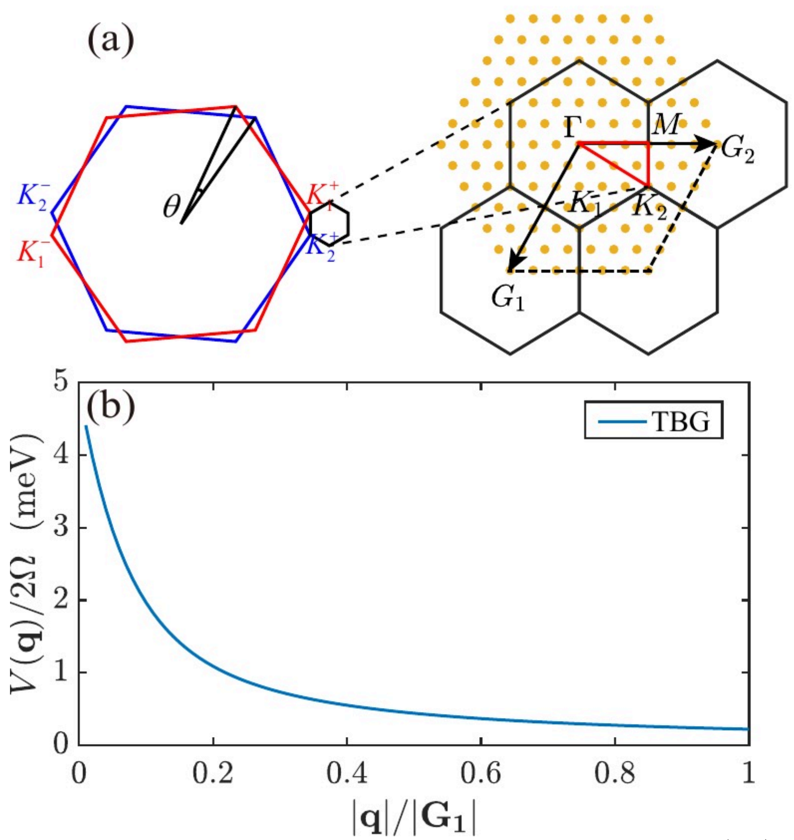
CPL 38, 077305 (2021)



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

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

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

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

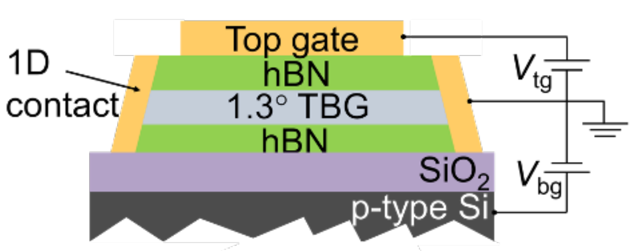
overlap of H_0 eigenstate

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

Single gate

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

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



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

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

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

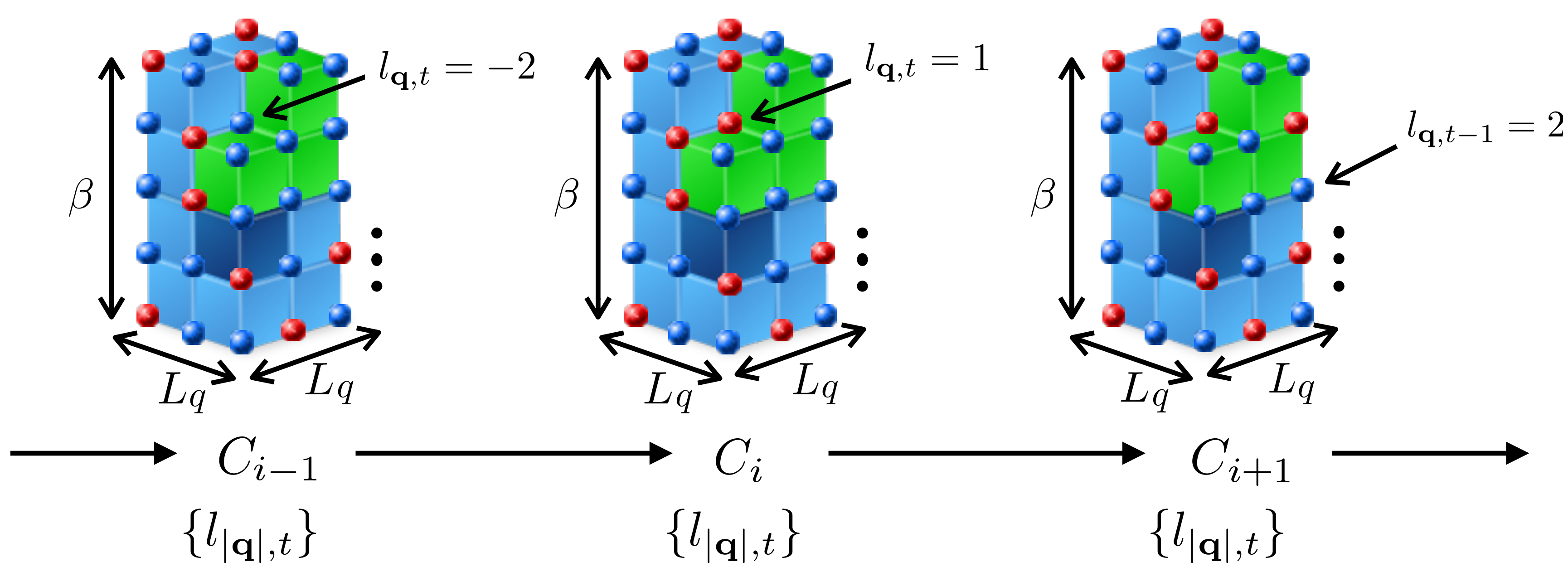
CPL 38, 077305 (2021)

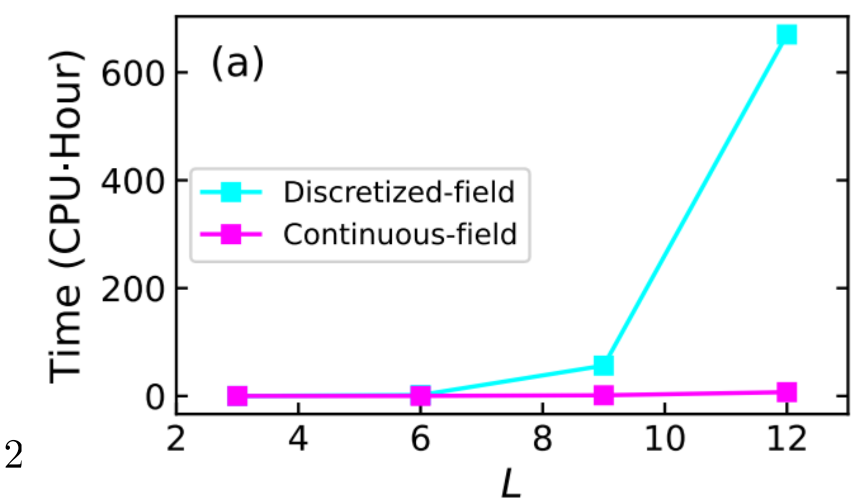
$$Z = \mathrm{Tr}\{\prod_{\tau} e^{-\Delta\tau\, H_{int}(\tau)}\} = \mathrm{Tr}\{\prod_{\tau} \exp\{-\frac{\Delta\tau}{4\Omega}\sum_{\mathbf{G},\mathbf{q}\in mBZ} V(\mathbf{q}+\mathbf{G})\cdot[\underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}}+\delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{A_{\mathbf{Q}}} - \underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}}-\delta\rho_{\ma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

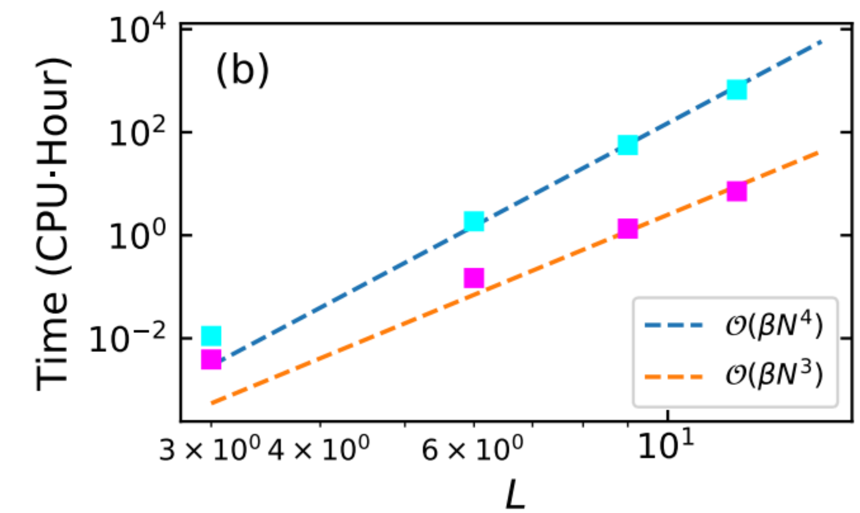
$$\exp(-\alpha_1(\mathbf{Q})A_{\mathbf{Q}}^2) = \frac{1}{4}\sum_{\{l_{\mathbf{Q},\tau,1}\}} \gamma(l_{\mathbf{Q},\tau,1})\ \exp(i\eta(l_{\mathbf{Q},\tau,1})\sqrt{\alpha_1(\mathbf{Q})}\ A_{\mathbf{Q}})) + O(\Delta\tau^4) \quad \{l_{\mathbf{Q},\tau,1}, l_{\mathbf{Q},\tau,2}\} \quad \alpha_1(\mathbf{Q})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

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

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







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

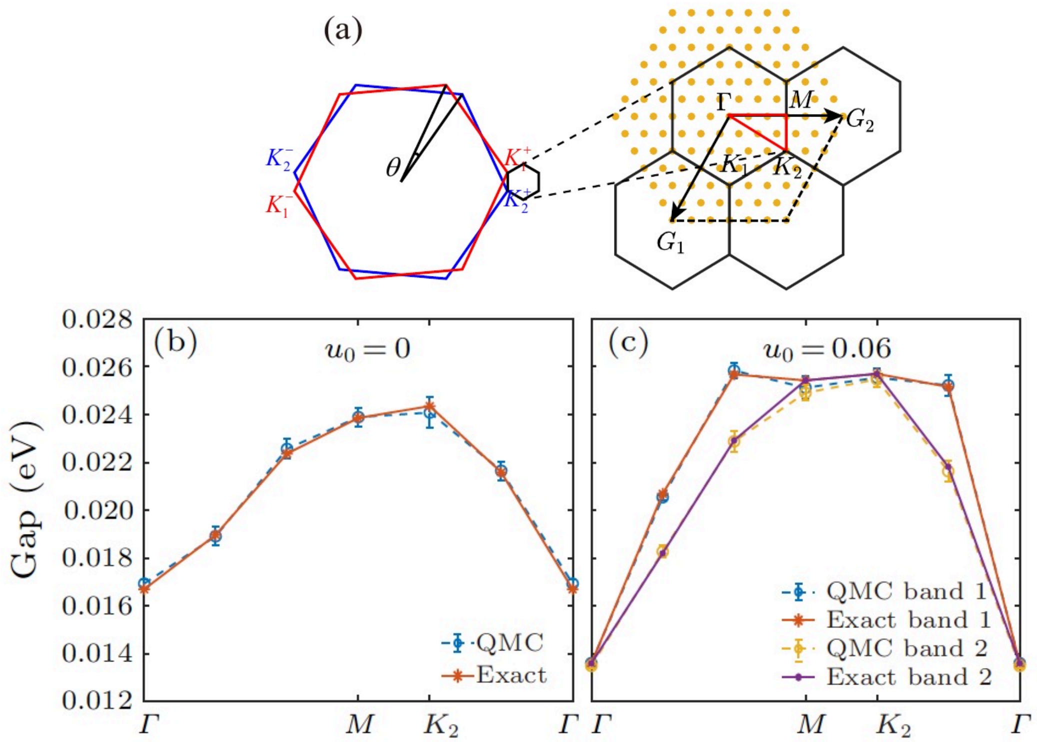
$O(N^3)$ $\qquad O(\beta N^4)$

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,†]

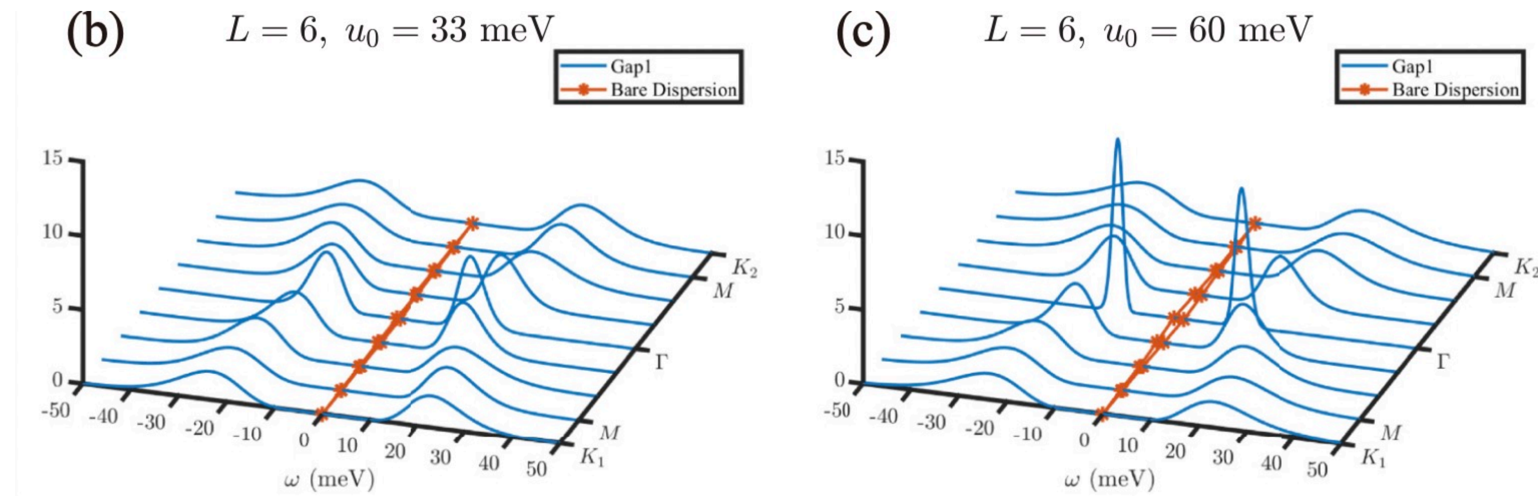
CPL 38, 077305 (2021)



single-particle excitations

PRB 105, L121110 (2022)

$T = 0.667$ meV



Bosonic collective excitations

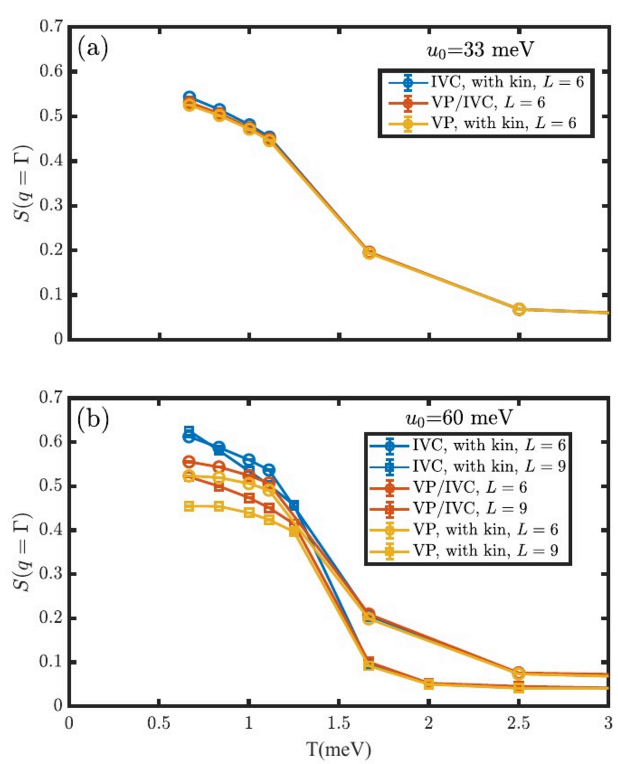
$$\mathcal{O}_a(\mathbf{q}) = \sum_{\mathbf{k}} d^{\dagger}_{\mathbf{k}+\mathbf{q}} M_a d_{\mathbf{k}}$$

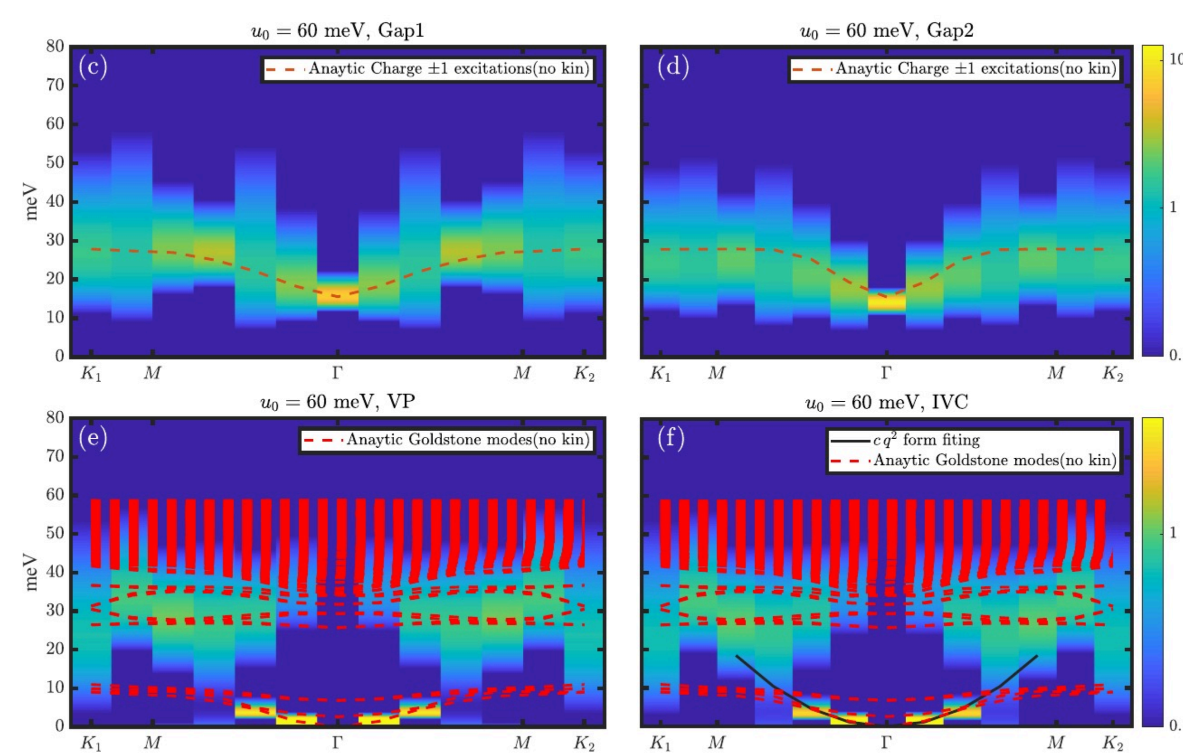
$$M_a = \tau_z \eta_0$$

for valley polarized state

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

for intervalley coherent state



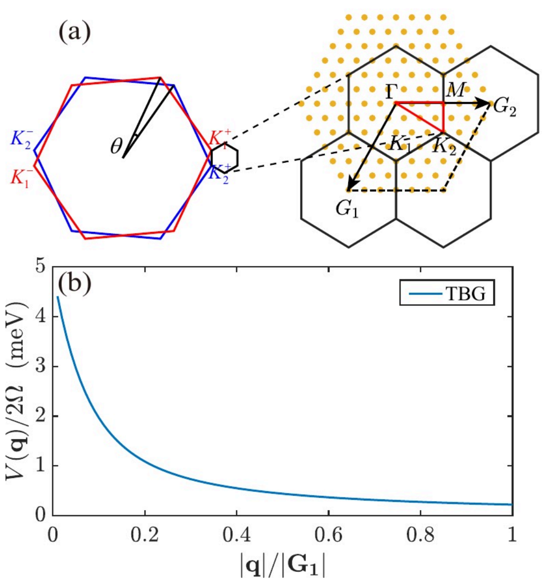


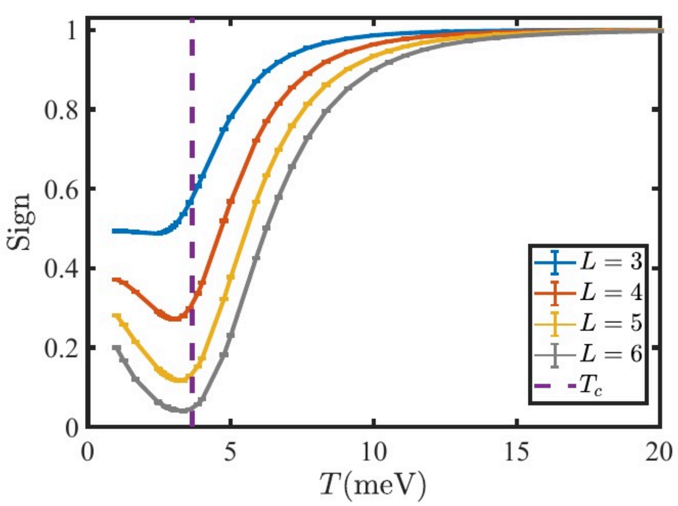
Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

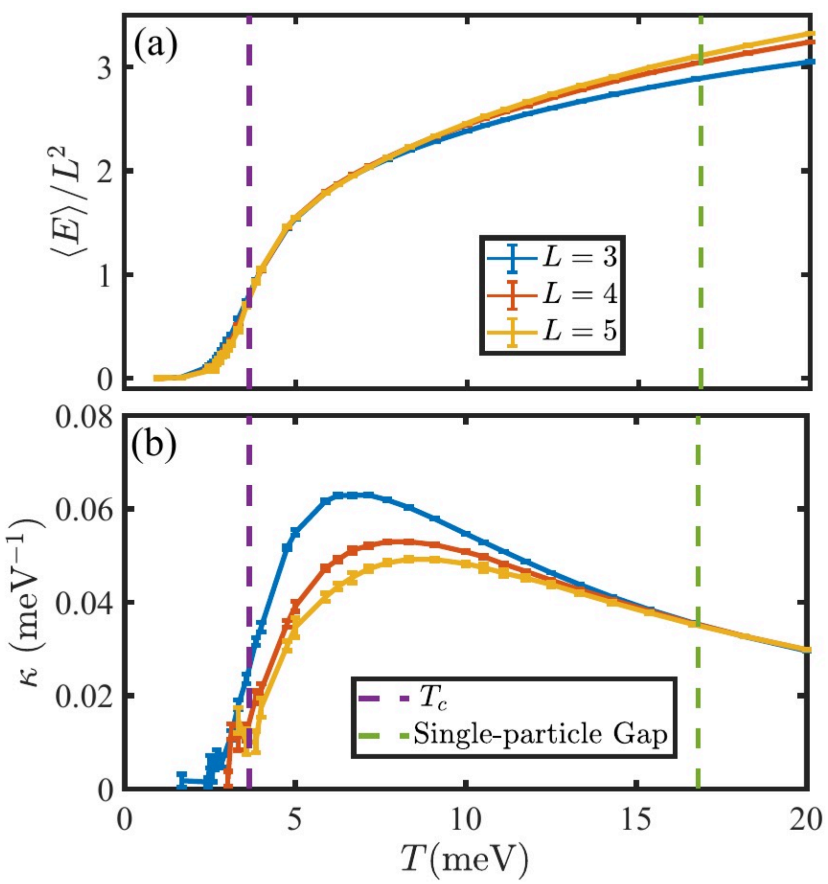
Gaopei Pan,[1,2] Xu Zhang,[3] Hongyu Lu,[3] Heqiu Li,[4] Bin-Bin Chen,[3] Kai Sun,[5,*] and Zi Yang Meng[3,†]

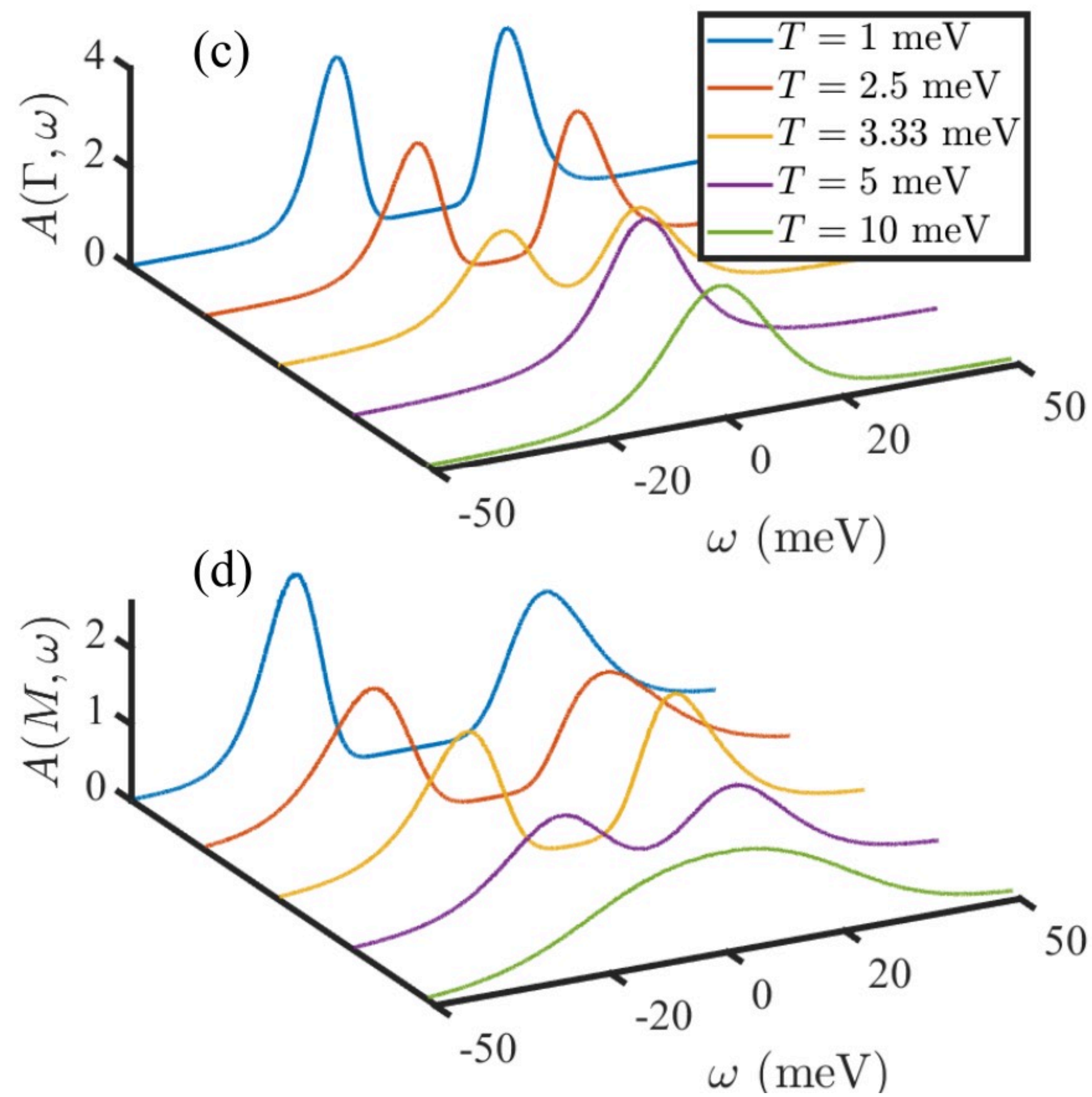
momentum-space QMC
Single valley and single spin

PRL 130, 016401 (2023)









$T_c = 3.65(5)$ 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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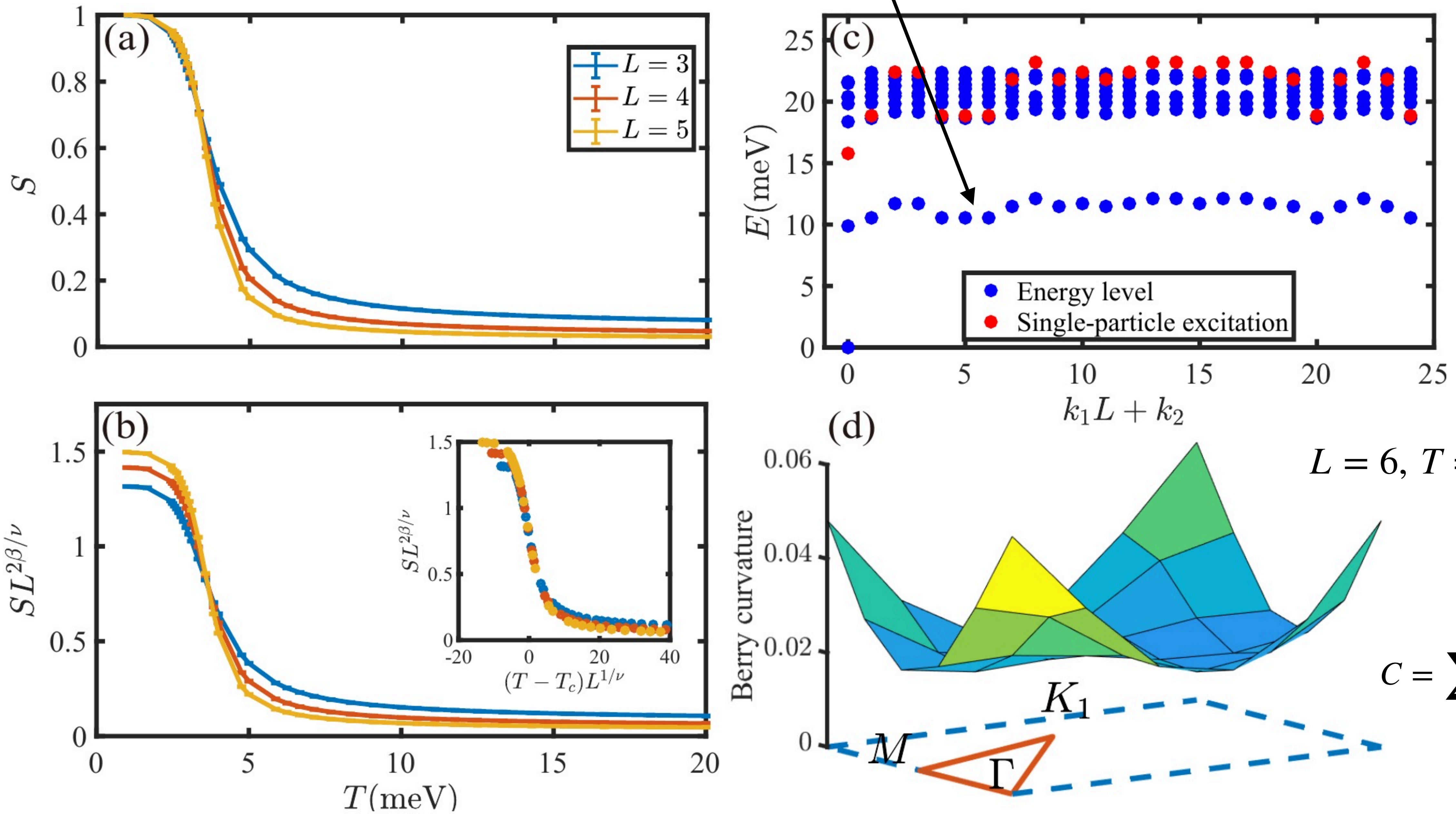
PRL 130, 016401 (2023)

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

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],
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CPL 38, 077305 (2021)

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

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

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

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

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

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

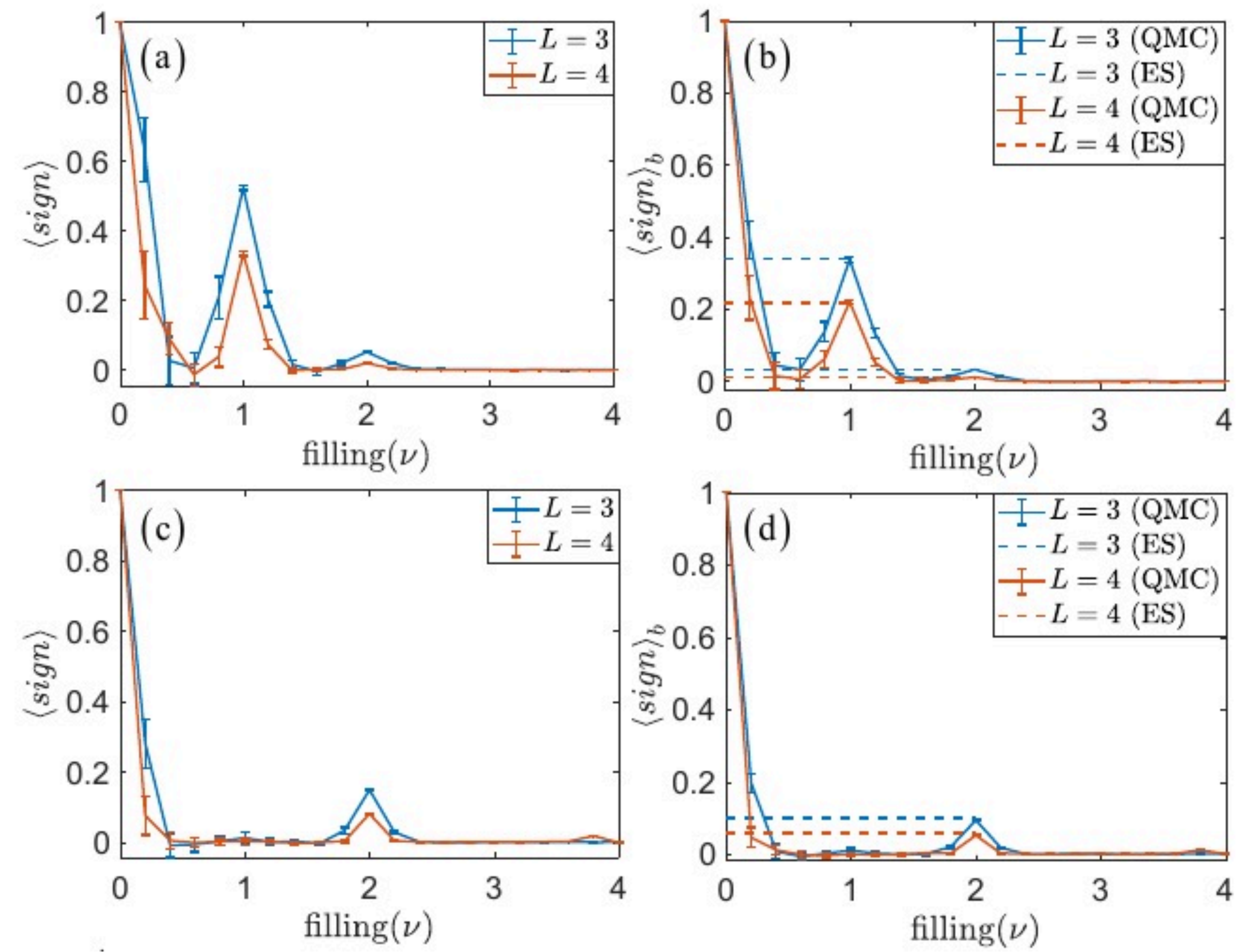
Fermionic Monte Carlo Study of a Realistic Model of Twisted Bilayer Graphene, Johannes S. Hofmann, et al., PRX 12, 011061 (2022)

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}



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

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

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

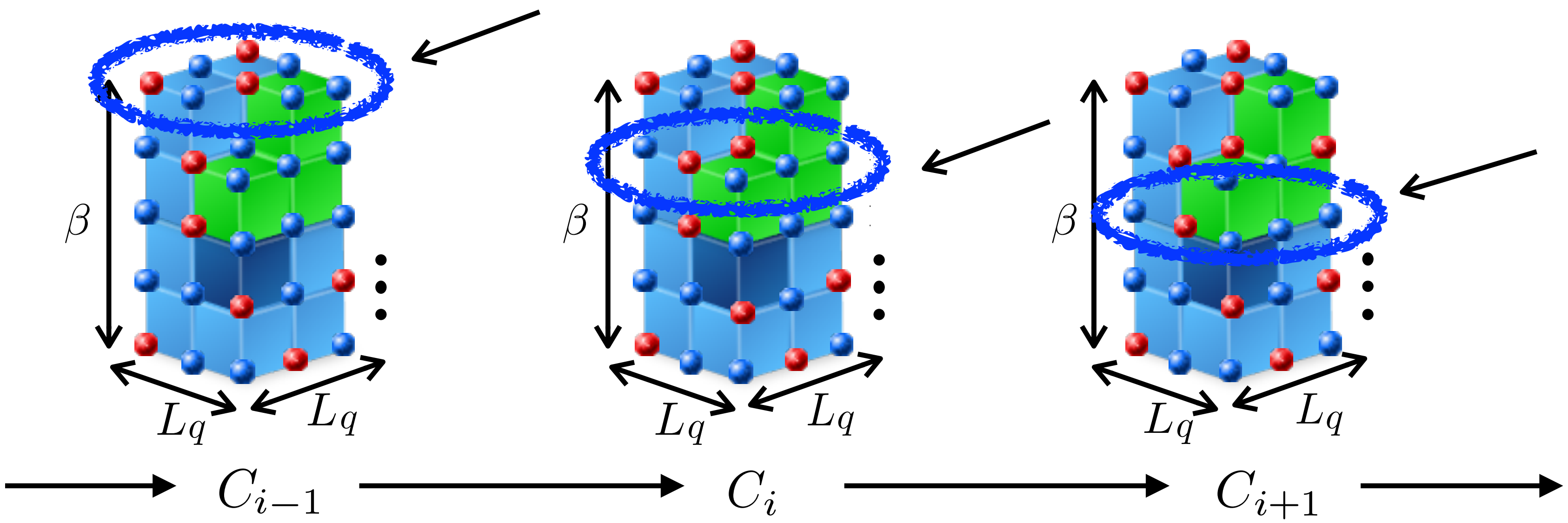
Continuous Field Momentum-Space QMC

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

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

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

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



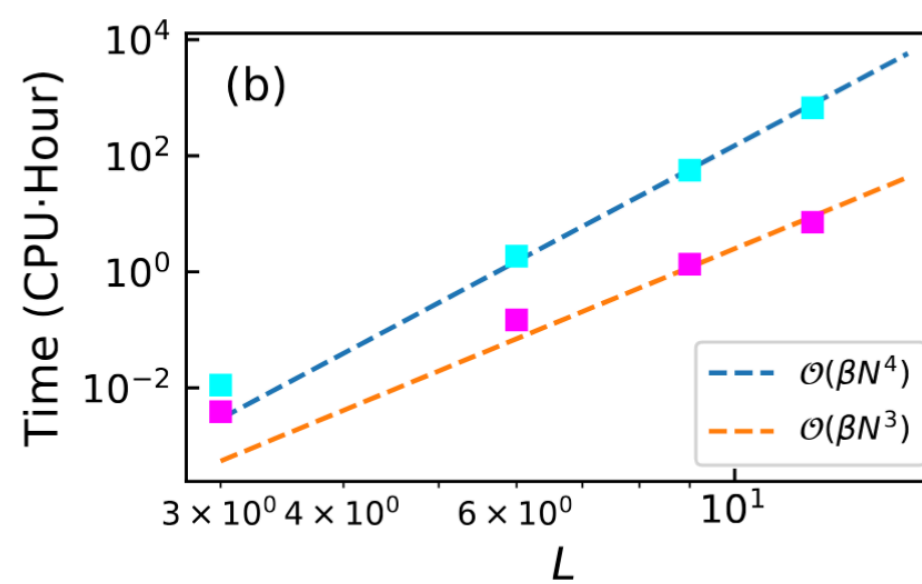
$\{\phi_{\tau,\mathbf{Q},\gamma}, p_{\tau,\mathbf{Q},\gamma}\}$ $\{\phi_{\tau,\mathbf{Q},\gamma}, p_{\tau,\mathbf{Q},\gamma}\}$ $\{\phi_{\tau,\mathbf{Q},\gamma}, p_{\tau,\mathbf{Q},\gamma}\}$

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

sparse matrix
O(N^2)

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

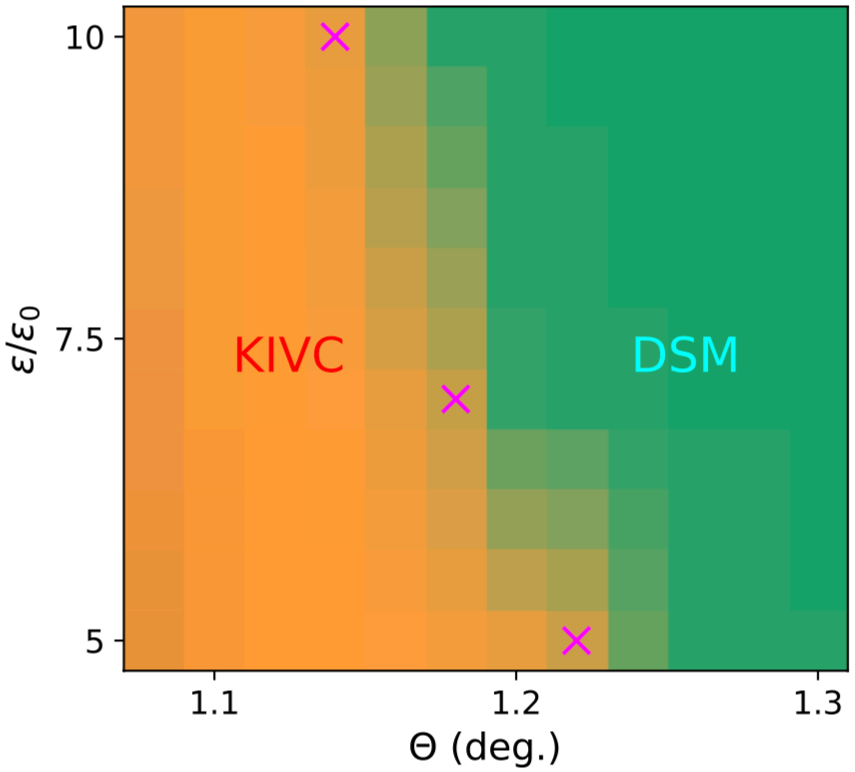
$O(N^2)$ $O(N^3)$

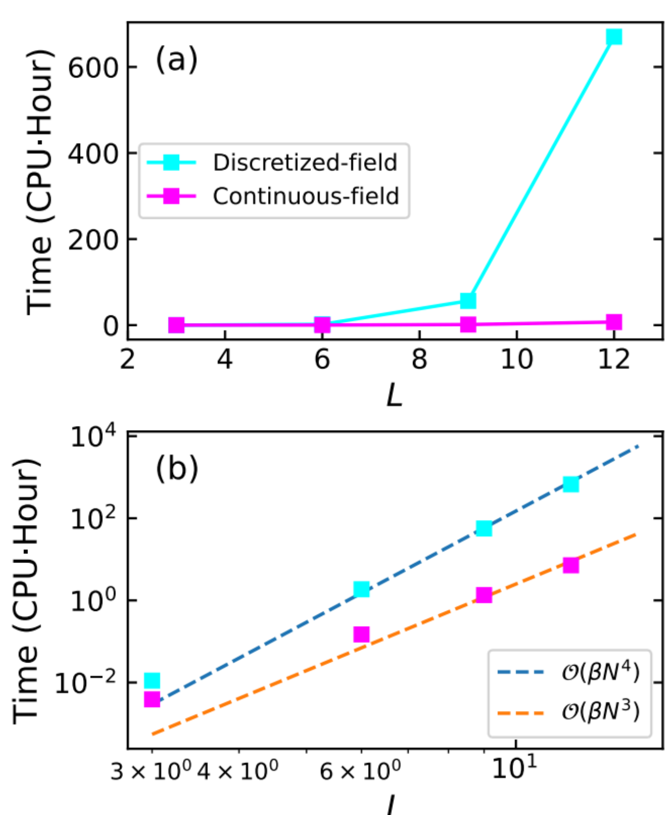


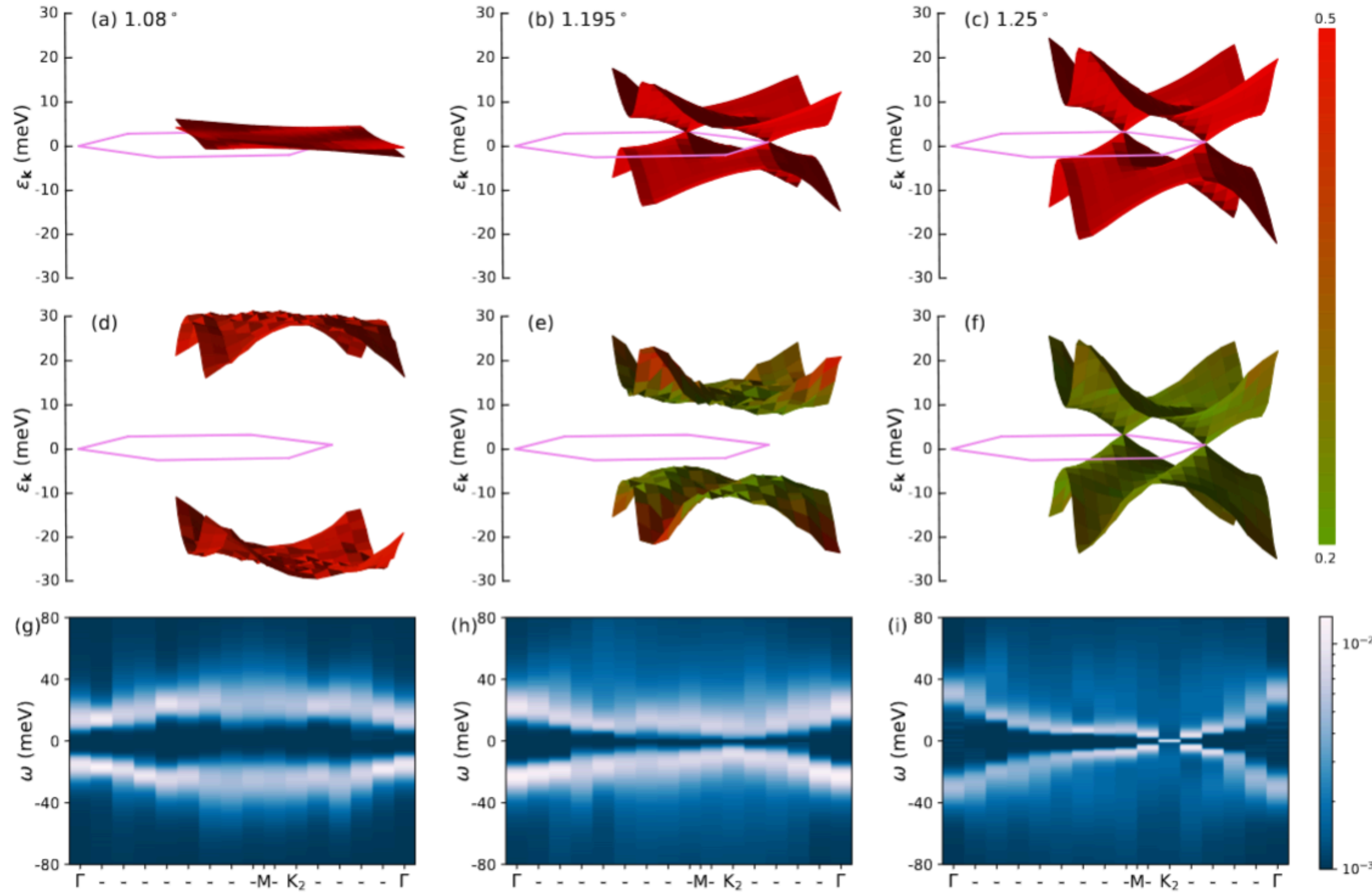
Angle-Tuned Gross-Neveu Quantum Criticality in Twisted Bilayer Graphene: A Quantum Monte Carlo Study

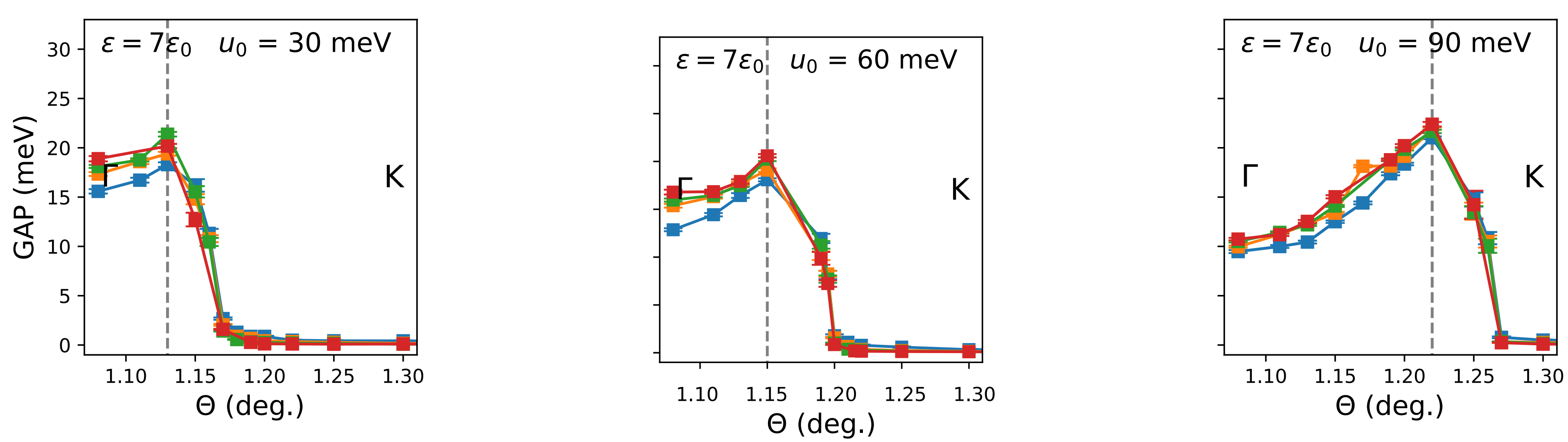
Cheng Huang,[1] Nikolaos Parthenios,[2,3] Maksim Ulybyshev,[4] Xu Zhang,[1,5] Fakher F. Assaad,[4,6] Laura Classen,[2,3,*] and Zi Yang Meng[1,†]

Nat. Comm. 16, 7176 (2025)









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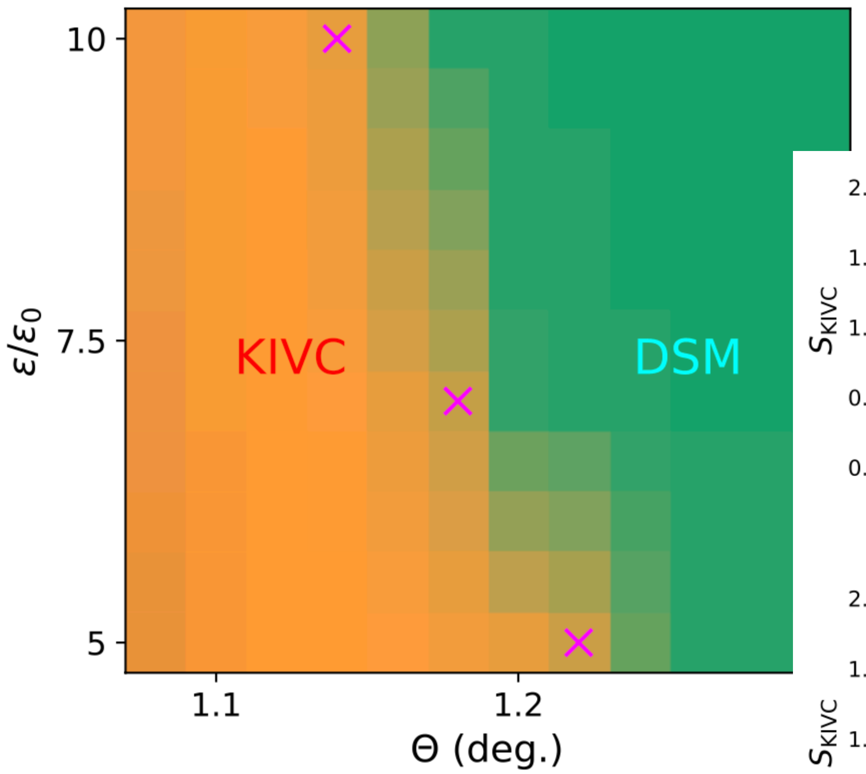

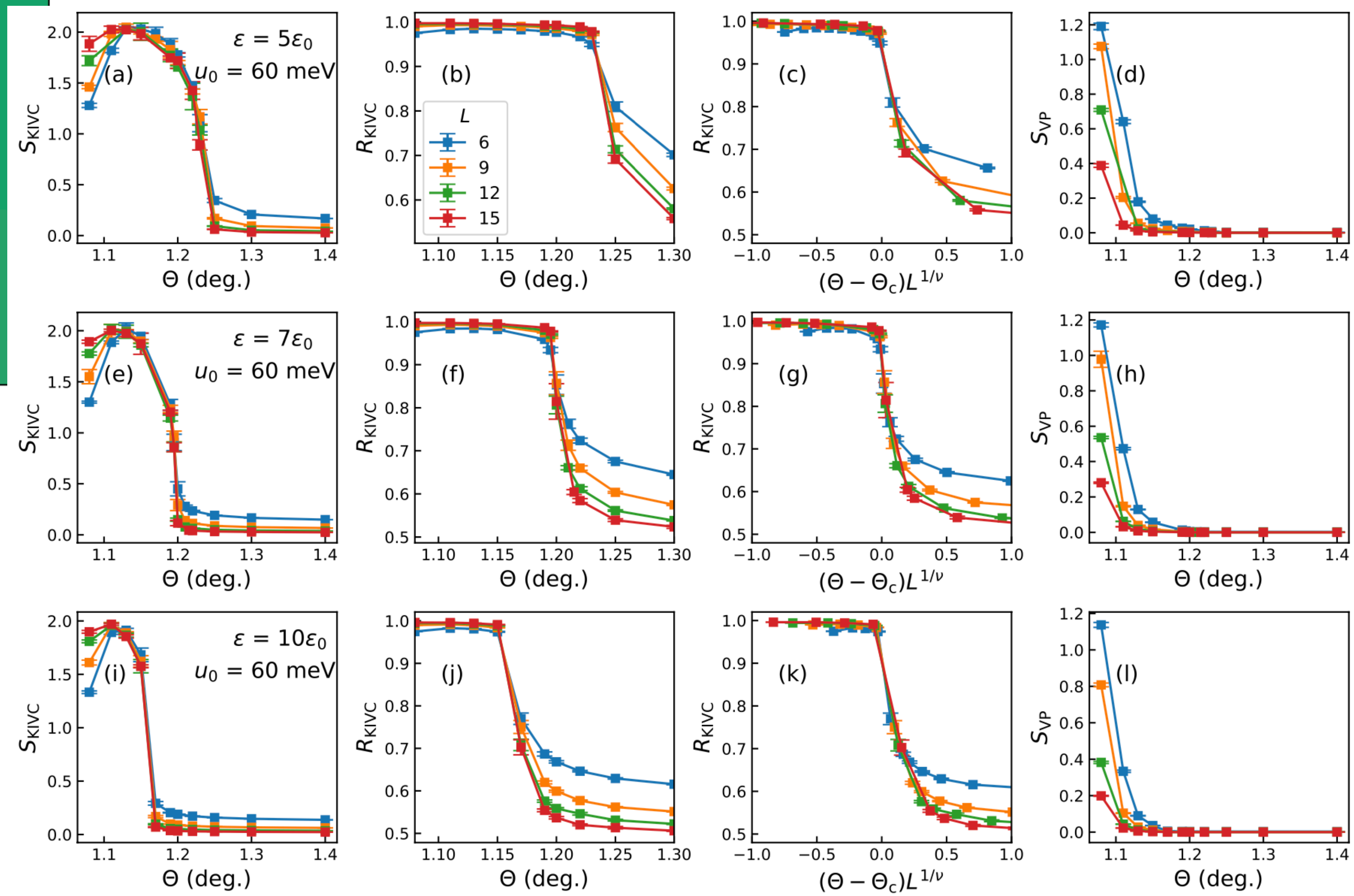

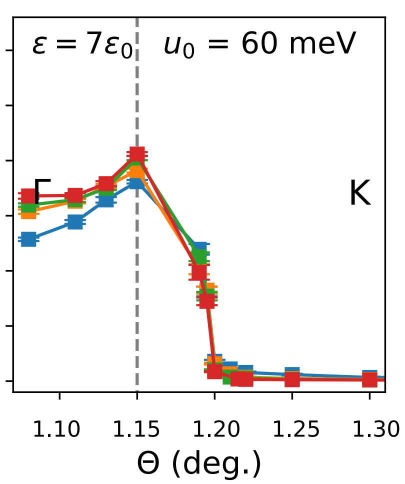

Content

1. Momentum-space QMC for twisted bilayer graphene

- CPL 38, 077305 (2021) [momentum-space QMC, 6 x 6]
- PRL 130, 016401 (2023) [Thermodynamic responses]
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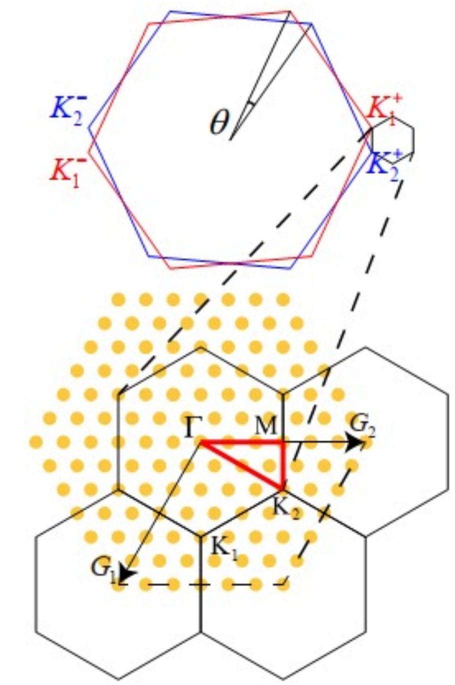

2. Quantum Fisher information in frustrated magnets

- Nat. Comm. in press (2026) [quantum spin ice]
- arXiv: 2603.19951 (2026) [kagome quantum spin liquid]
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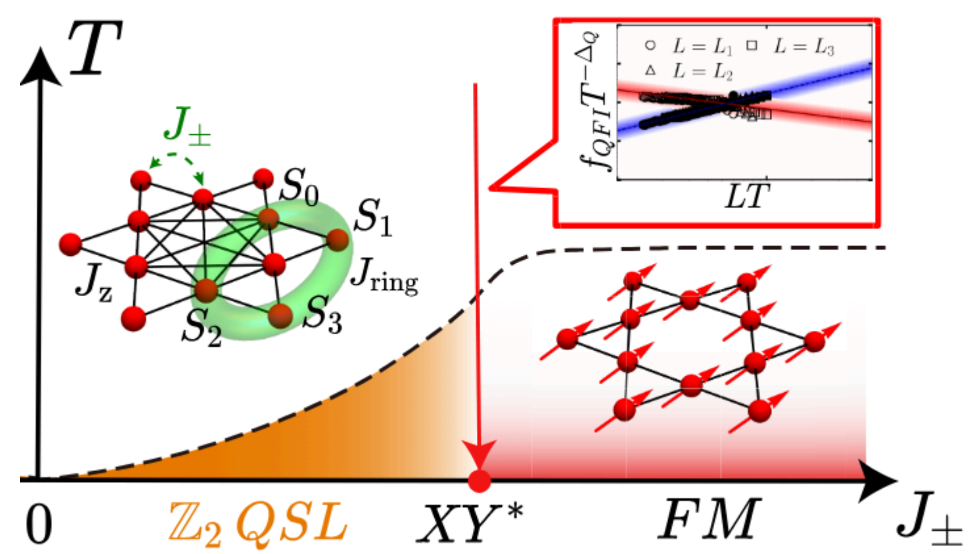
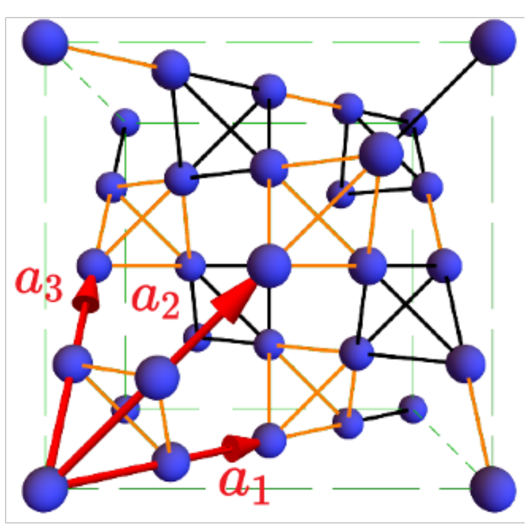
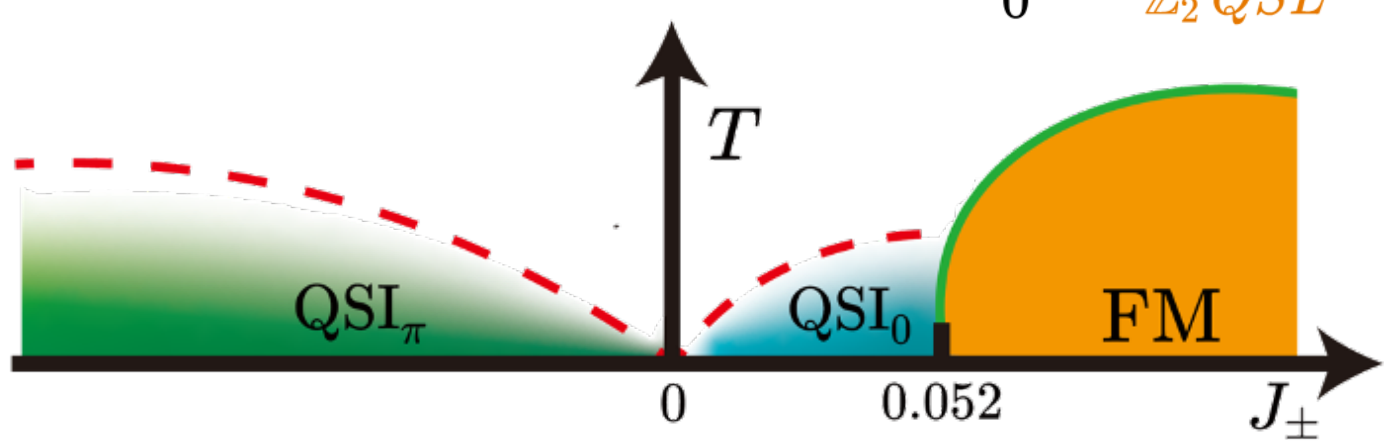






Quantum Fisher Information as a Thermal Probe in Frustrated Magnets through Insights from Quantum Spin Ice

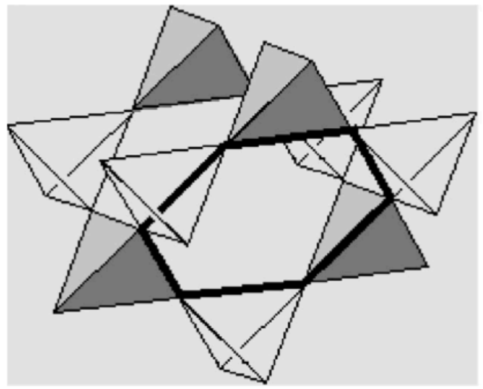
Chengkang Zhou,[1,*] Zhengbang Zhou,[2,*] Félix Desrochers,[2,3] Yong Baek Kim,[2] and Zi Yang Meng[1]

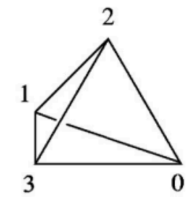
Nat. Comm. in press (2026)

$$\mathcal{H}=\mathcal{H}_I+\mathcal{H}',$$

$$\mathcal{H}_I=\frac{J_z}{2}\sum_t (S_t^z)^2,$$

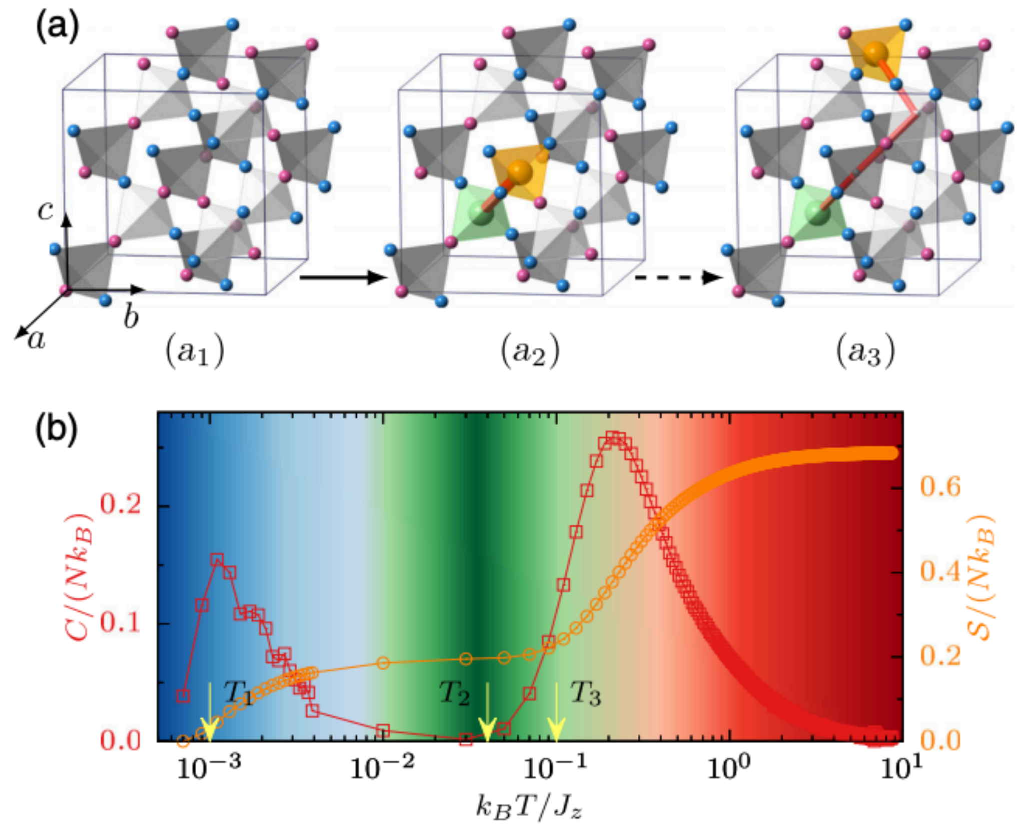
$$\mathcal{H}'=\frac{J_\perp}{2}\sum_{\langle ij\rangle}(S_i^+S_j^-+\mathrm{H.c.}),$$





- Dynamics of Topological Excitations in a Model Quantum Spin Ice, Huang, Deng, Wang, Meng, PRL 120, 167202 (2018)

$$\mathcal{H}=\sum_{\langle i,j\rangle}-J_\pm(S_i^+S_j^-+\mathrm{H.c.})+J_zS_i^zS_j^z.$$



$$(\frac{J_\pm}{J_z})_c=0.052$$

$$\frac{J_\pm}{J_z}=0.046$$

$$T_1=0.001J_z$$

$$T_2=0.04J_z$$

$$T_3=0.1J_z$$

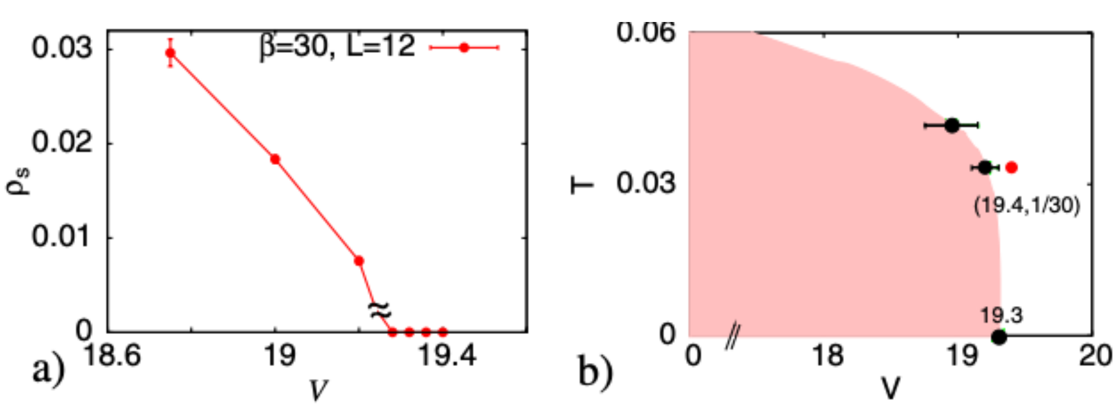
- Pyrochlore photons: The U(1) spin liquid in a S=1/2 three-dimensional frustrated magnet, Hermele, Fisher, Balents, PRB 69, 064404 (2004)

$$\mathcal{H}_p=\frac{U}{2}\sum_{\langle\mathbf{rr}'\rangle}(n_{\mathbf{rr}'}-1/2)^2-K\sum_{\hexagon}\cos(\phi_1-\phi_2+\phi_3-\phi_4+\phi_5-\phi_6).$$

$$\mathcal{H}_p=\frac{U}{2}\sum_{\langle\mathbf{rr}'\rangle}e_{\mathbf{rr}'}^2-K\sum_{\hexagon}\cos\left(\sum_{\mathbf{rr}'\in\hexagon}a_{\mathbf{rr}'}\right).$$

- Unusual Liquid State of Hard-Core Bosons on the Pyrochlore Lattice, Banerjee, Isakov, Damle, Kim, PRL 100, 047208 (2008)

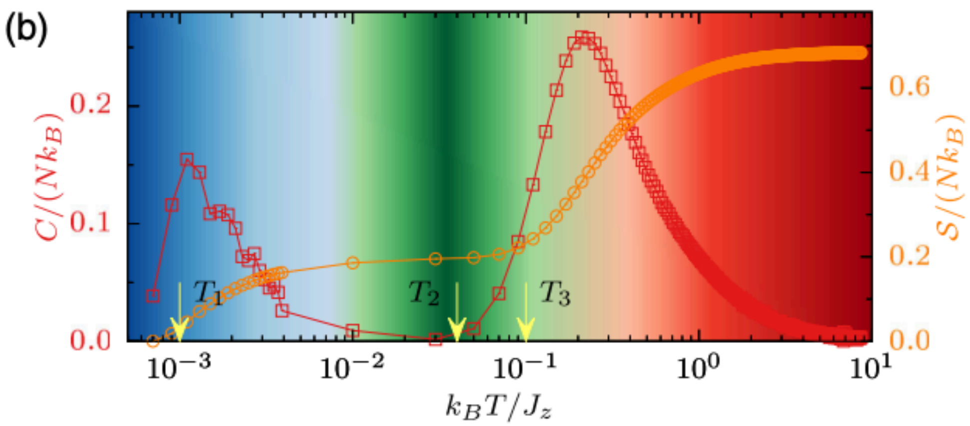
$$H=\sum_{\langle ij\rangle}[V(n_i-1/2)(n_j-1/2)-t(b_i^\dagger b_j+b_ib_j^\dagger)]$$



Dynamics of Topological Excitations in a Model Quantum Spin Ice

Chun-Jiong Huang,[1,2,3] Youjin Deng,[1,2,3,*] Yuan Wan,[4,5,†] and Zi Yang Meng[5,6,‡]

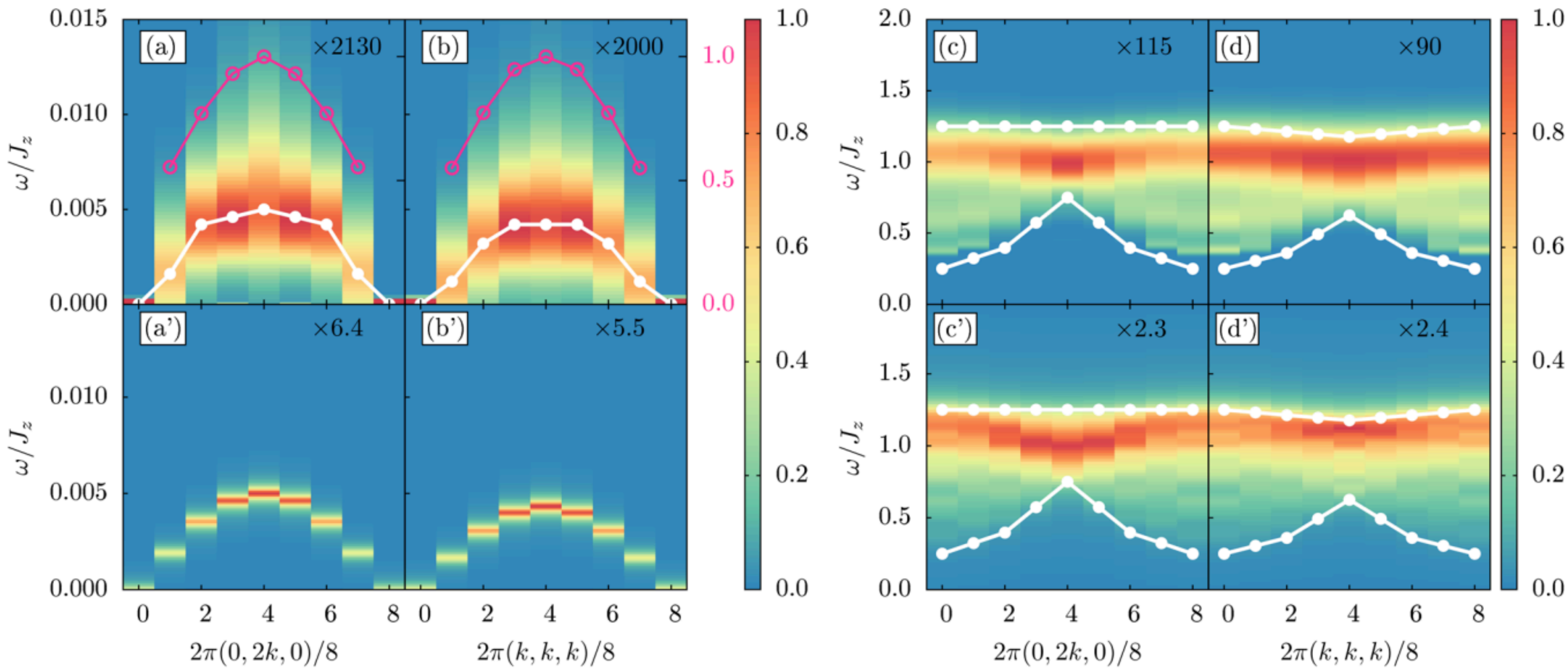
PRL 120, 167202 (2018)



$$\mathcal{H} = \sum_{\langle i,j\rangle} -J_{\pm}(S_i^+ S_j^- + \text{H.c.}) + J_z S_i^z S_j^z.$$

$$S^{zz}_{\alpha\beta}(\mathbf{q},\tau) = \langle S^z_{-\mathbf{q},\alpha}(\tau) S^z_{\mathbf{q},\beta}(0)\rangle$$

$$S^{+-}_{\alpha\beta}(\mathbf{q},\tau) = \langle S^+_{-\mathbf{q},\alpha}(\tau) S^-_{\mathbf{q},\beta}(0)\rangle$$



$$J_{\pm}/J_z = 0.046, \quad T_1 = 0.001J_z, \quad 4\times8\times8\times8$$

Quantum Fisher Information as a Thermal Probe in Frustrated Magnets through Insights from Quantum Spin Ice

Chengkang Zhou,[1,*] Zhengbang Zhou,[2,*] Félix Desrochers,[2,3] Yong Baek Kim,[2] and Zi Yang Meng[1]

Nat. Comm. in press (2026)

$\rho = \sum_n p_n |n\rangle\langle n|$ $\quad F_Q[\rho, O] = 2\sum_{m,n} \frac{(p_m - p_n)^2}{p_m + p_n} |\langle m|O|n\rangle|^2$ $\quad O = S^\alpha_{\mathbf{q}} := \sum_i S^\alpha_{\mathbf{R}_i} e^{i\mathbf{q}\cdot\mathbf{R}_i}$

$f_Q(O) := F_Q[\rho, O]/N, \quad \Delta\lambda = \lambda_{\max} - \lambda_{\min}$

$$f_Q(S^\alpha_{\mathbf{q}}, T) = 4\int_0^\infty d\omega \tanh\left(\frac{\omega}{2T}\right)\left(1 - e^{-\omega/T}\right) A^\alpha(\mathbf{q}, \omega)$$

$$\text{nQFI}(O) := \frac{f_Q(O)}{(\Delta\lambda)^2} > m \Longrightarrow \text{entanglement depth } \geq m + 1$$

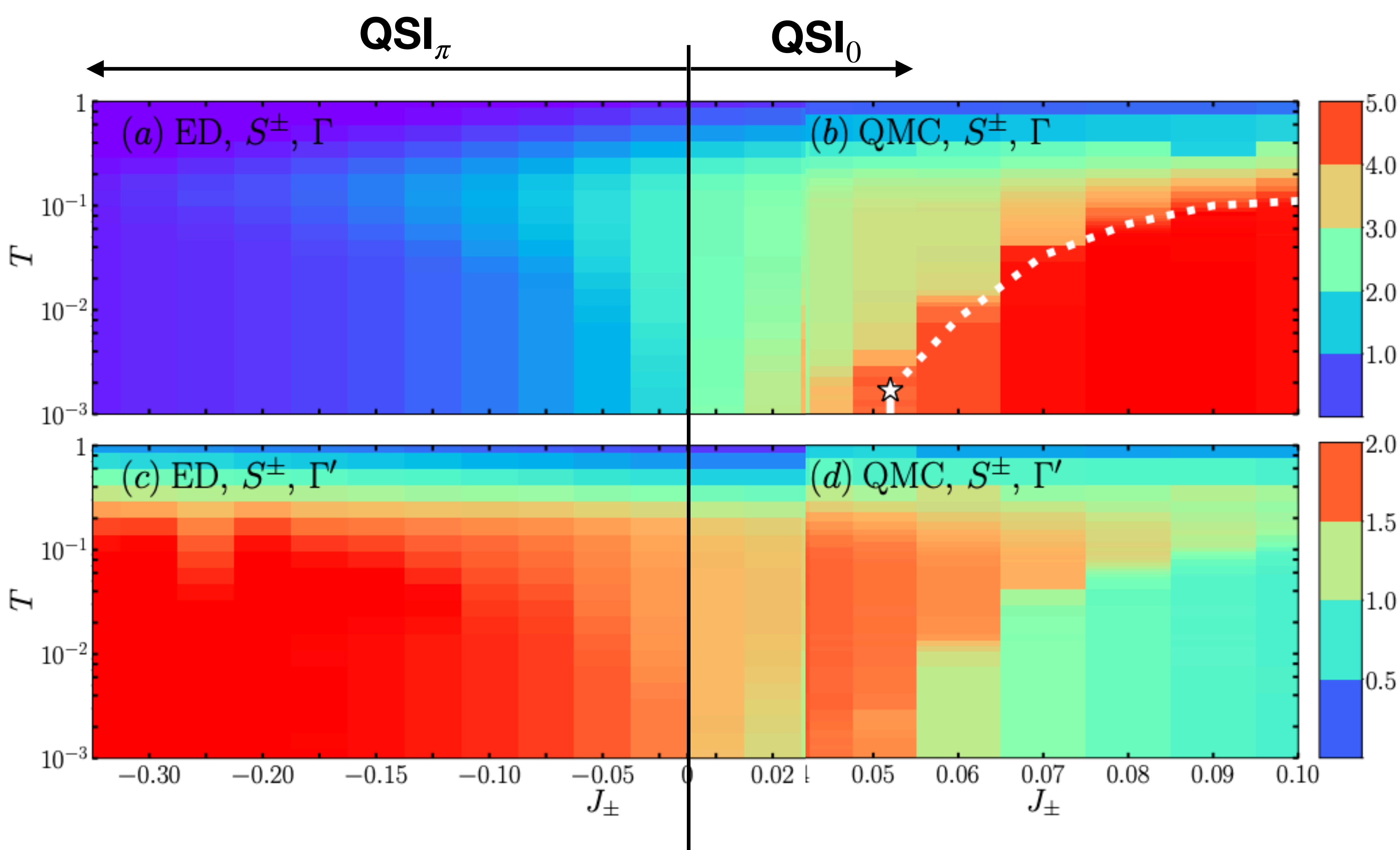
$$A^\alpha(\mathbf{q}, \omega) := \frac{1}{2\pi N}\int dt \langle S^{\alpha\dagger}_{\mathbf{q}}(t) S^\alpha_{\mathbf{q}}(0)\rangle e^{i\omega t}$$

$f_Q(S^\pm_q, T)$

$q = \Gamma = (0,0,0)$

$q = \Gamma' = (4\pi, 4\pi, 0)$

ED, 16-site cluster
QMC, 4×4^3 sites



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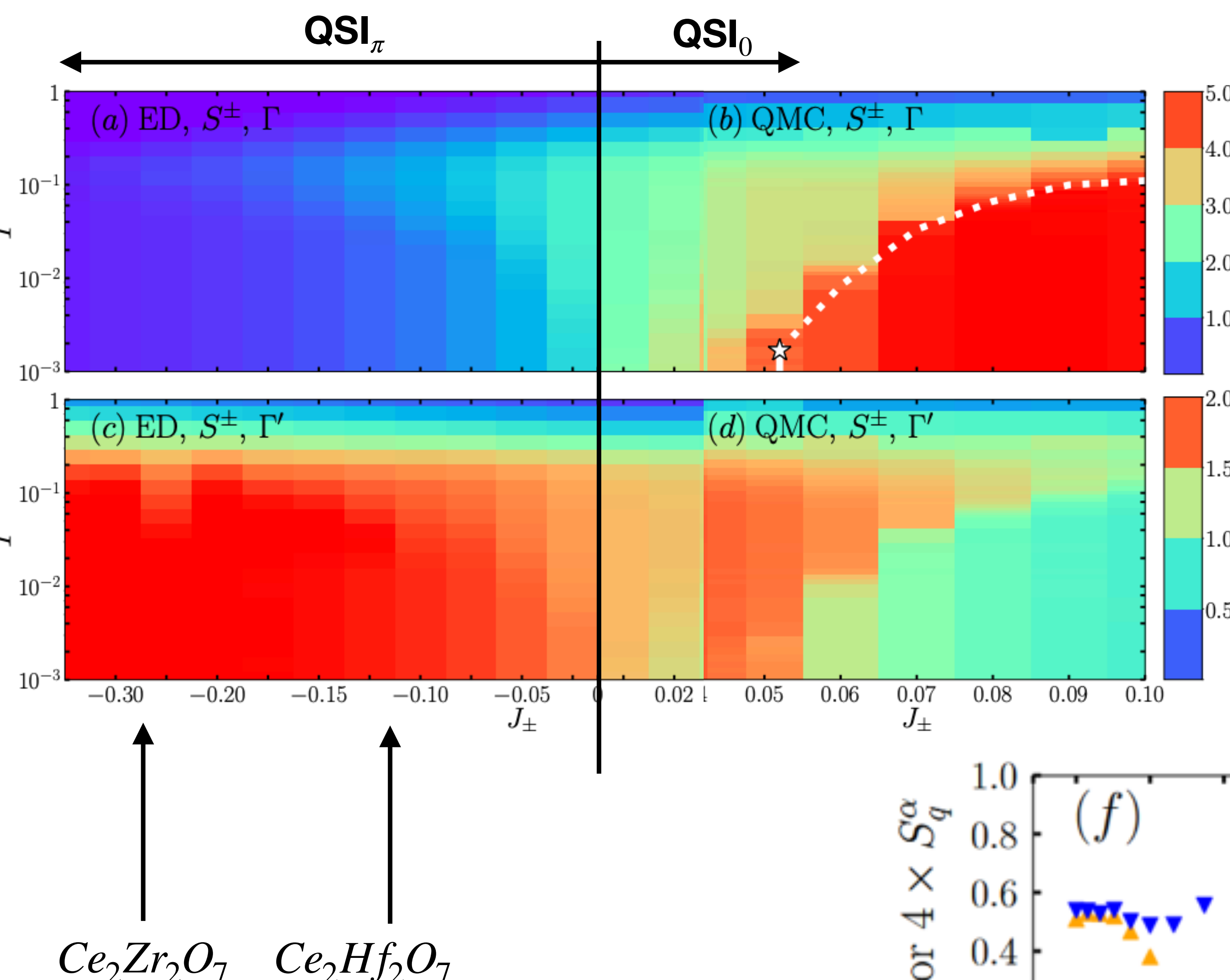
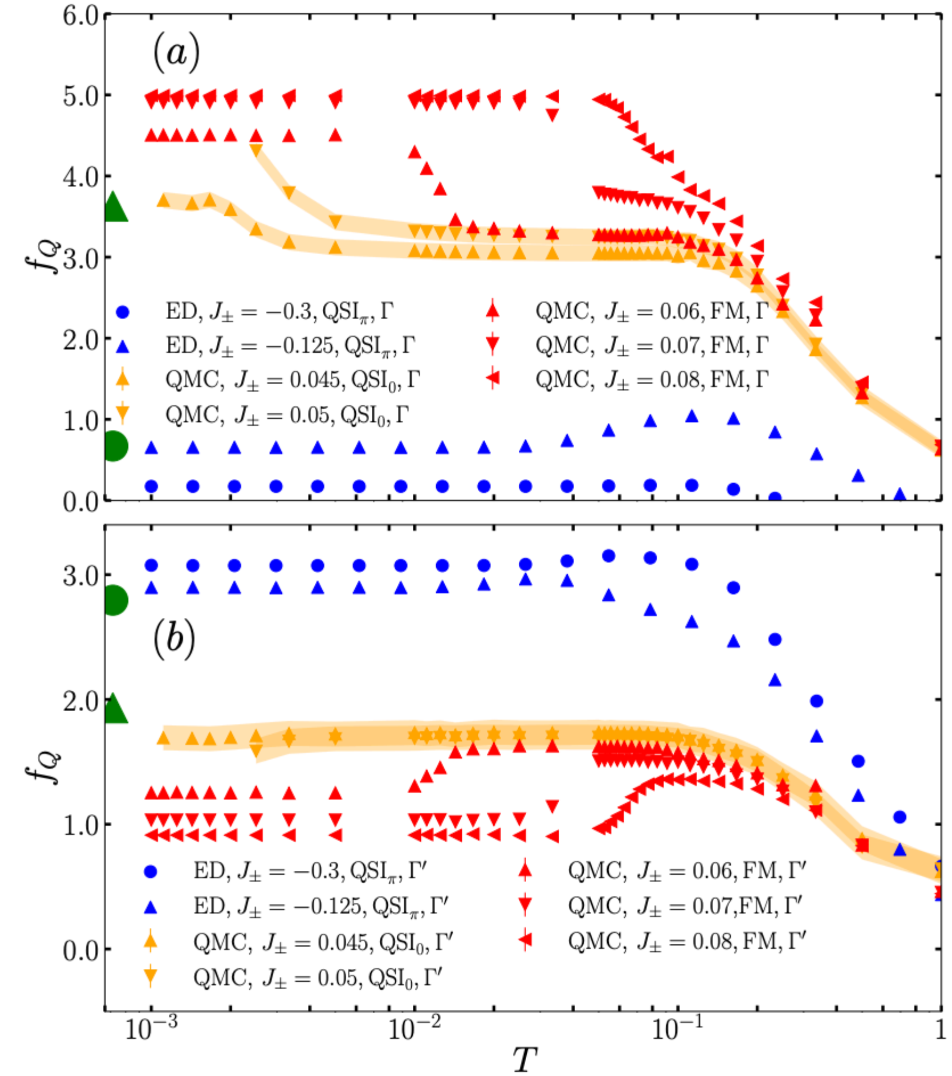
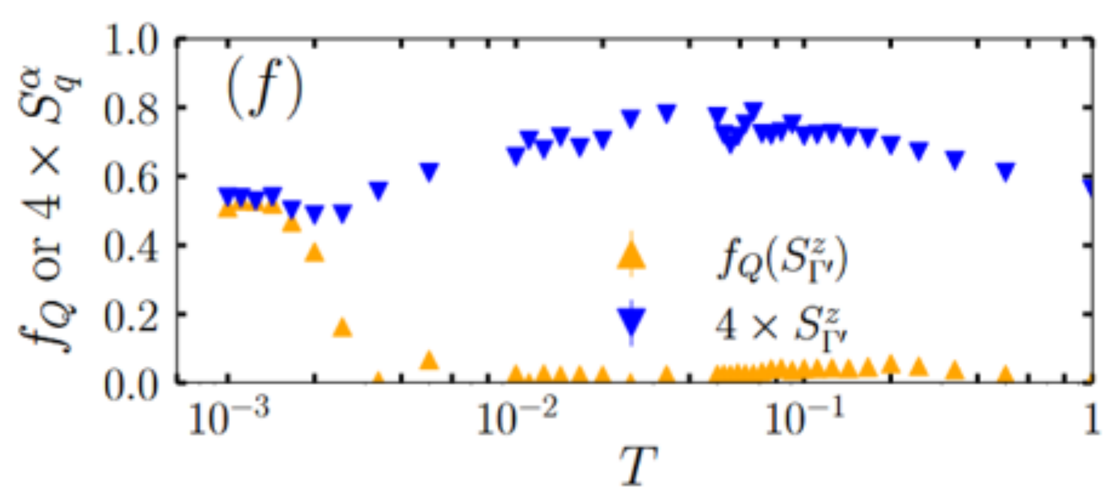
$$f_Q(S^{\alpha}_{\mathbf{q}}, T) = 4\int_0^{\infty} d\omega \tanh\left(\frac{\omega}{2T}\right)\left(1 - e^{-\omega/T}\right)A^{\alpha}(\mathbf{q},\omega)$$

$$A^{\alpha}(\mathbf{q},\omega) := \frac{1}{2\pi N}\int dt \langle S^{\alpha\dagger}_{\mathbf{q}}(t) S^{\alpha}_{\mathbf{q}}(0)\rangle e^{i\omega t}$$







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Chengkang Zhou,[1,*] Zhengbang Zhou,[2,*] Félix Desrochers,[2,3] Yong Baek Kim,[2] and Zi Yang Meng[1]

Nat. Comm. in press (2026)

Ce-based dipolar–octupolar (DO) pyrochlore $Ce_2Zr_2O_7$

neutron scattering couples to dipolar moments $S^{\pm}$

from local to global frame

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \frac{1}{N}\sum_{\mu\nu}\left(\hat{\mathbf{z}}_\mu \cdot \hat{\mathbf{z}}_\nu - \frac{(\hat{\mathbf{z}}_\mu \cdot \mathbf{Q})(\hat{\mathbf{z}}_\nu \cdot \mathbf{Q})}{|\mathbf{Q}|^2}\right)\langle \tau^z_{-\mathbf{q},\mu}(t)\tau^z_{\mathbf{q},\nu}(0)\rangle := A^{\mathrm{DO}}(\mathbf{q},t)$$

$$f(S_q^{DO}, T) \qquad q = \Gamma' = (4\pi, 4\pi, 0)$$

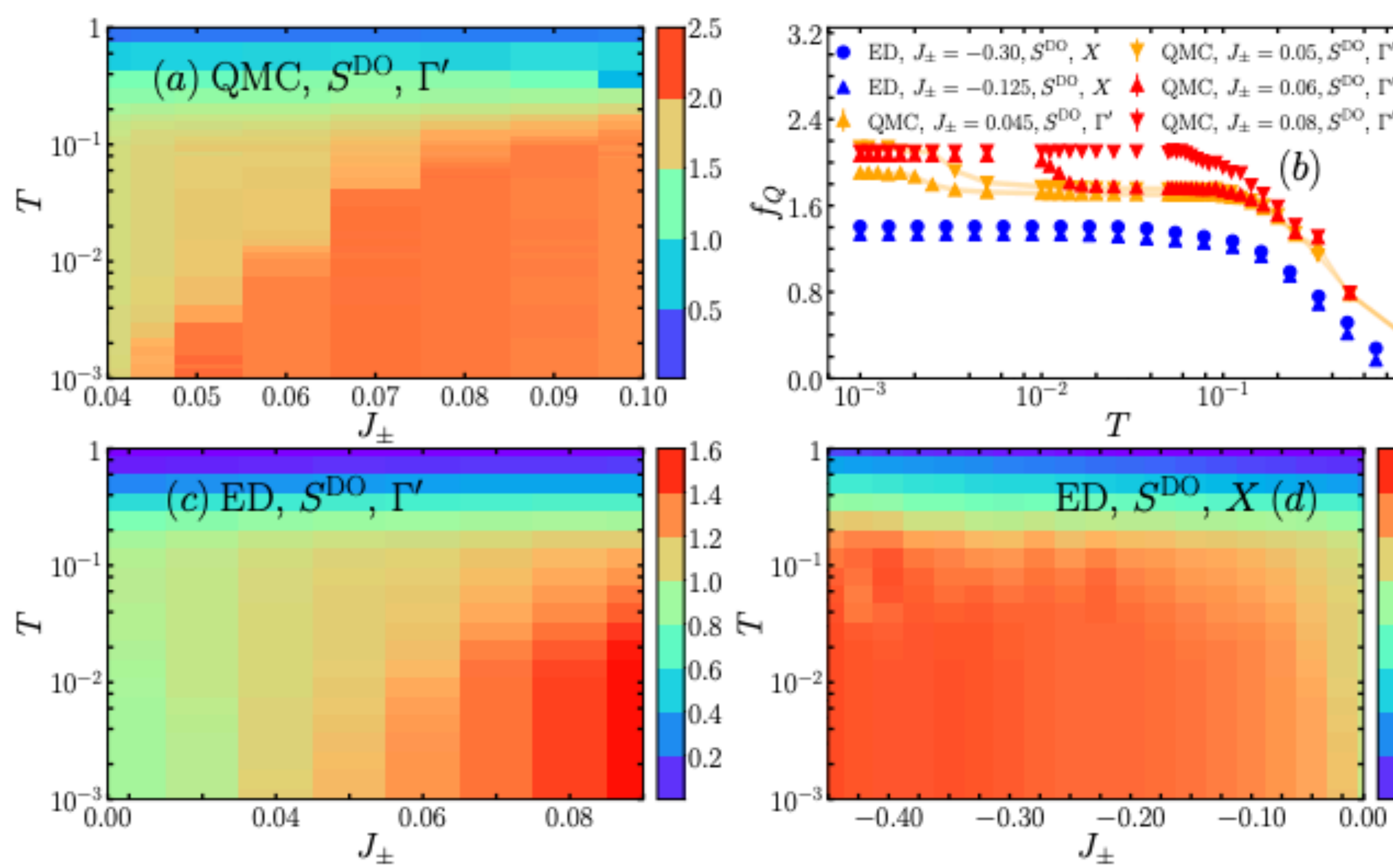
$$q = X = (0,0,2\pi)$$

$$f_Q(S^\alpha_{\mathbf{q}}, T) = 4\int_0^\infty d\omega \tanh\left(\frac{\omega}{2T}\right)\left(1 - e^{-\omega/T}\right)A^\alpha(\mathbf{q},\omega)$$

$$\mathrm{nQFI}(S^{\mathrm{DO}}_{\mathbf{q}}) = \tfrac{3}{2} f_Q(S^{\mathrm{DO}}_{\mathbf{q}})$$

$$\mathrm{nQFI}(S^{\mathrm{DO}}_{\Gamma'}, T) \gtrsim 2.2$$

QSI$_0$ > 3 partite entangled



$$\mathrm{nQFI}(S^{\mathrm{DO}}_X, T) \gtrsim 2.3$$

QSI$_\pi$ > 3 partite entangled

Quantum Fisher Information as a Probe of Critical Scaling in Frustrated Magnets: Signatures from Kagome Quantum Spin Liquid

Zhengbang Zhou,[1,*] Chengkang Zhou,[2,3,*] Menghan Song,[2,3] Yong Baek Kim,[1] and Zi Yang Meng[2,3]

- Fractionalization in an easy-axis Kagome antiferromagnet, Balents, Fisher, Girvin, PRB 65, 224412 (2002)
- Spin-Liquid Phase in a Spin-1/2 Quantum Magnet on the Kagome Lattice, Isakov, Kim, Paramekanti, PRL 97, 207204 (2006)
- arXiv: 2603.19951 (2026)

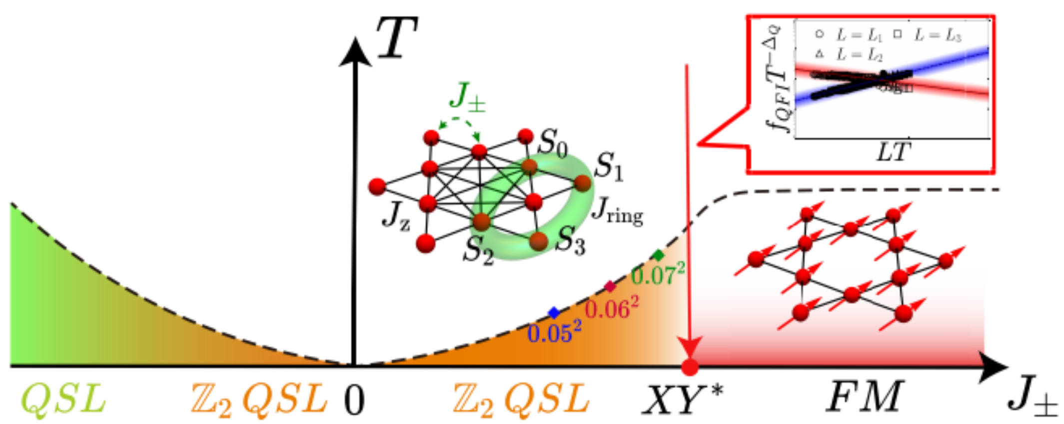
$$H = -J_{\pm}\sum_{\langle i,j\rangle}(S_i^+S_j^- + S_i^-S_j^+) + \frac{J_z}{2}\sum_{\hexagon}\left(\sum_{i\in\hexagon} S_i^z\right)^2$$

Ring Exchange in BFG model regime:

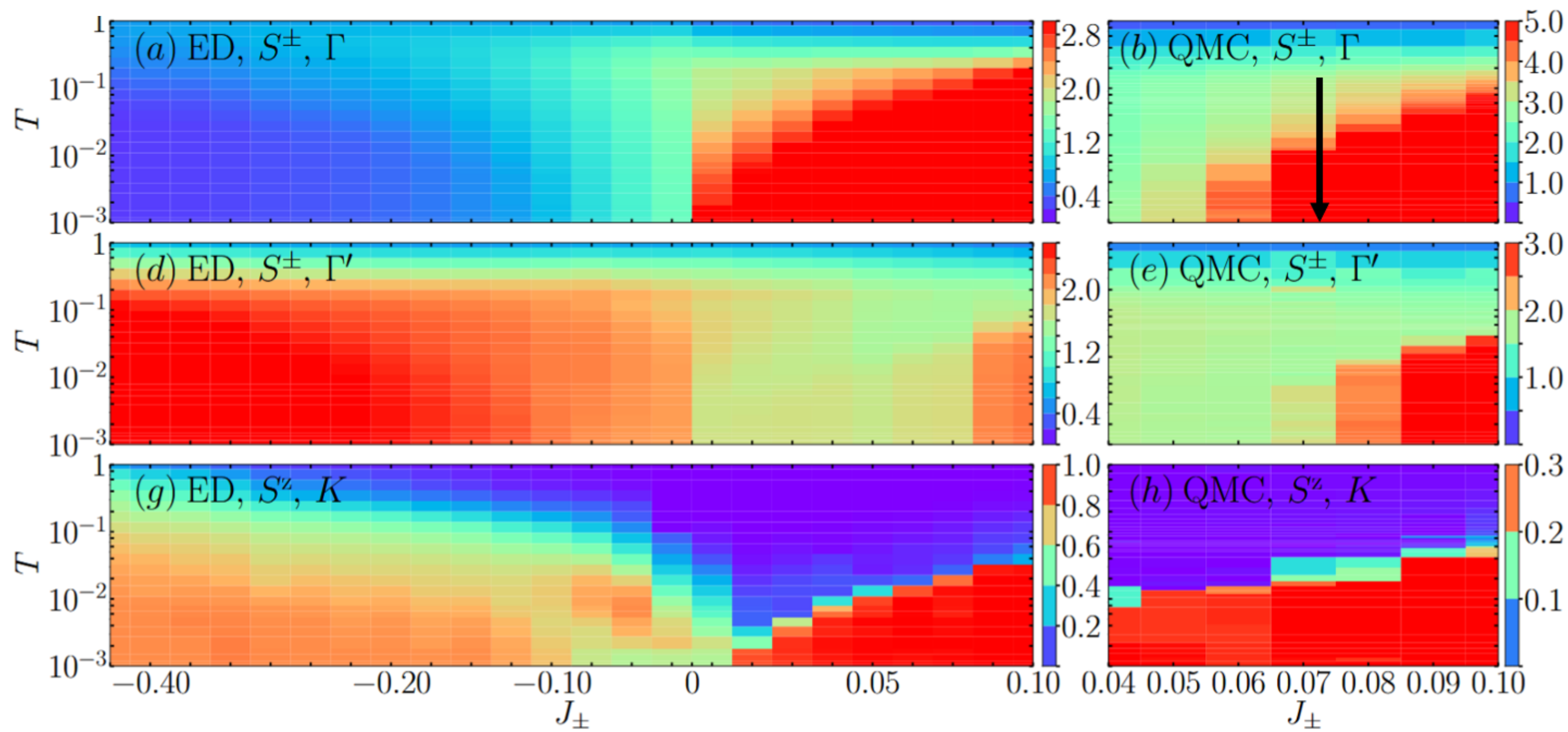
$$H_{ring} = J_{ring}\sum_{\langle 0,1,2,3\rangle}(S_0^+S_1^-S_2^+S_3^- + S_0^-S_1^+S_2^-S_3^+)$$

$$J_{ring} = \frac{J_{\pm}^2}{J_z}, T\sim J_{ring}$$

If $J_z = 1, J_{\pm} = 0.07$, then $T\sim 0.0049$



BFG — Big Friendly Giant



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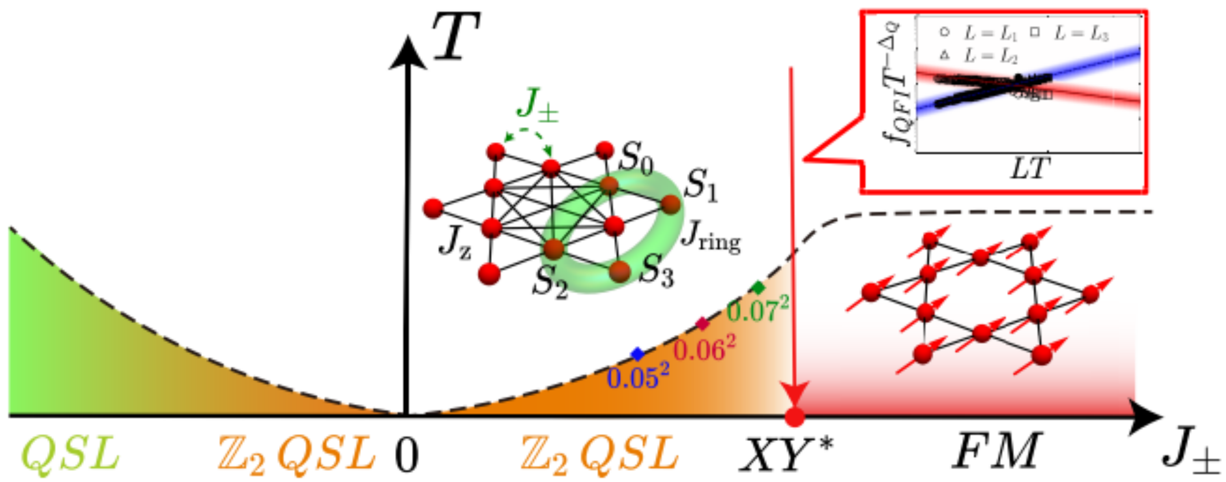


$$f_Q = \lambda^{\Delta_Q}\phi(T\lambda^z, L^{-1}\lambda, h\lambda^{1/\nu})$$

$h = \frac{J_\pm}{J_z} - (\frac{J_\pm}{J_z})_c = 0$ $\quad z = 1 \quad$ $\lambda = L$ at low temperature ($L \ll 1/T$)

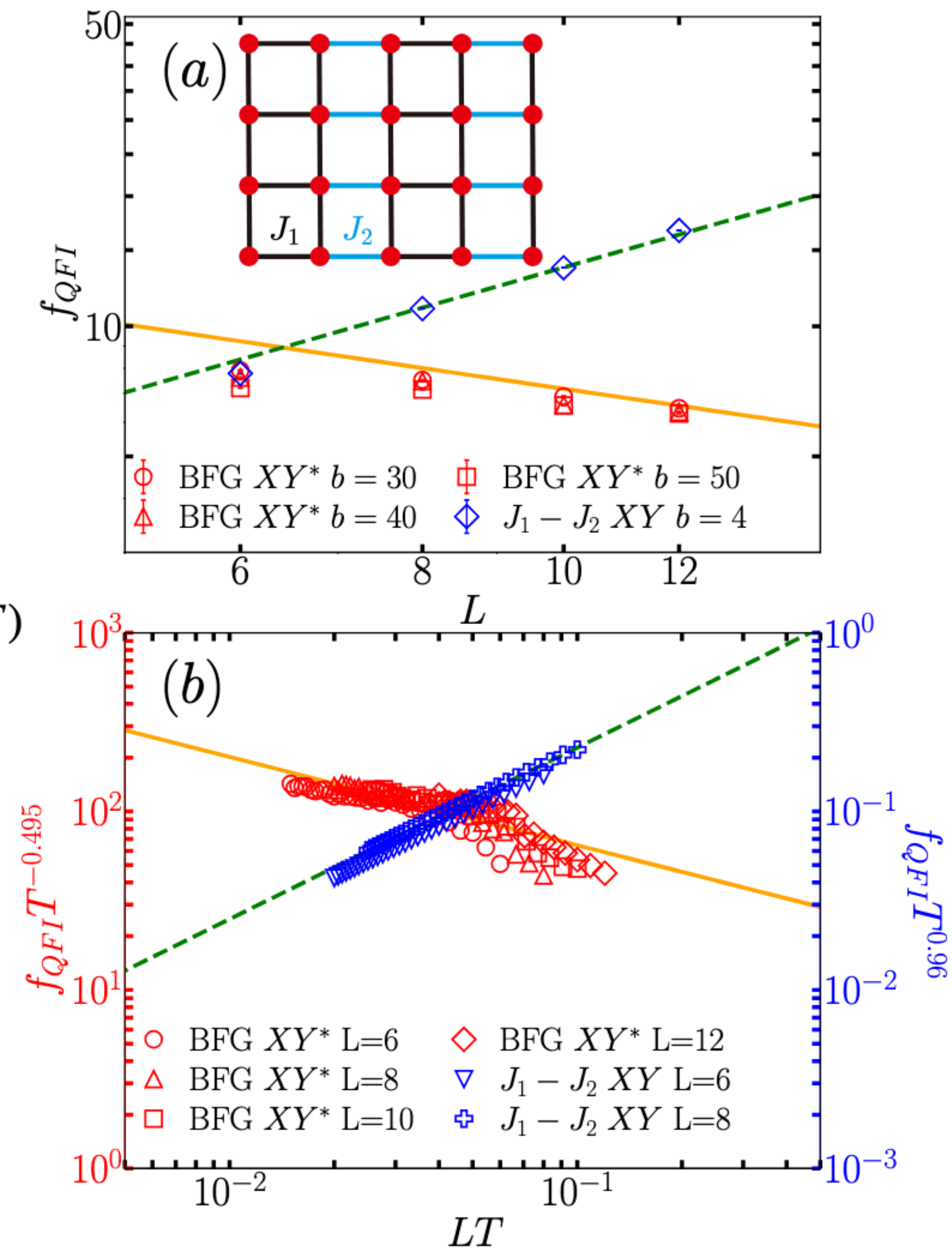
$$T = 1/(bL)$$

$$f_Q = L^{\Delta_Q}\phi(1/b)$$

$\Delta_Q = d - 2\Delta = 2 - (1+\eta) = -0.495$ (2+1) XY*

$\Delta_Q = d - 2\Delta = 2 - (1+\eta) = 0.96$ (2+1) XY

$$f_Q T^{\Delta_Q} = (TL)^{\Delta_Q}\phi(TL)$$



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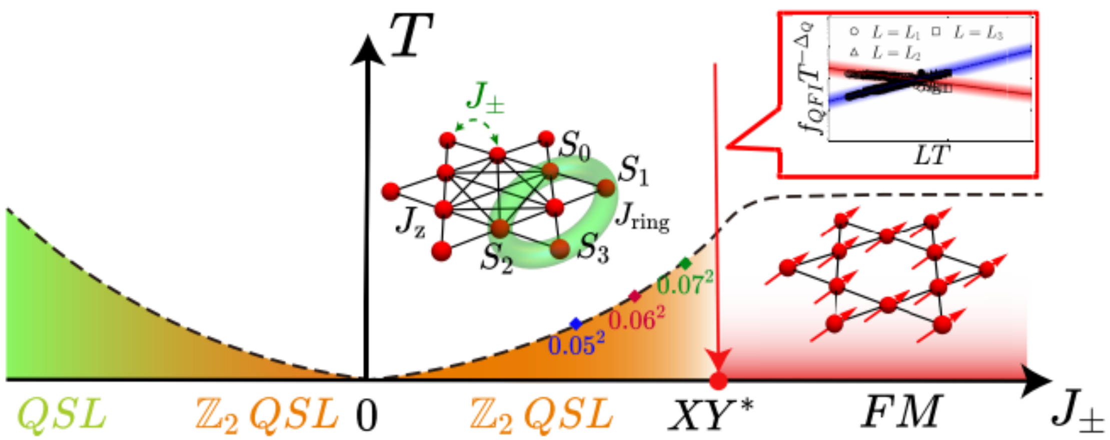

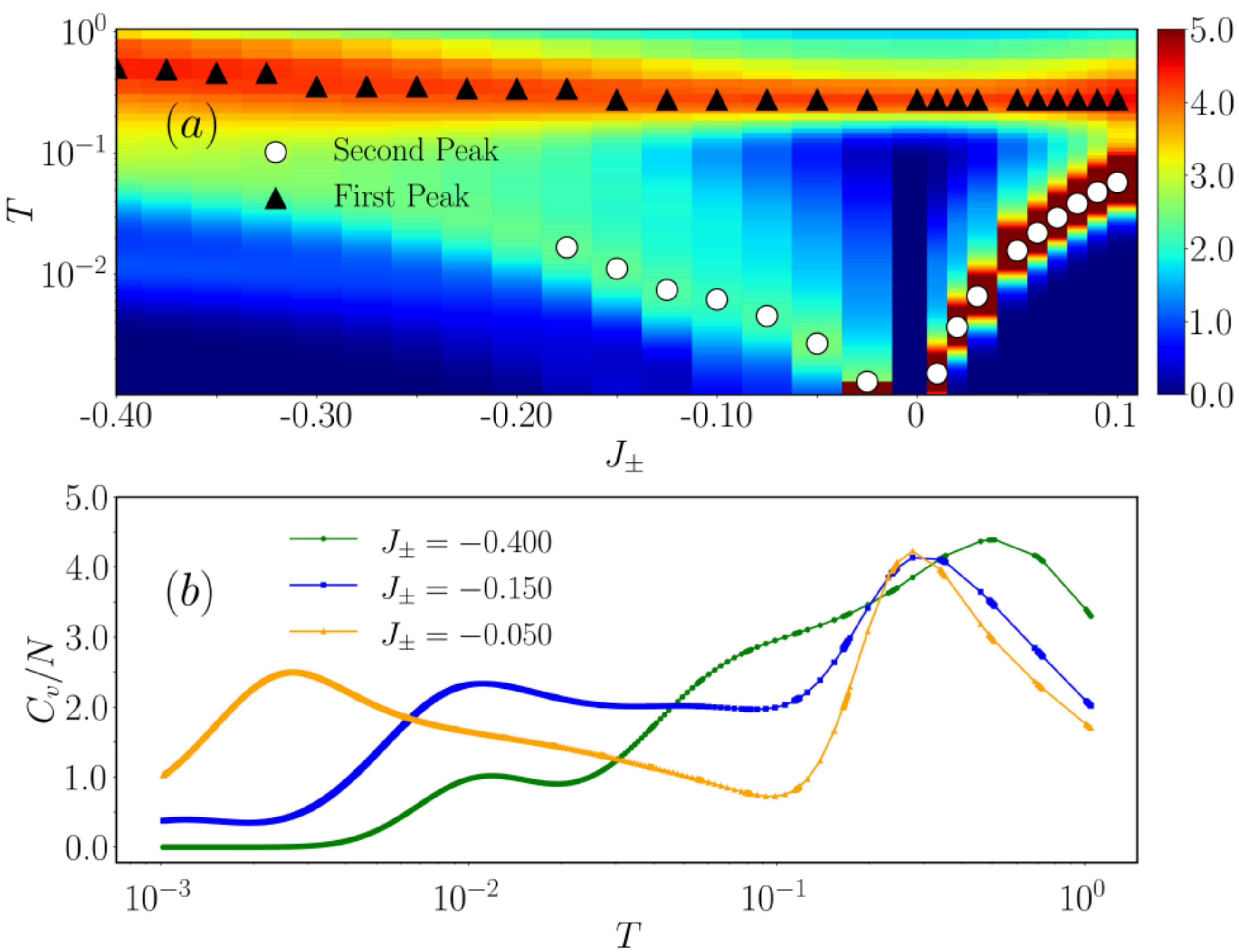

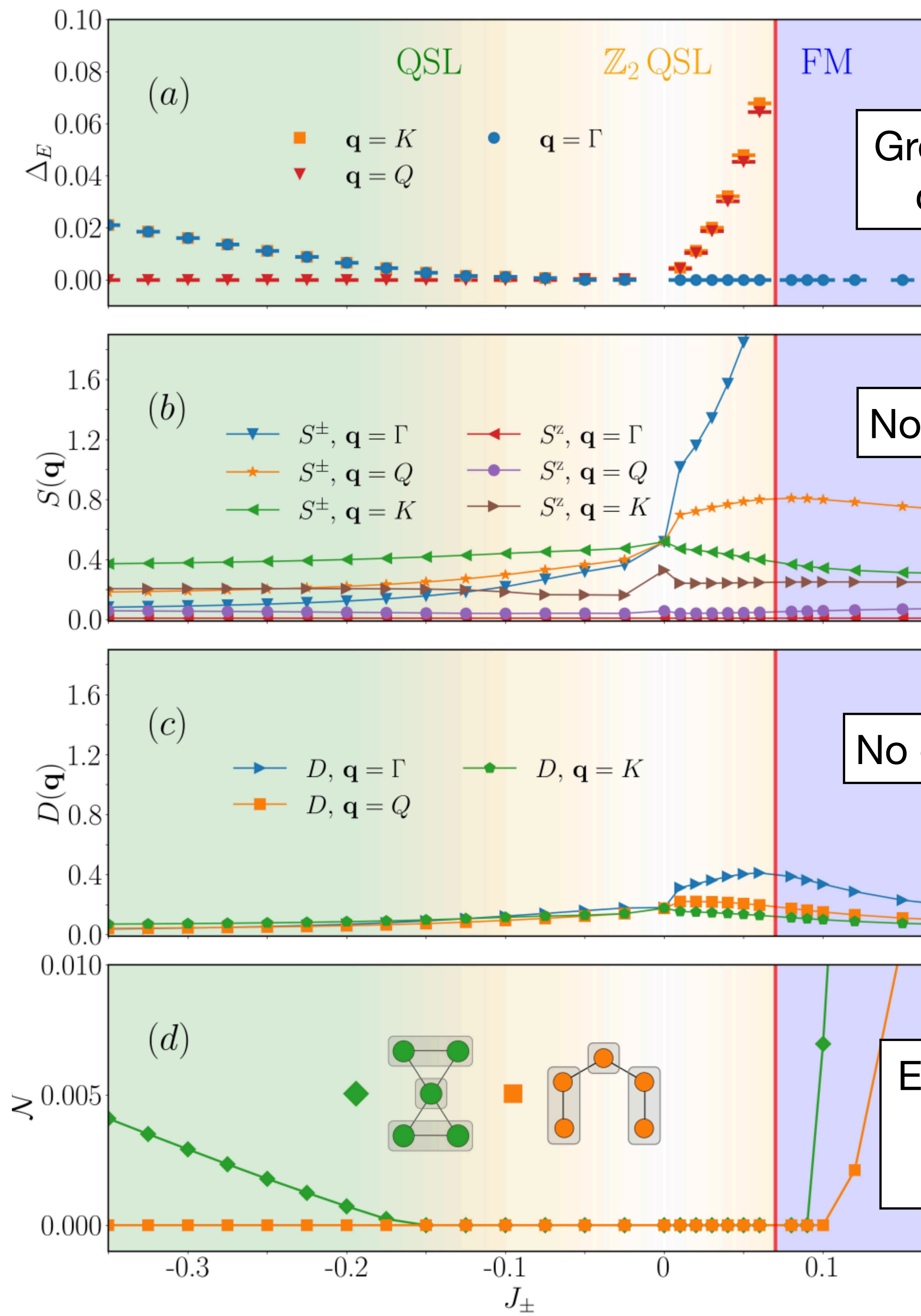

Ground state changes

No spin order

No dimer order

Entanglement Structure changes

Content

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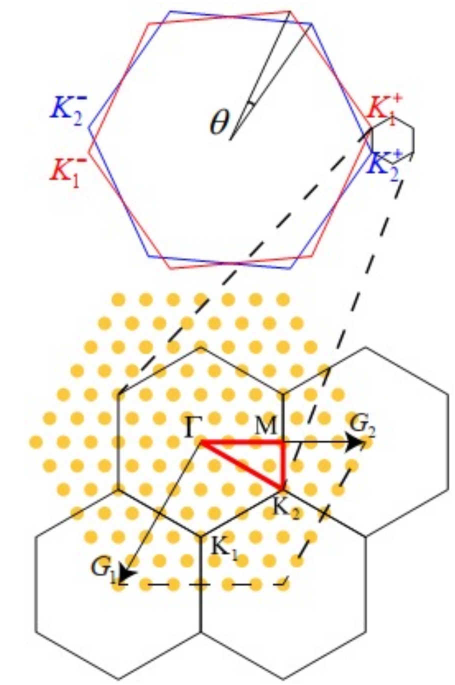

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