Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Quantum Monte Carlo: Discussion

Zi Yang Meng and Fakher F. Assaad Exotic quantum matter from quantum spin liquids to novel field theories, Pollica 26 June 2024

Outline

Quantum Monte Carlo

Applications

Dynamical properties of quantum magnets

Z_2 and U(1) spin liquids

Kitaev materials

Heavy fermions

……

Quantum Monte Carlo

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \sum_C W(C)$$

C Configuration space : Set of Feynman Diagrams (CT-INT)

World lines (SSE, Loop)

Auxiliary fields (Determinant Monte Carlo)

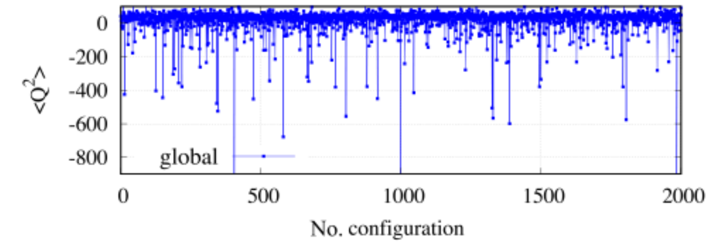
....

W(C) *Weight* of a configuration.

Conditions on the choice of configuration space: $W(C')/W(C)$ has to be computable in polynomial time.

Quantum Monte Carlo

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \sum_C W(C)$$



If:

1. $W(C) > 0$
2. Distribution has no fat tails
3. One can generate N independent configurations with probability $P(C) = \frac{W(C)}{\sum_C W(C)}$

Then:

$$\langle O \rangle_P = \sum_C P(C) O(C) \simeq \frac{1}{N} \sum_{i=1}^{N} O(C_i) = X$$

$$\mathcal{P}(X) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} \exp\left[-\frac{(X - \langle O \rangle_P)^2}{2\sigma^2} \right] \quad \text{with} \quad \sigma^2 = \frac{1}{N} \left(\langle O^2 \rangle_P - \langle O \rangle_P^2 \right).$$

Quantum Monte Carlo: Sign problem

$$\langle O \rangle = \frac{\sum_C W(C) O(C)}{\sum_C W(C)} = \frac{\frac{\sum_C |W(C)| \frac{W(C)}{|W(C)|} O(C)}{\sum_C |W(C)|}}{\frac{\sum_C W(C)}{\sum_C |W(C)|}}$$

$$\frac{W(C)}{|W(C)|} = \mathrm{sign(C)} \qquad \langle \mathrm{sign} \rangle = \frac{\sum_C W(C)}{\sum_C |W(C)|} \propto e^{-\alpha \beta V} \qquad \frac{\Delta \langle \mathrm{sign} \rangle}{\langle \mathrm{sign} \rangle} \ll 1 \qquad \text{CPU time} \propto e^{2\alpha\beta V}$$

<u>Solution ?</u>

Change methods (DMRG and co → Frank's discussion)

Change formulation so as to minimize α (Polynomial sign problem in flat bands)

Confront the sign problem (Lefschetz thimbles and Complex Langevin QCD)

Go approximative (Fixed node QMC in real or slater determinant space)

....

QMC examples (successful & unsuccessful) in quantum magnets

Pride and Prejudice

ZI YANG MENG & FAKHER ASSAAD


QMC examples (successful & unsuccessful) in quantum magnets
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Model-Design and Numerical Simulations

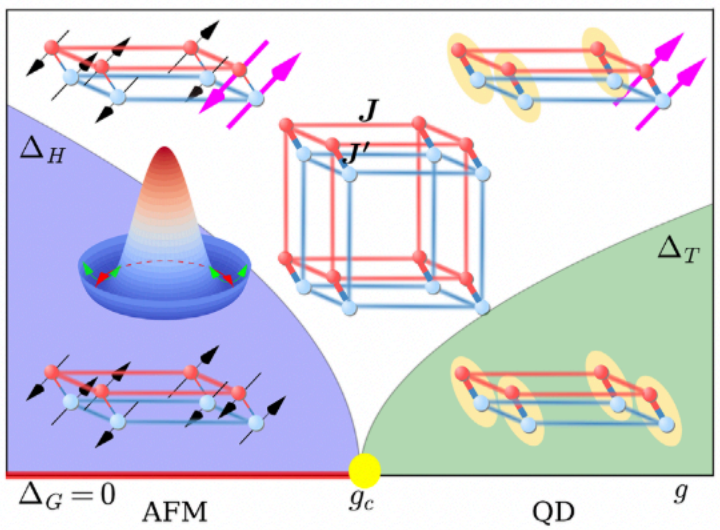
- Magnetic phase transitions and Dynamical properties (amplitude mode)
- Kagome models and Z2 quantum spin liquid (BFG)
- Pyrochlore models and U1 quantum spin liquid (Quantum Spin ice)
- Dirac fermion/spinon coupled with U1 gauge field
- YCu3-Br/Cl and SCBO
- Polynomial Sign problem
- ……

Magnetic phase transitions and amplitude mode

PRL **118,** 147207 (2017) PHYSICAL REVIEW LETTERS

Amplitude Mode in Three-Dimensional Dimerized Antiferromagnets

Yan Qi Qin,[1] B. Normand,[2] Anders W. Sandvik,[3] and Zi Yang Meng[1]



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

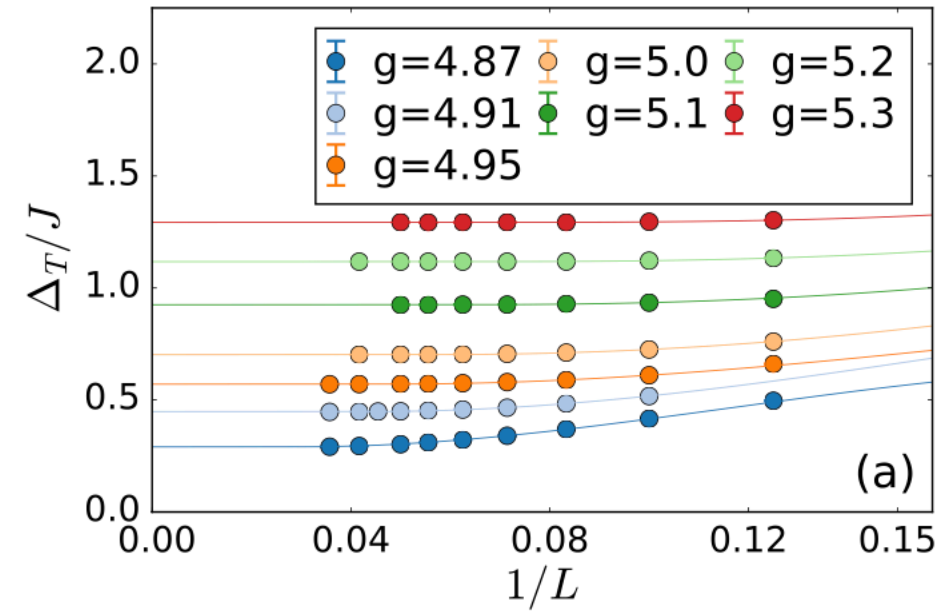
$$S^z_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}}(S^{1z}_r - S^{2z}_r)$$

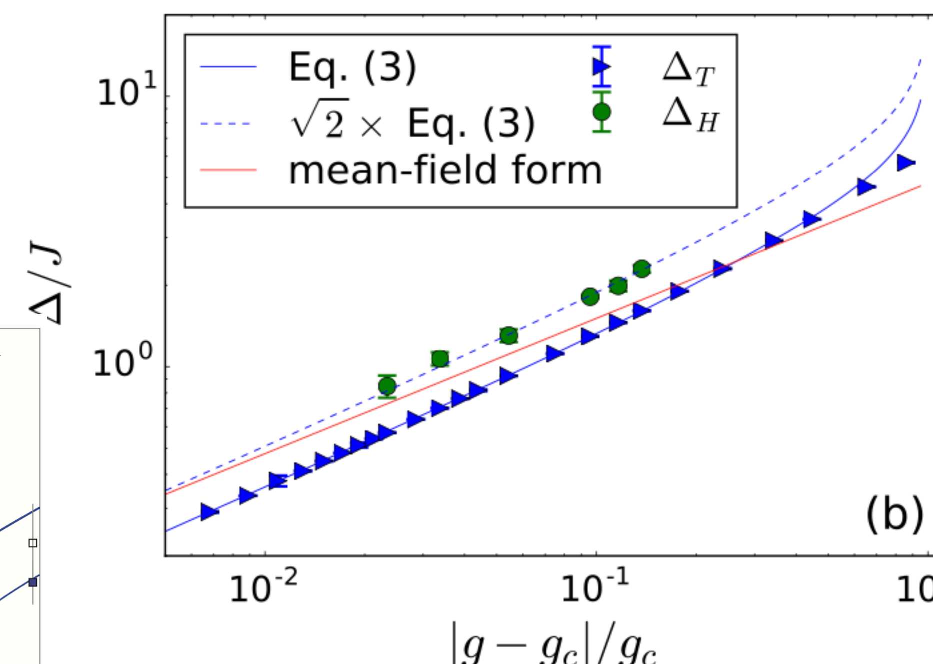
Log-corrections

$$\Delta_T \sim (|g-g_c|/g_c)^{\nu} \ln^{-\hat{\nu}}(|g-g_c|/g_c),$$

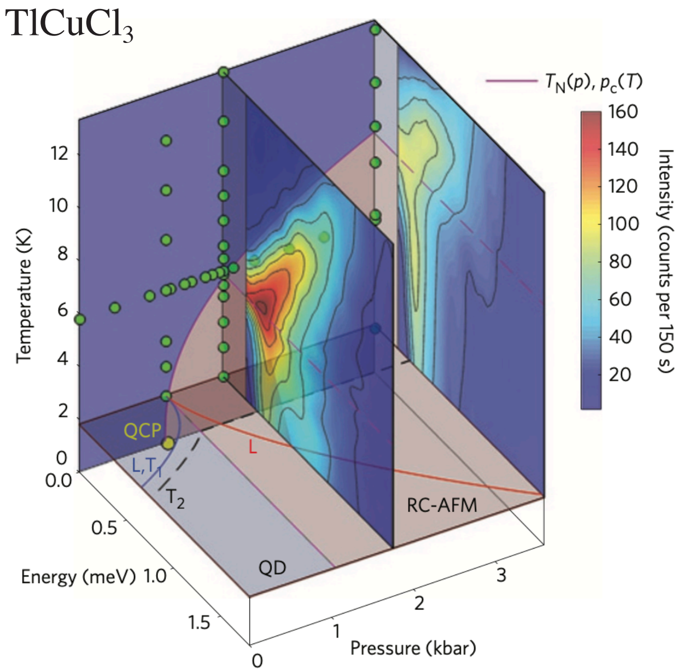
$$\nu = \frac{1}{2} \quad \hat{\nu} = \frac{N+2}{2(N+8)} = \frac{5}{22}\Big|_{N=3}$$

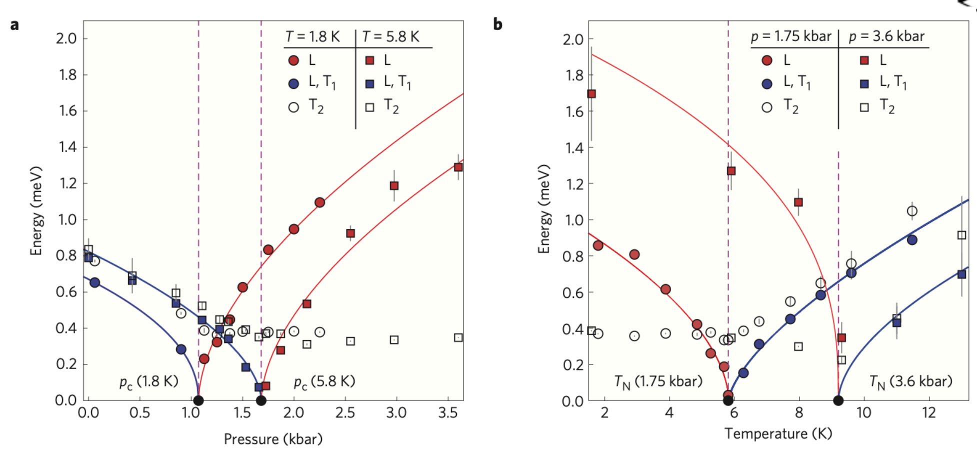
$g_c \approx 4.837$





TlCuCl$_3$





P. Merchant, B. Normand, K. W. Kramer, M. Boehm, D. F. McMorrow, and C. Ruegg, Nat. Phys. 10, 373 (2014).

Magnetic phase transitions and amplitude mode

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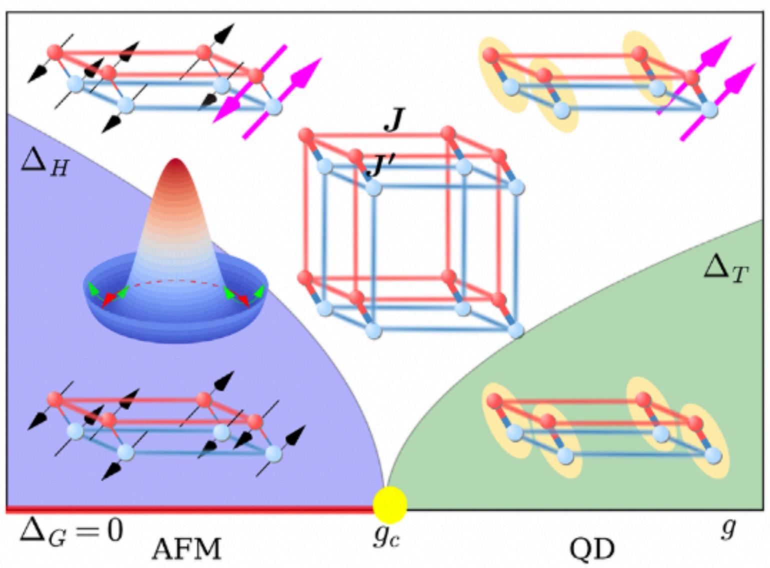

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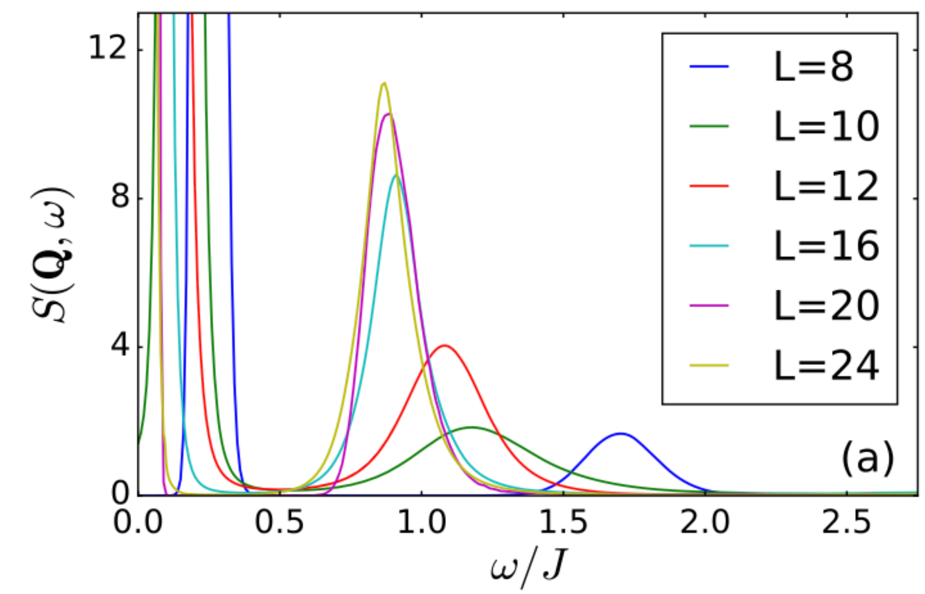
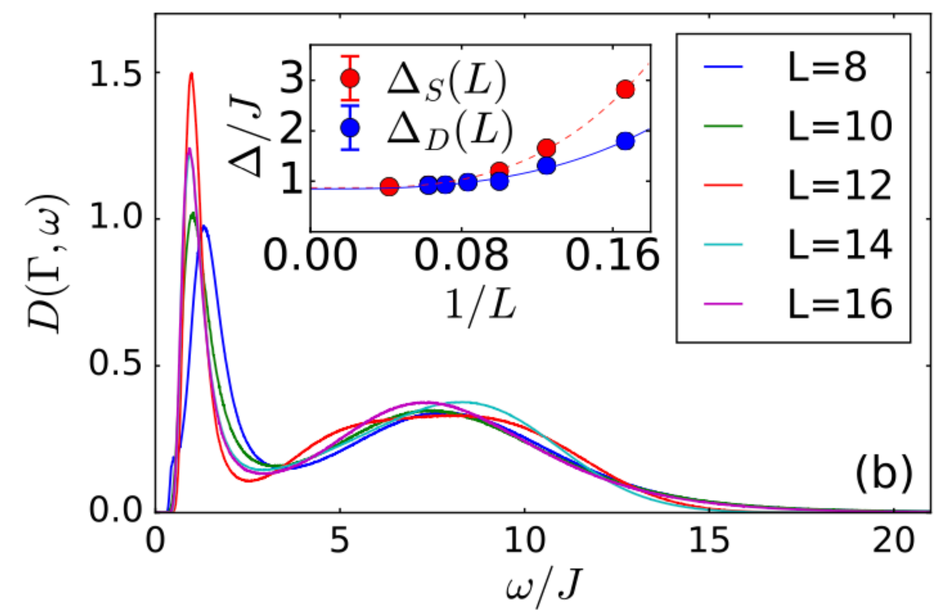
$$S^z_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}} (S^{1z}_r - S^{2z}_r)$$

$$D(\Gamma,\tau) = \langle B_\Gamma(\tau) B_\Gamma(0)\rangle,$$

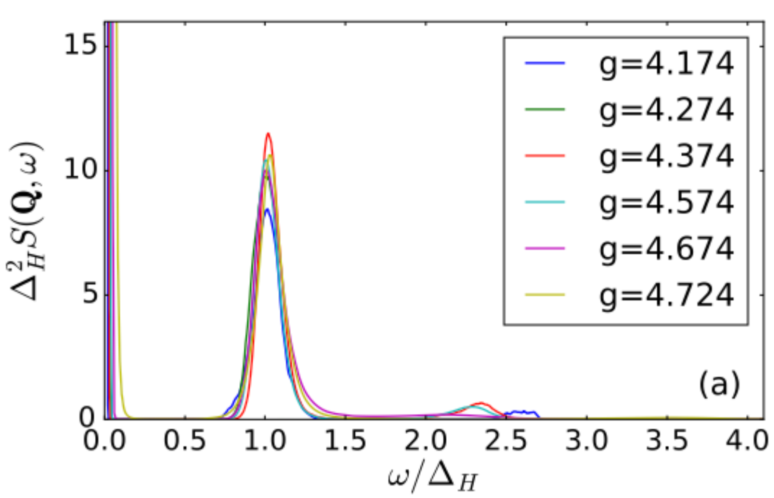
$$B_\Gamma = \frac{1}{\sqrt{N}} \sum_r B_r, \quad B_r = \mathbf{S}^1_r \cdot \mathbf{S}^2_r - \langle \mathbf{S}^1_r \cdot \mathbf{S}^2_r \rangle$$

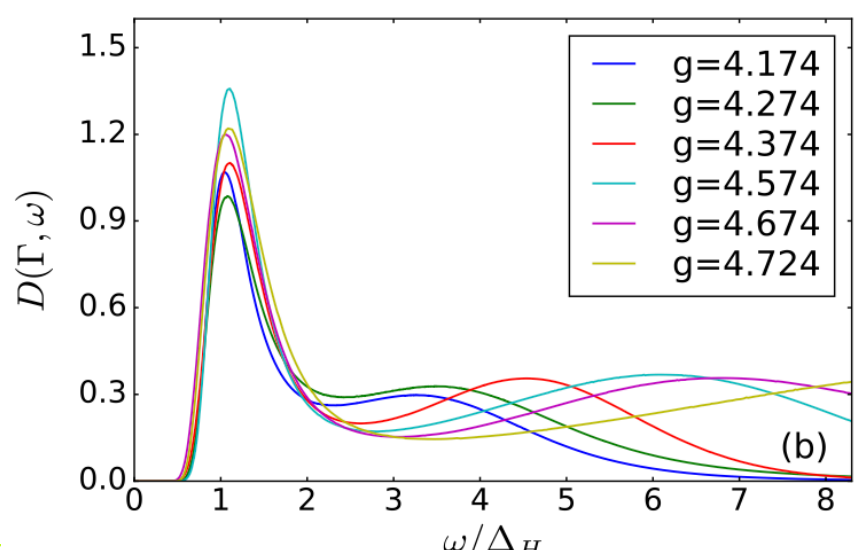
$g \approx g_c - 0.1$





Scaling of the scalar susceptibility $D(\Gamma,\omega) \sim \Delta_H^{d+z-2/\nu} \Phi(\omega/\Delta_H),$





- D. Podolsky and S. Sachdev, Phys. Rev. B 86, 054508 (2012).
- S. Gazit, D. Podolsky, and A. Auerbach, Phys. Rev. Lett. 110, 140401 (2013).
- M. Lohöfer and S. Wessel, Phys. Rev. Lett. 118, 147206 (2017).

Spectra in dimension crossover

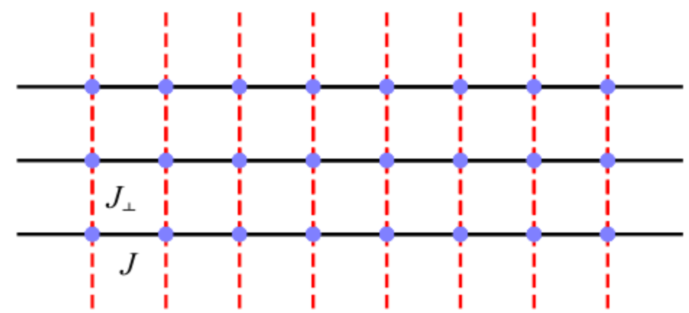
PHYSICAL REVIEW LETTERS **126**, 227201 (2021)

Amplitude Mode in Quantum Magnets via Dimensional Crossover

Chengkang Zhou,[1] Zheng Yan,[1,2] Han-Qing Wu,[3] Kai Sun,[4,*] Oleg A. Starykh,[5,†] and Zi Yang Meng[1,‡]

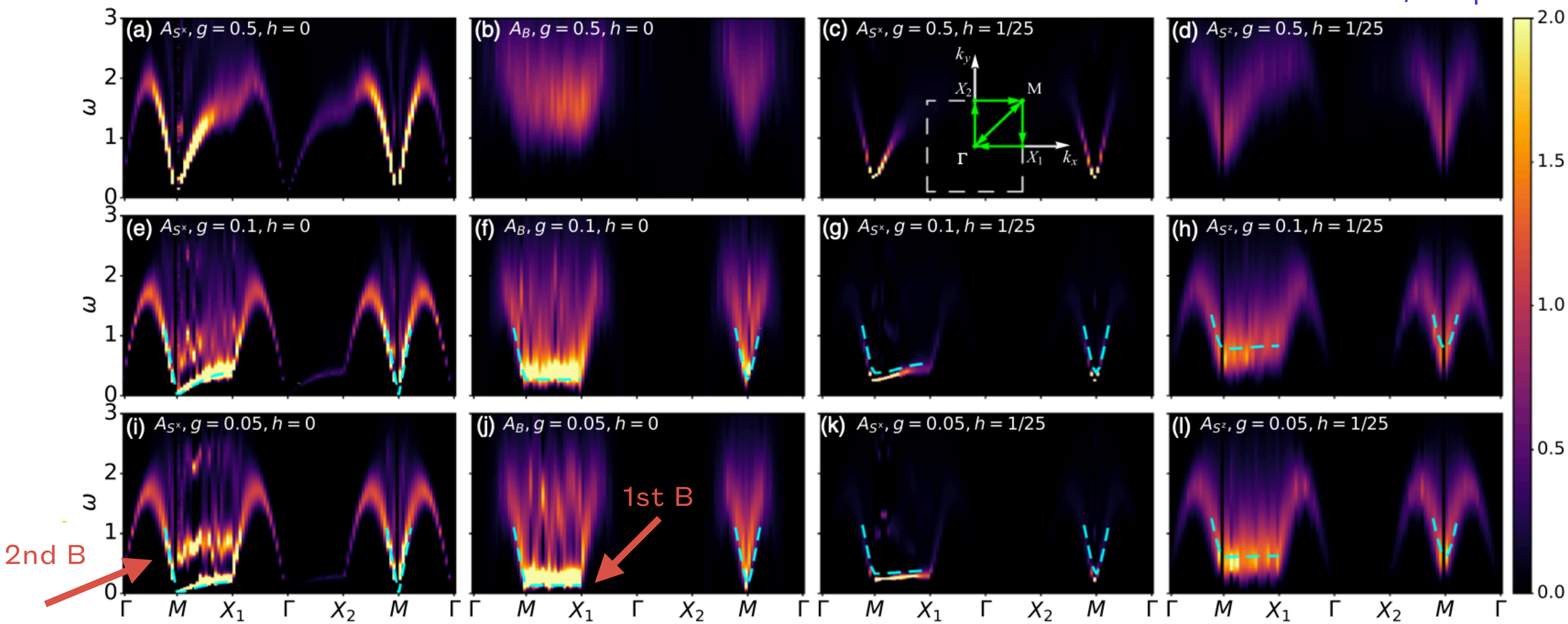
$$H = J\sum_{\langle i,j\rangle_x} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\langle i,j\rangle_y} \mathbf{S}_i \cdot \mathbf{S}_j - h\sum_i (-1)^i S_i^z,$$

QMC+ chain-mean-field of sine-Gorden



$g = J_\perp / J$

Phase | First breather | Phase | Second breather / Amplitude



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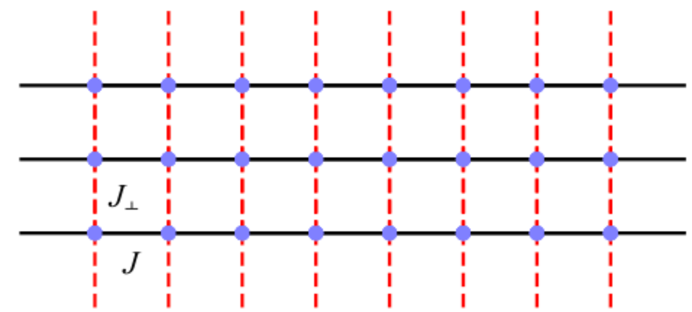


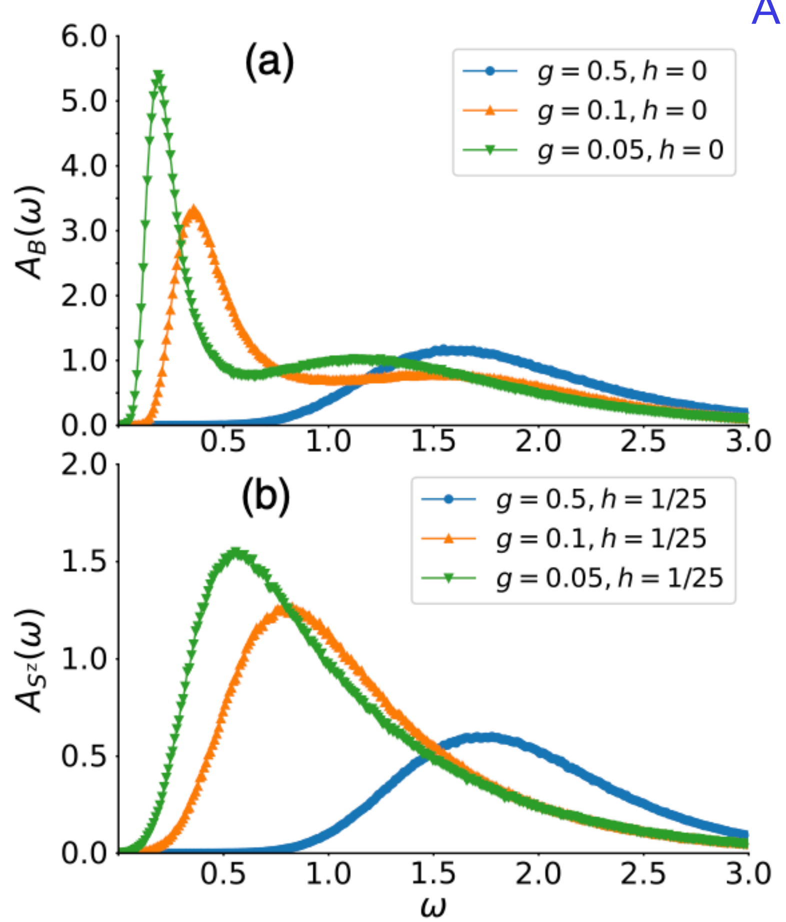
close to $k_x = \pi$

$$\omega_{S^x} = \omega_{S^y} = \Delta_0\sqrt{1 + b_h + \cos k_y + \frac{v^2(k_x-\pi)^2}{\Delta_0^2}}$$

$$\omega_{S^z} = \Delta_0\sqrt{3(1+b_h) + \frac{Z_2}{Z_1}\cos k_y + \frac{v^2(k_x-\pi)^2}{\Delta_0^2}}$$

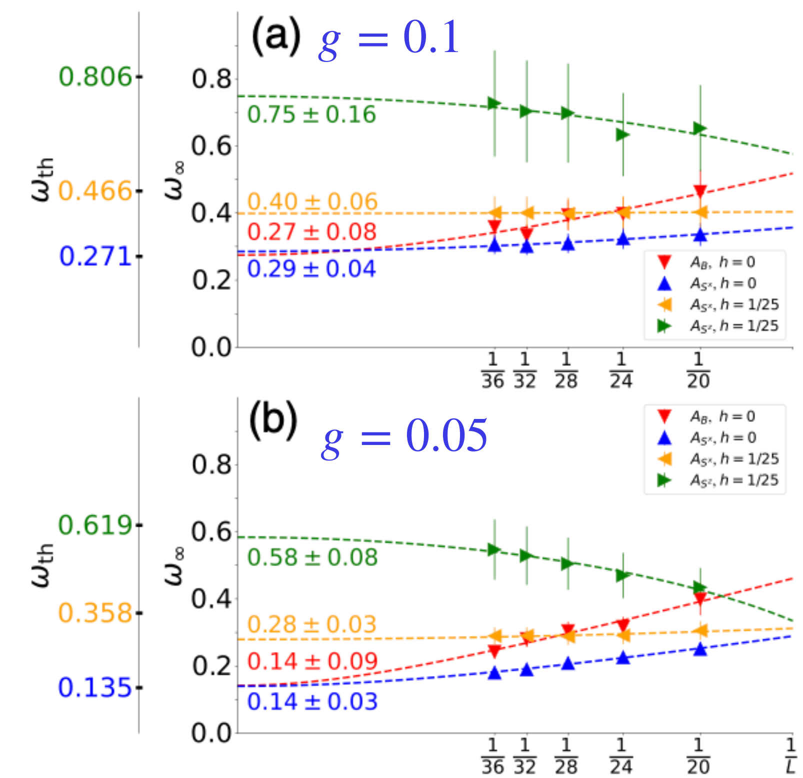
$$\omega_B = \Delta_0\sqrt{1 + b_h + \frac{v^2(k_x-\pi)^2}{\Delta_0^2}}.$$

$(\pi, \pi/2)$



Bond mode, first breather, Δ_0

Amplitude mode, second breather, $\sqrt{3}\Delta_0$



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- ……

Kagome quantum spin liquid

PHYSICAL REVIEW B, VOLUME 65, 224412 (2002)

Fractionalization in an easy-axis Kagome antiferromagnet

L. Balents,[1] M. P. A. Fisher,[2] and S. M. Girvin[2,3]

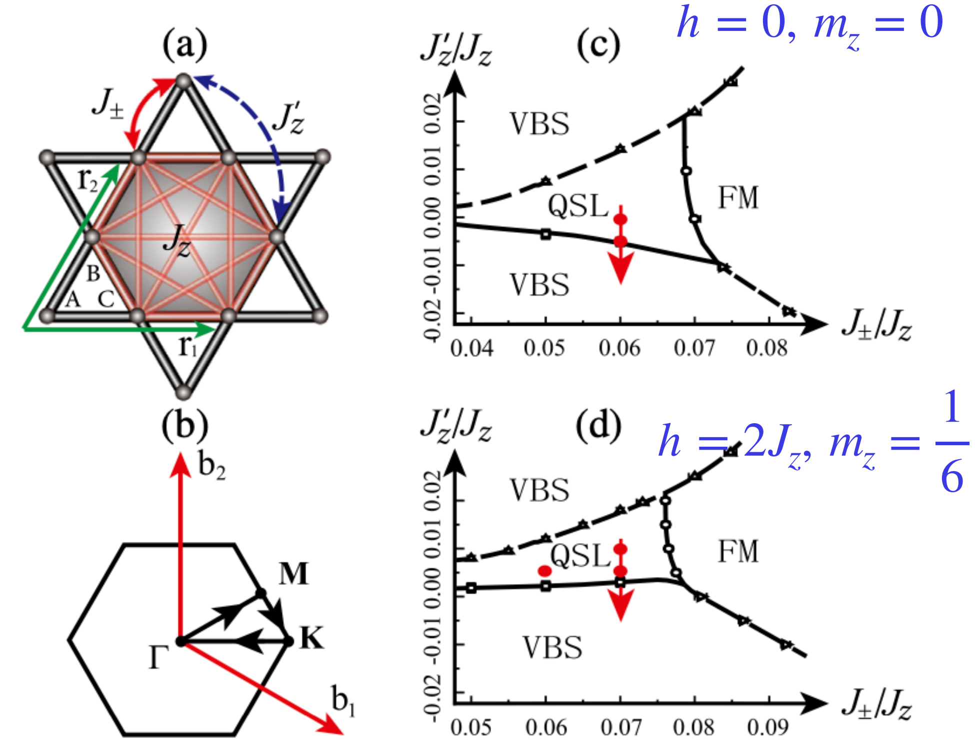
PHYSICAL REVIEW LETTERS **121**, 077201 (2018)

Dynamical Signature of Symmetry Fractionalization in Frustrated Magnets

Guang-Yu Sun,[1,2] Yan-Cheng Wang,[3] Chen Fang,[1,4] Yang Qi,[5,6,7] Meng Cheng,[8] and Zi Yang Meng[1,4]

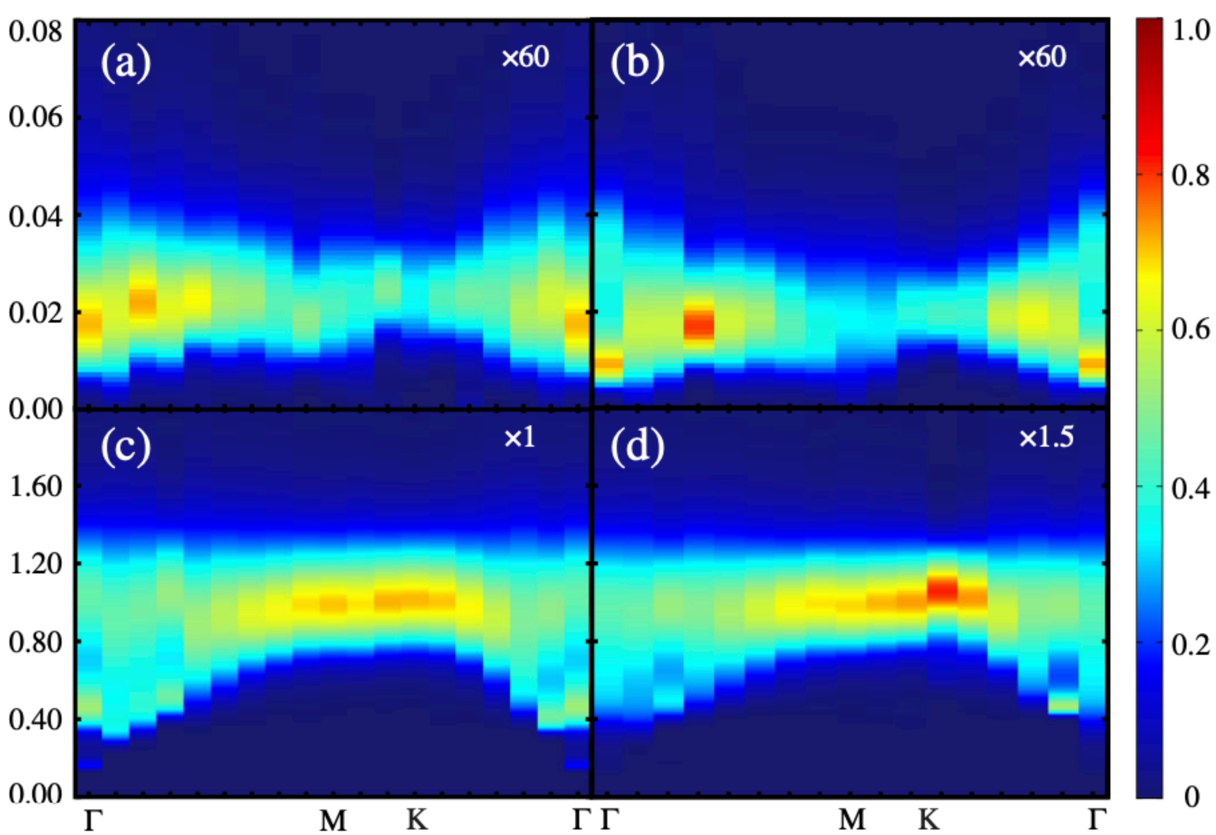
$$H = -J_{\pm}\sum_{\langle i,j\rangle}(S_i^+S_j^- + \mathrm{H.c.}) + \frac{J_z}{2}\sum_{\hexagon}\Big(\sum_{i\in\hexagon}S_i^z\Big)^2 + J_z'\sum_{\langle i,j\rangle'}S_i^zS_j^z - h\sum_i S_i^z,$$

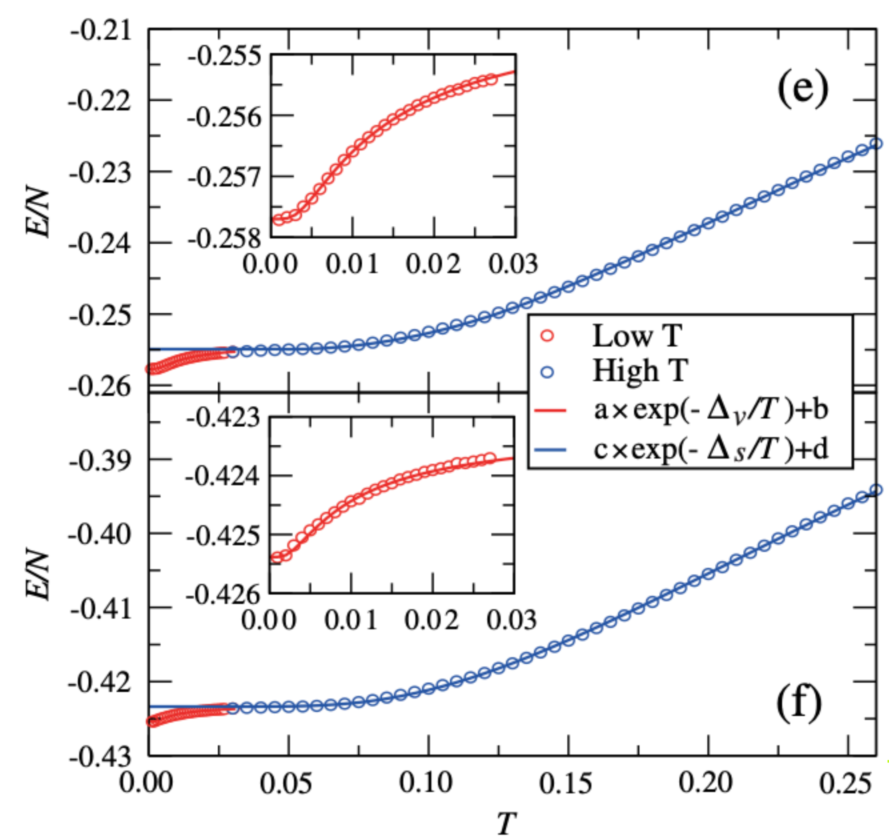
$$S^{\pm}_{\alpha\beta}(\mathbf{q},\tau) = \langle S^+_{-\mathbf{q},\alpha}(\tau)S^-_{\mathbf{q},\beta}(0)\rangle, \quad S^{zz}_{\alpha\beta}(\mathbf{q},\tau) = \langle S^z_{-\mathbf{q},\alpha}(\tau)S^z_{\mathbf{q},\beta}(0)\rangle.$$



$h = 0,\ m_z = 0$

$h = 2J_z,\ m_z = \frac{1}{6}$





$\Delta_s \sim 0.4$

$\Delta_v \sim 0.01$

- S. V. Isakov, R. G. Melko, and M. B. Hastings, Science 335, 193 (2012).
- J. Becker and S. Wessel, Phys. Rev. Lett. 121, 077202 (2018).

Kagome quantum spin liquid

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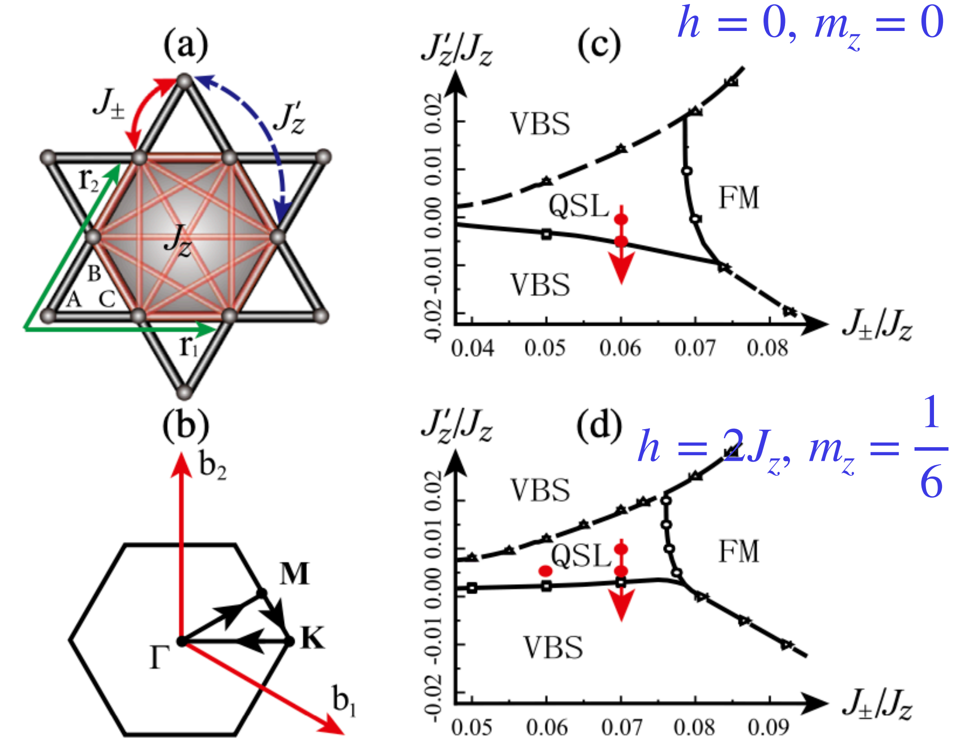

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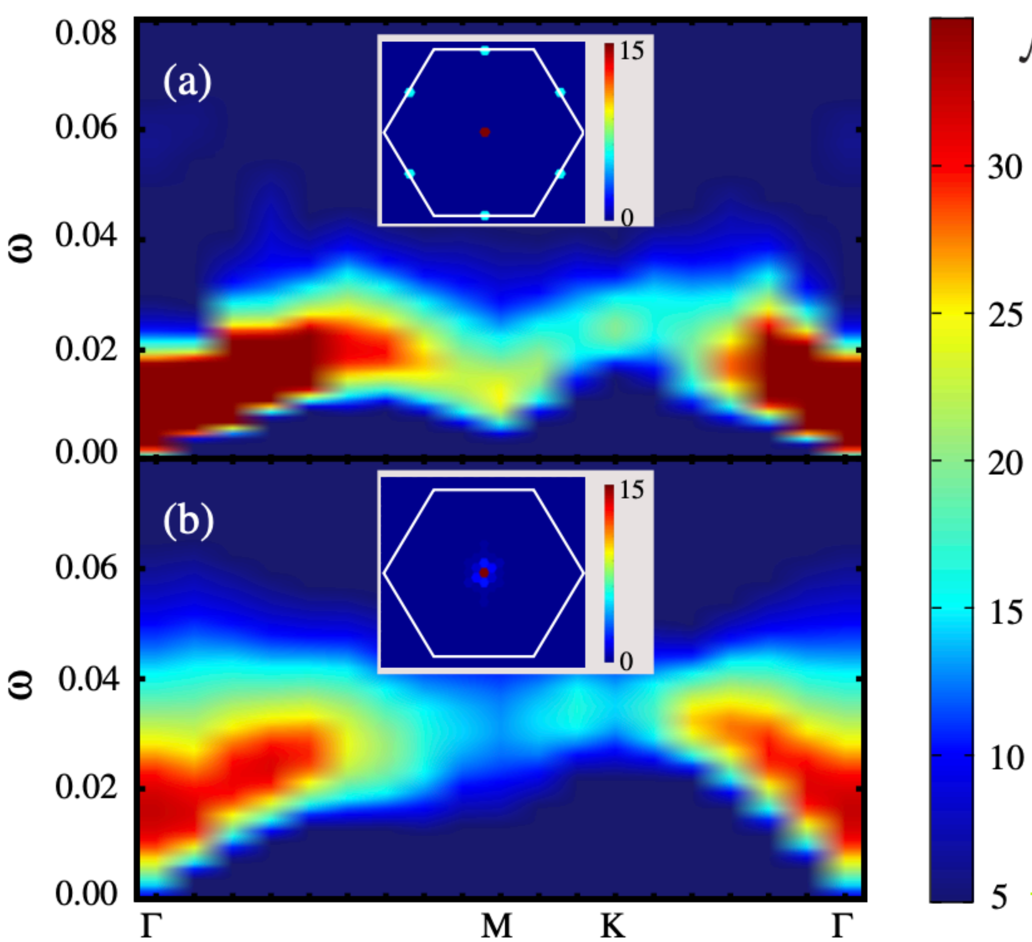
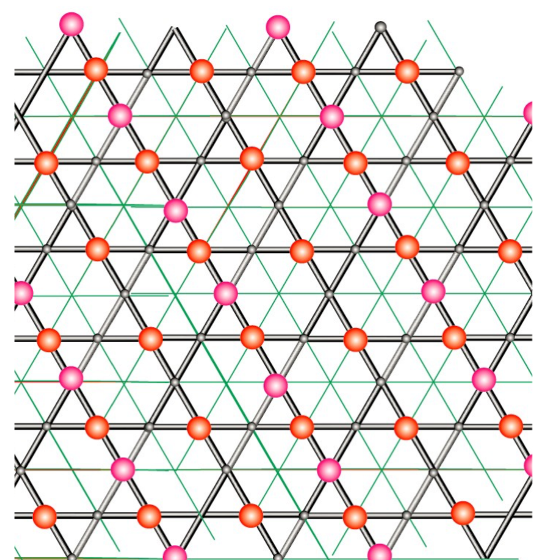
Translation symmetry fractionalisation $\quad T_1^{(a)}T_2^{(a)} = -T_2^{(a)}T_1^{(a)},$



$$\mathcal{N}(\mathbf{q},\omega) = \mathcal{N}(\mathbf{q}+\mathbf{K},\omega),\ 2\mathbf{K} = \mathbf{G}$$



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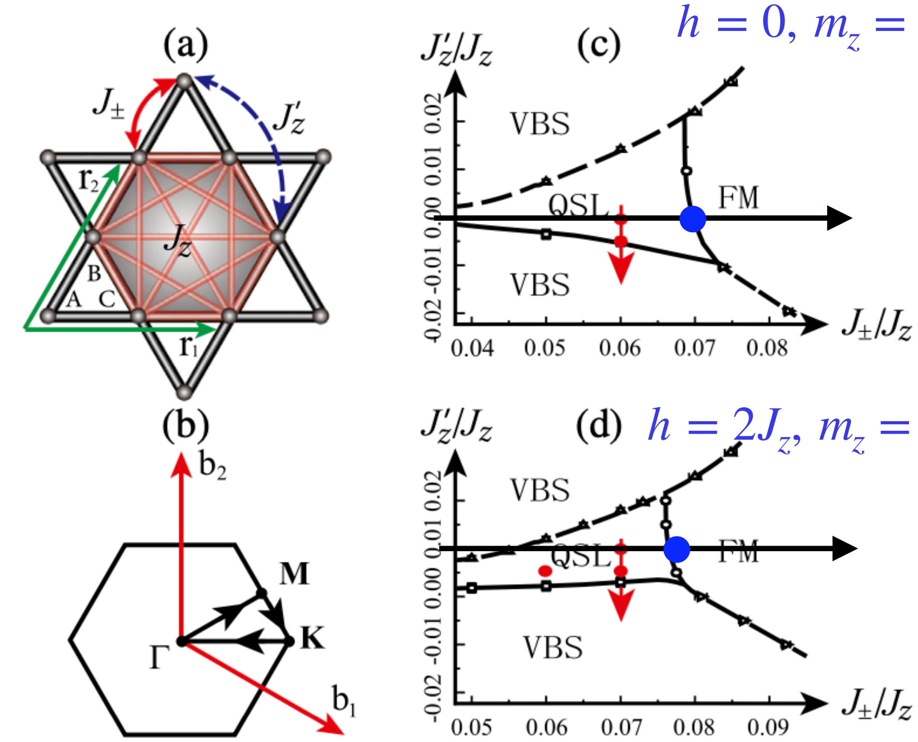

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Translation symmetry fractionalisation

$$T_1^{(a)}T_2^{(a)} = -T_2^{(a)}T_1^{(a)},$$

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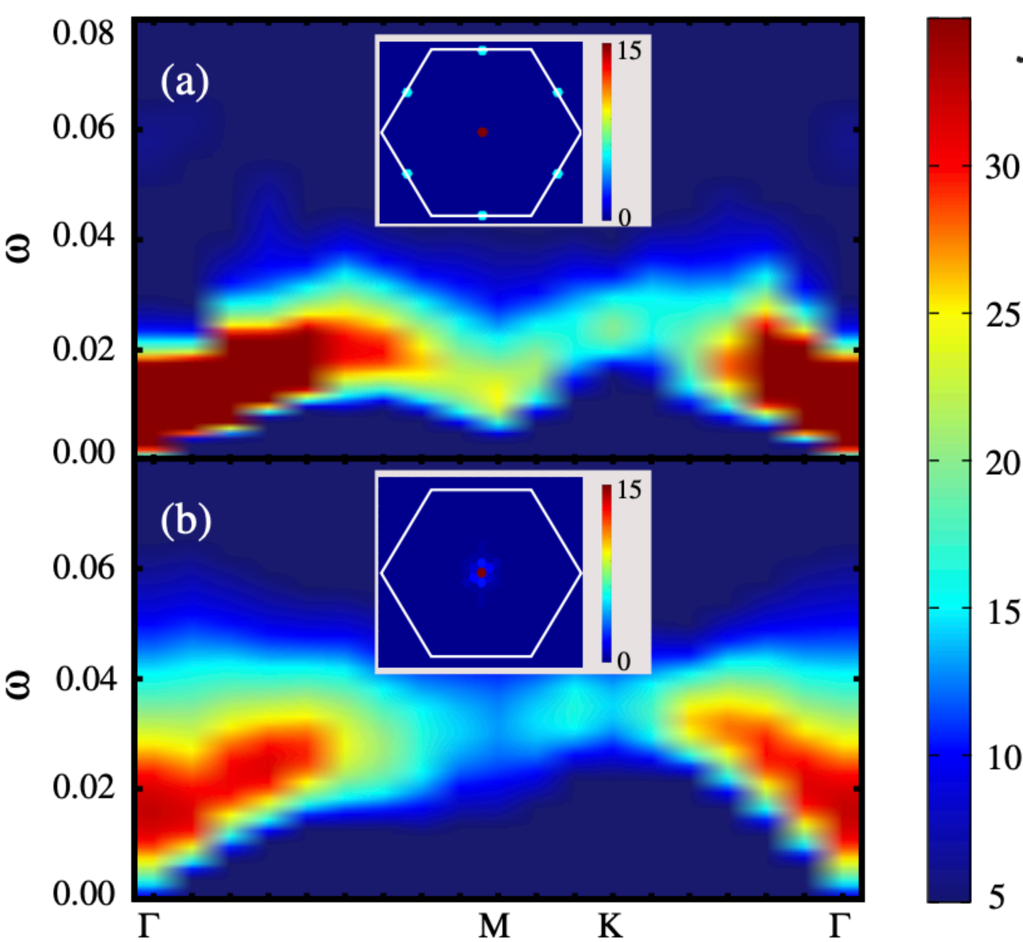

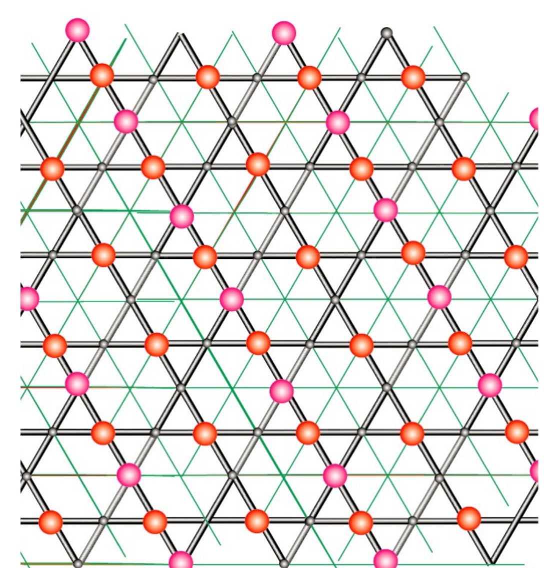

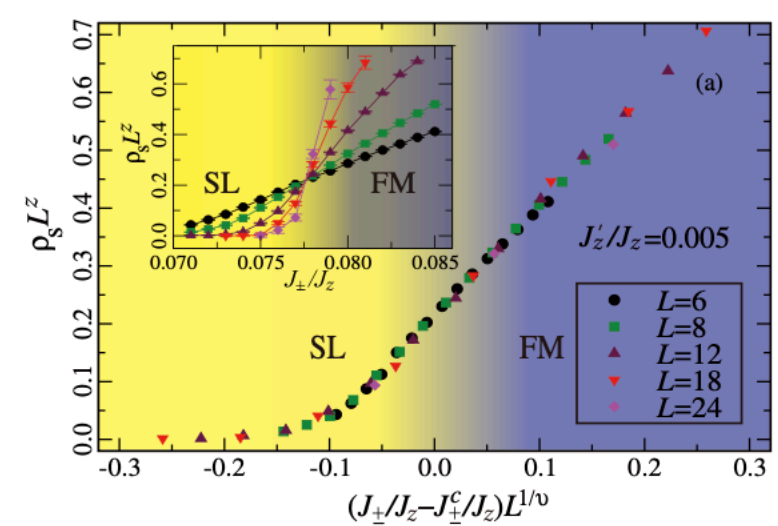

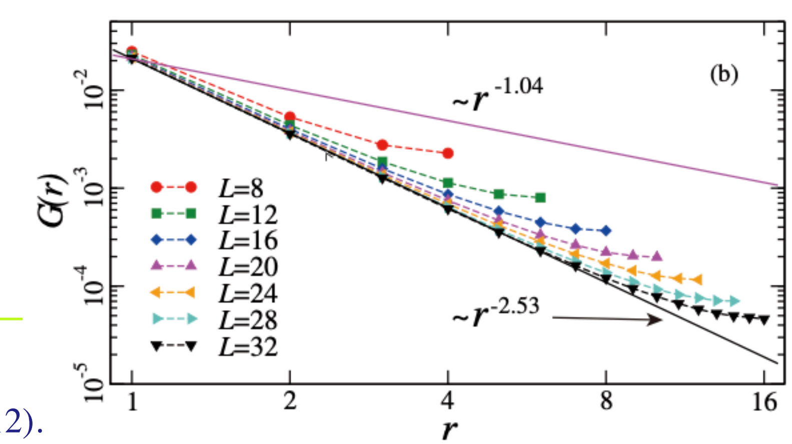

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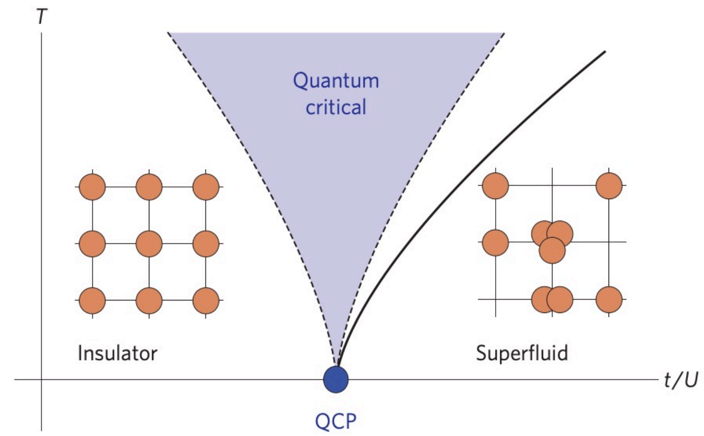
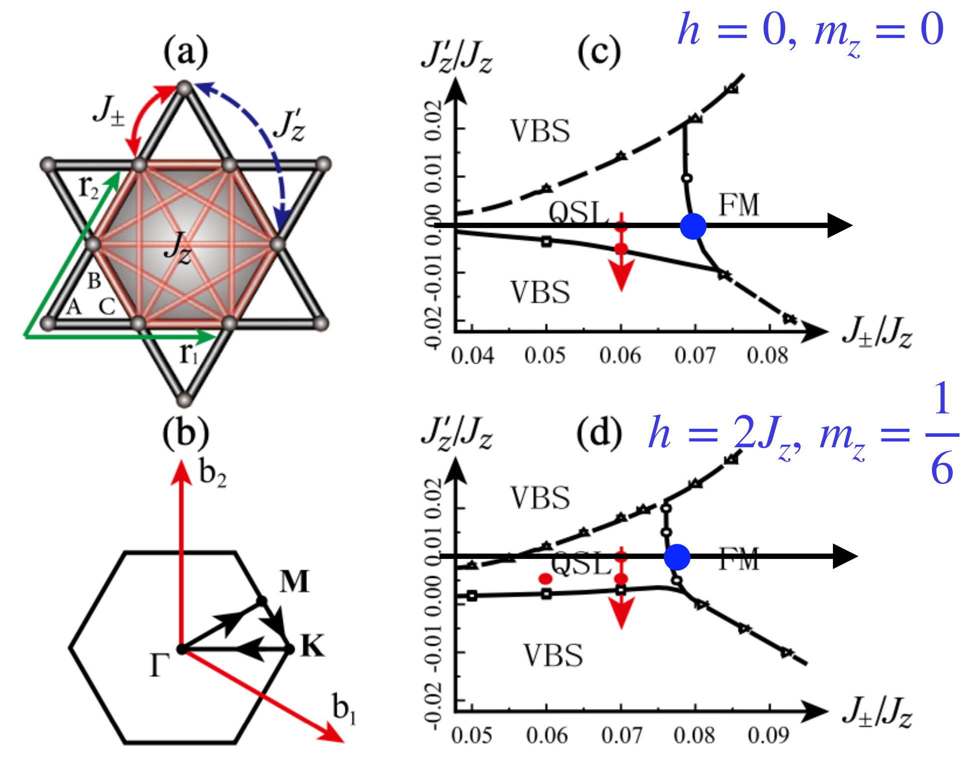
Kagome quantum spin liquid

nature physics
ARTICLES
PUBLISHED ONLINE: 23 MARCH 2014 | DOI: 10.1038/NPHYS2913

The dynamics of quantum criticality revealed by quantum Monte Carlo and holography

William Witczak-Krempa[1]*, Erik S. Sørensen[2] and Subir Sachdev[3]

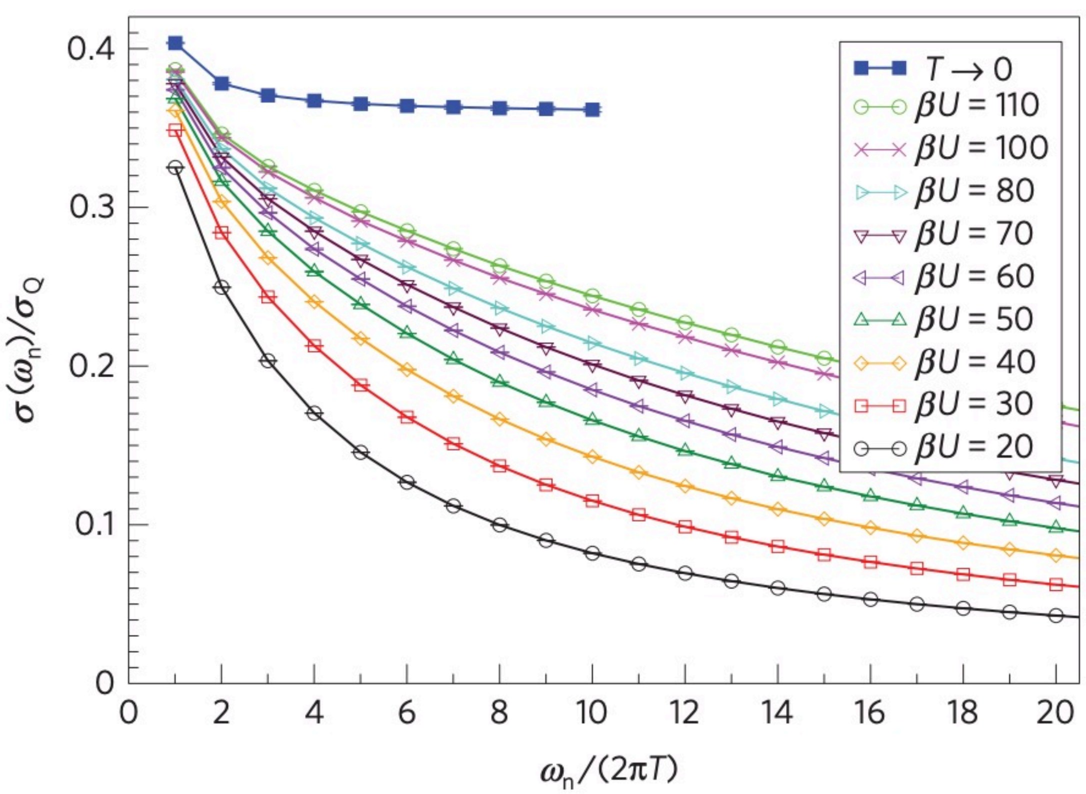




PHYSICAL REVIEW B **90**, 245109 (2014)

Conformal field theories at nonzero temperature: Operator product expansions, Monte Carlo, and holography

Emanuel Katz,[1] Subir Sachdev,[2,3] Erik S. Sørensen,[4] and William Witczak-Krempa[3]



$$\sigma(i\omega_n) = -\frac{i}{\omega_n}\langle J_x(\omega_n) J_x(-\omega_n)\rangle$$

$$\sigma(i\omega_n) = \sigma_\infty + b_1\left(\frac{T}{\omega_n}\right)^{3-\frac{1}{\nu}} + b_2\left(\frac{T}{\omega_n}\right)^3 + \cdots$$

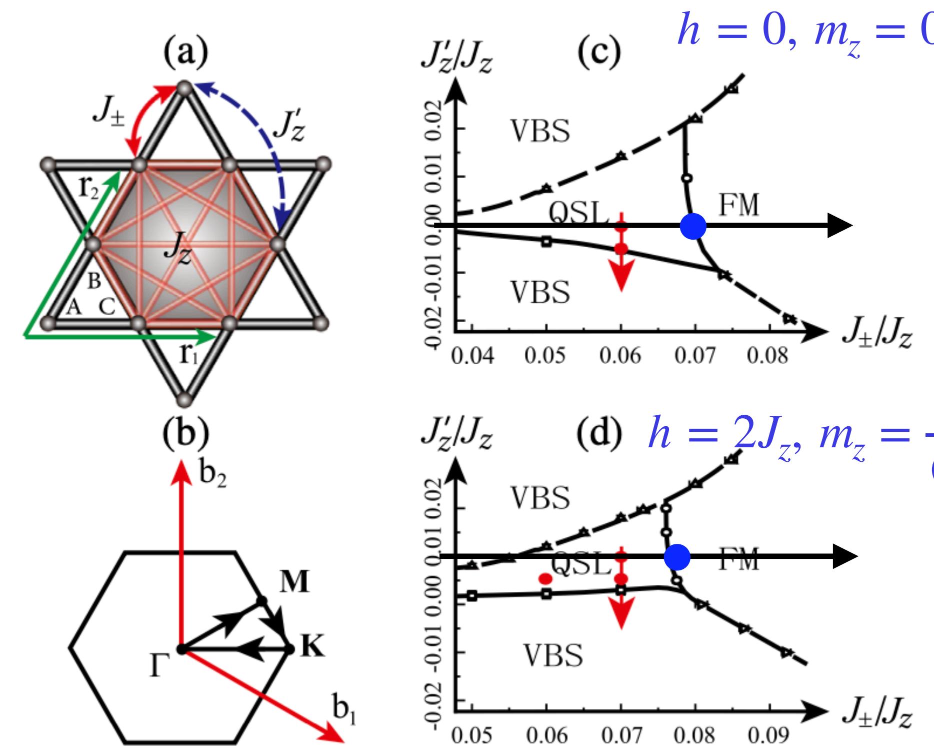
Low temperature limit: $\omega_n \gg T$ $\quad\quad \sigma_{XY}(\infty) \approx 0.36$

Kagome quantum spin liquid

nature COMMUNICATIONS

Fractionalized conductivity and emergent self-duality near topological phase transitions

Yan-Cheng Wang [1], Meng Cheng [2], William Witczak-Krempa [3,4] & Zi Yang Meng [5]



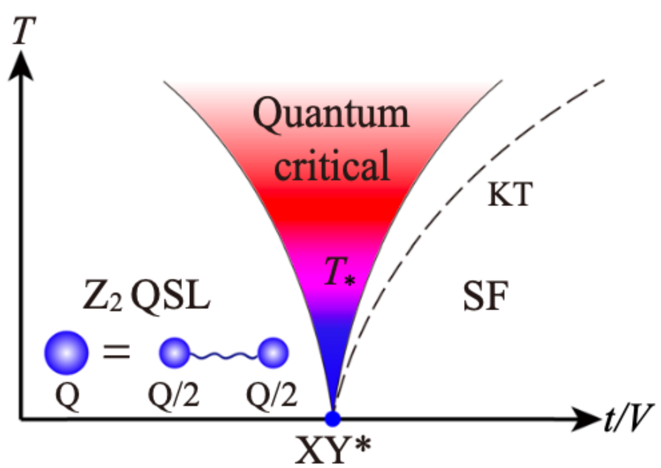
$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + \mathrm{h.c.}) + V \sum_{\hexagon} \Big(\sum_{i \in \hexagon} n_i \Big)^2 + V' \sum_{\langle i,j \rangle'} n_i n_j + \mu \sum_i n_i$$

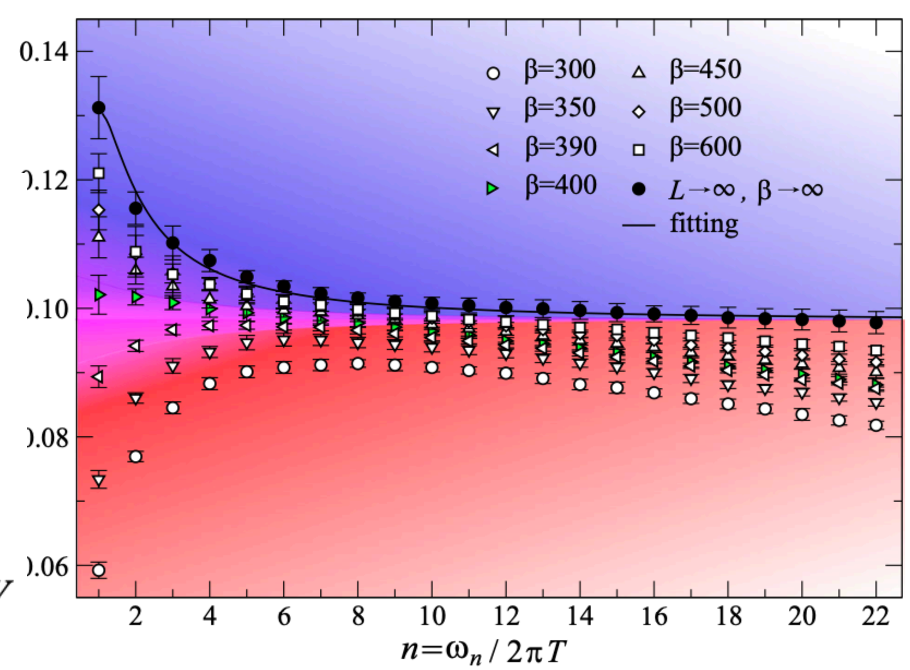
Particle-like conductivity

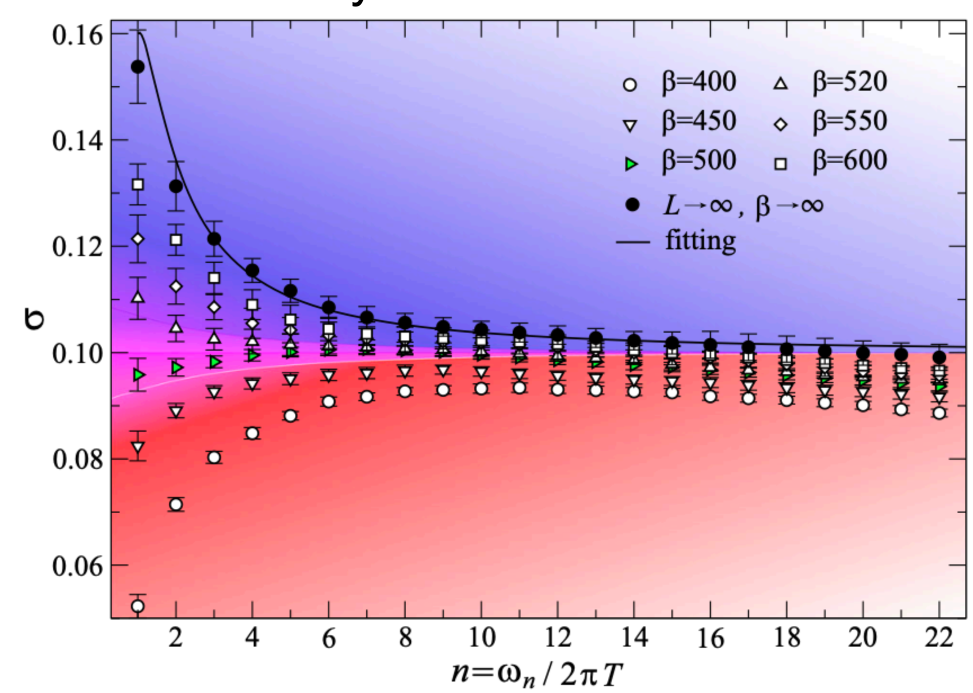
Vortex-like conductivity

Particle-Vortex duality at the scale of T*

$$\sigma_{XY^*}(\infty) = \frac{1}{4}\, \sigma_{XY}(\infty).$$







$$\sigma_{XY^*}(\infty) = 0.098(9)$$

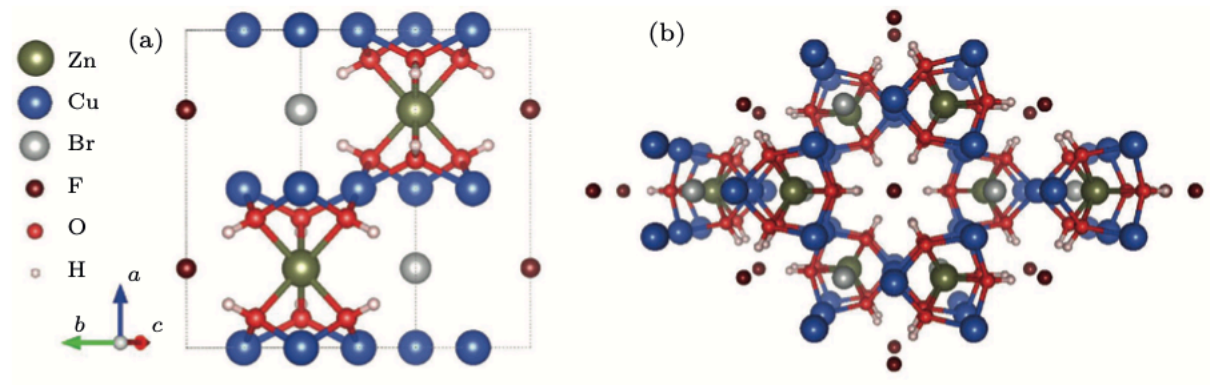
$$\sigma_{XY^*}(\infty) = 0.100(13)$$

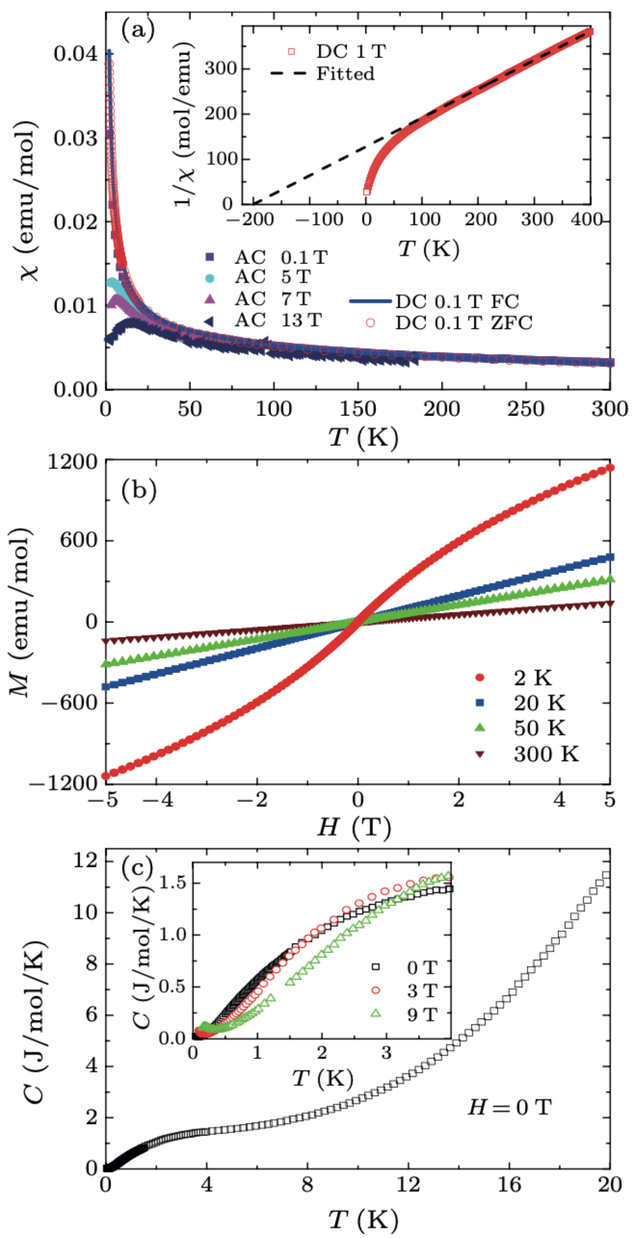
Kagome quantum spin liquid Cu3Zn(OH)6FBr

CHIN. PHYS. LETT. Vol. 34, No. 7 (2017) 077502 Express Letter

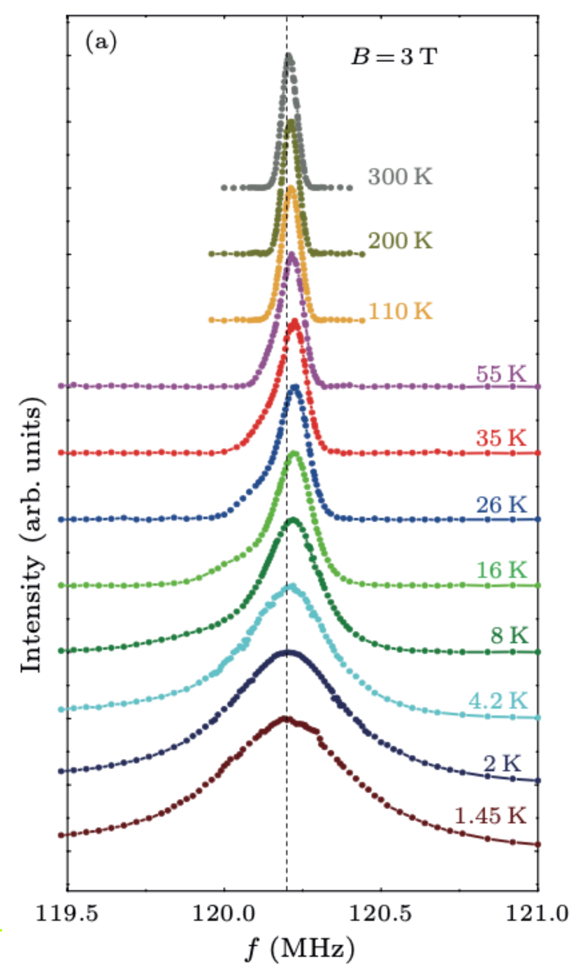
Gapped Spin-1/2 Spinon Excitations in a New Kagome Quantum Spin Liquid Compound $Cu_3Zn(OH)_6FBr$ *

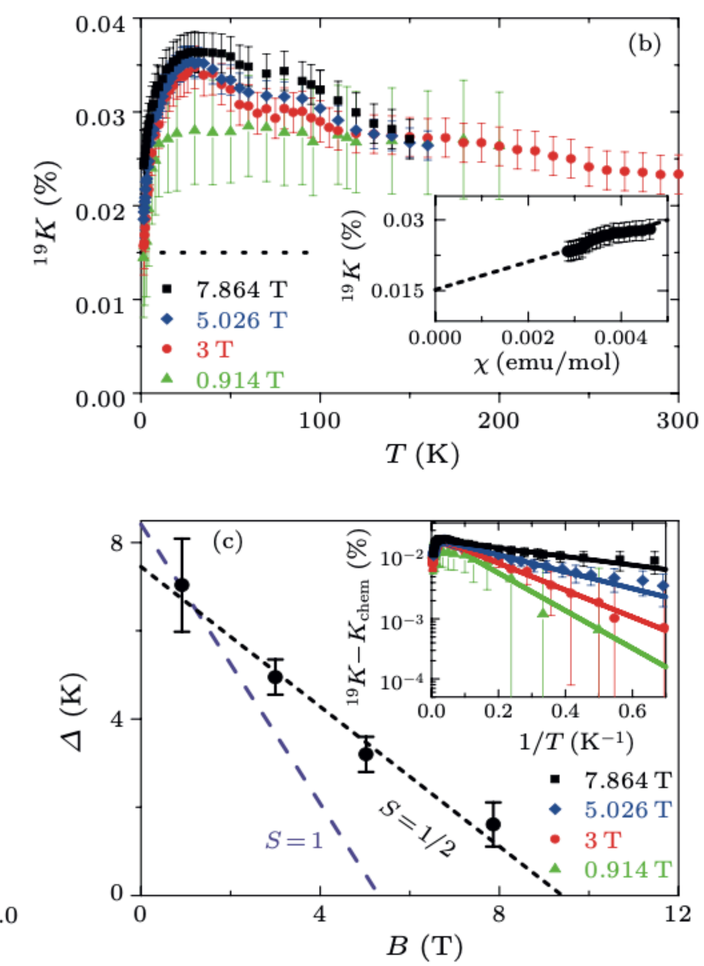
Youguo Shi, Shiliang Li, Guo-qing Zheng ... in IOP, CAS





F has nuclear spin I=1/2





PHYSICAL REVIEW B **105**, L121109 (2022)

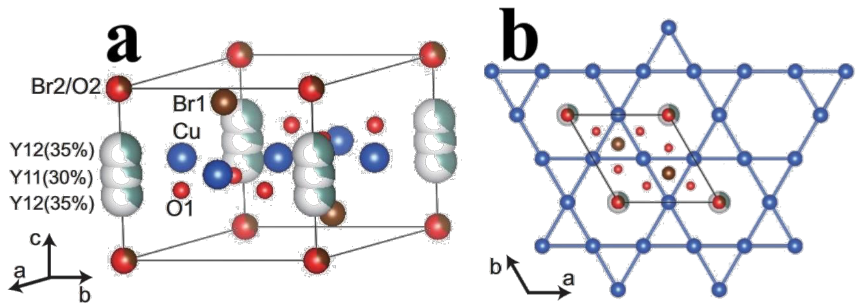
Letter

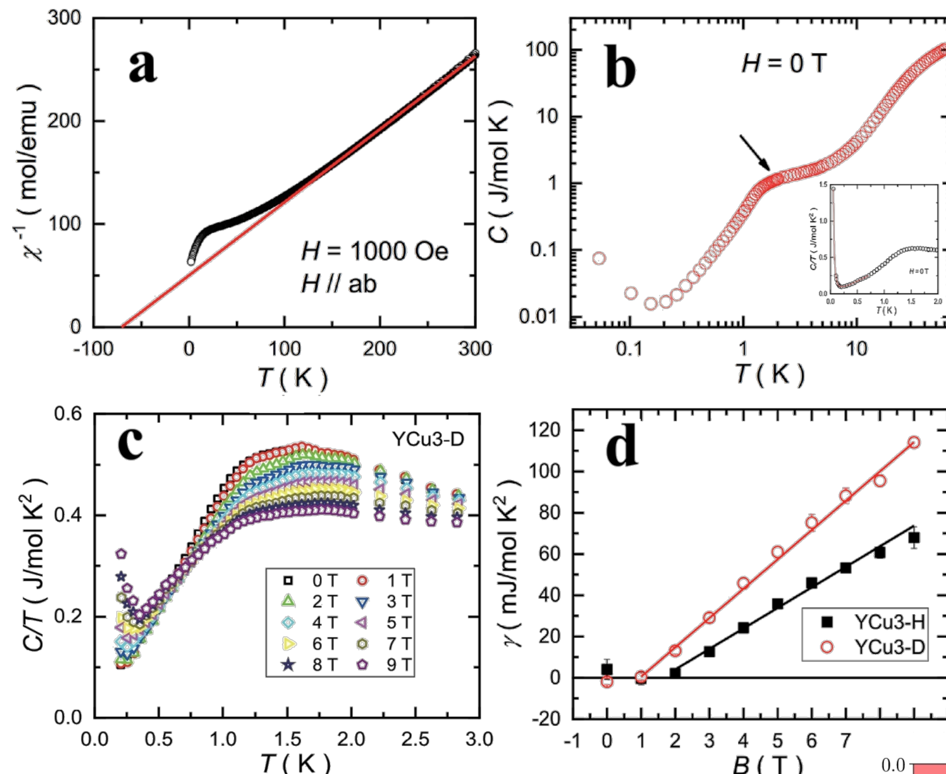
Kagome material YCu3-Br/Cl

Possible Dirac quantum spin liquid in the kagome quantum antiferromagnet $YCu_3(OH)_6Br_2[Br_x(OH)_{1-x}]$

Shiliang Li's group in IOP, CAS

$YCu_3(OH)_6Br_2[Br_{(1-x)}(OH)_x]$ (YCu_3-Br)



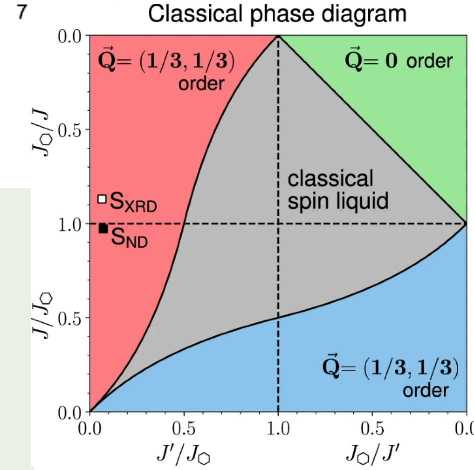


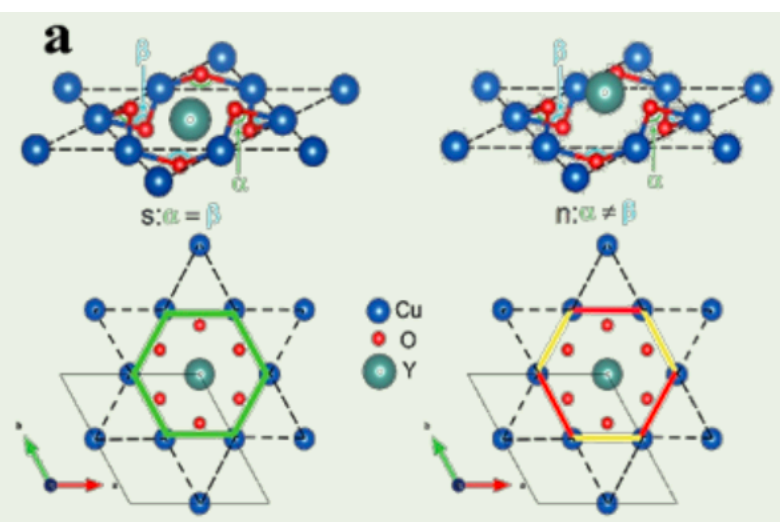
Magnetic ground states in kagome $YCu_3(OH)_6[(Cl_xBr_{1-x})_{3-y}(OH)_y]$

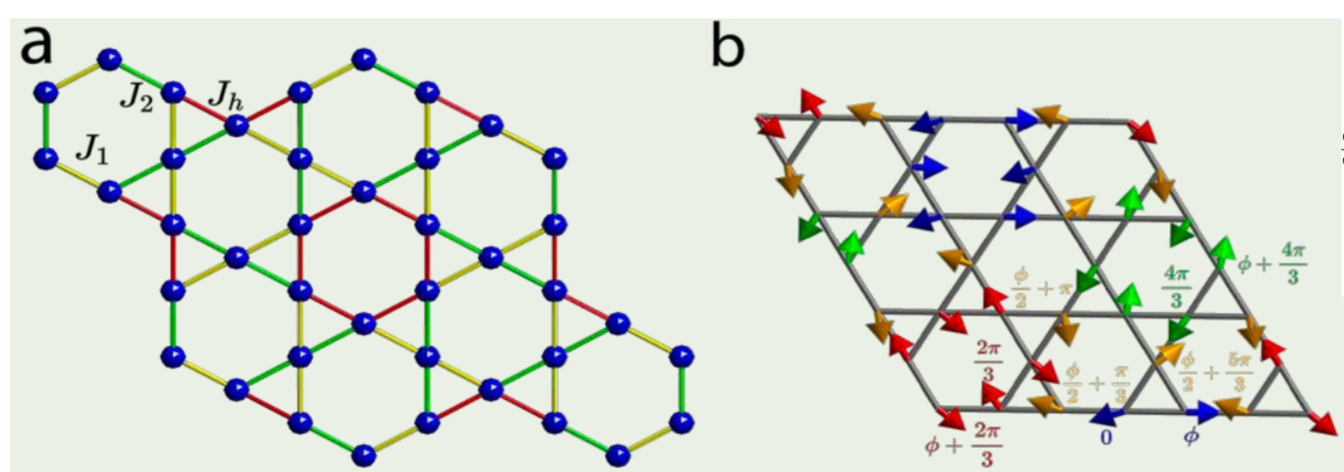
Aini Xu,[1,2] Qinxin Shen,[1,2] Bo Liu,[1,2] Zhenyuan Zeng,[1,2] Lankun Han,[1,2] Liqin Yan,[1,2] Jun Luo,[1] Jie Yang,[1] Rui Zhou,[1,*] and Shiliang Li[1,2,†]

arXiv:2311.13089

Classical phase diagram





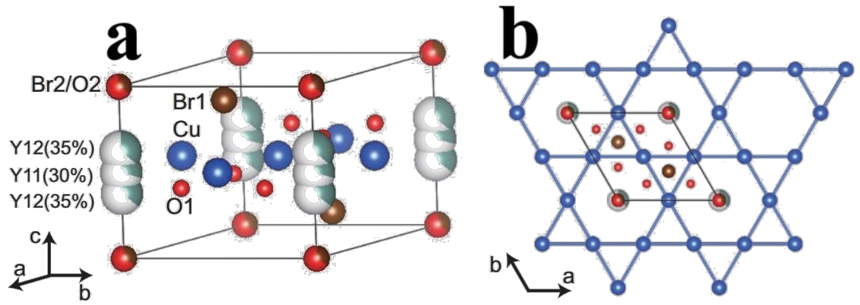


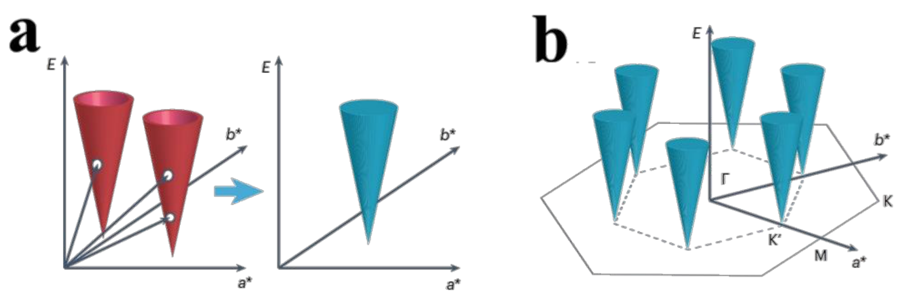
YCu3-Cl YCu3-Br

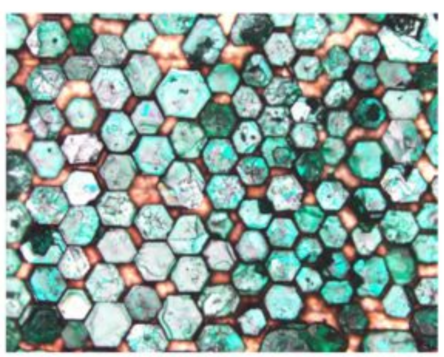
Hering, M., Ferrari, F., Razpopov, A. *et al.* Phase diagram of a distorted kagome antiferromagnet and application to Y-kapellasite. *npj Comput Mater* **8**, 10 (2022).

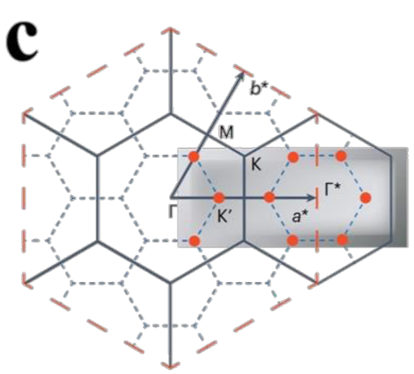
Kagome material YCu3-Br

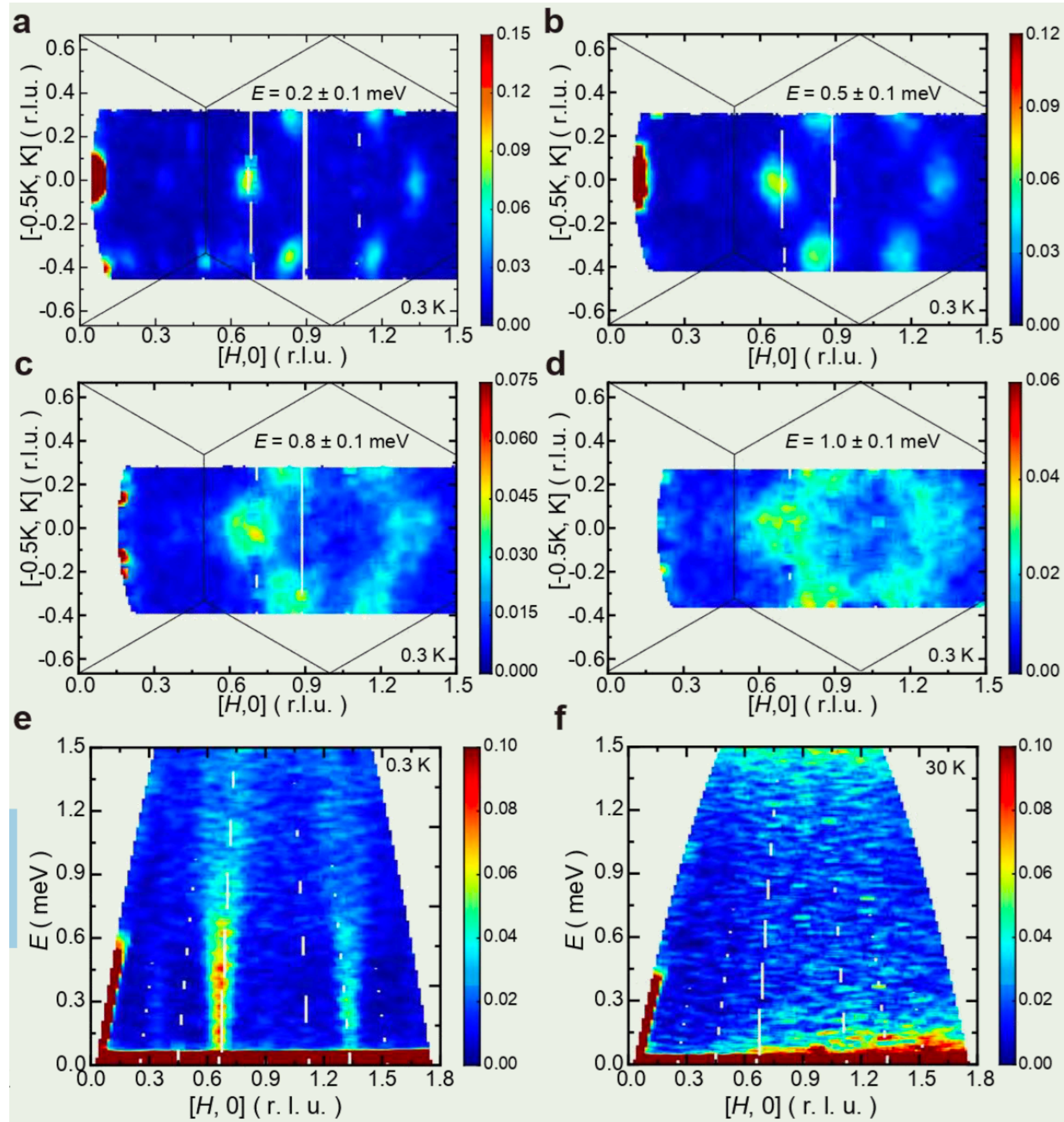
$YCu_3(OH)_6Br_2[Br_{(1-x)}(OH)_x]$ (YCu_3-Br)











nature physics

Article https://doi.org/10.1038/s41567-024-02495-z

Spectral evidence for Dirac spinons in a kagome lattice antiferromagnet

Zhenyuan Zeng[1,2], Chengkang Zhou[3], Honglin Zhou[1,2], Lankun Han[1,2], Runze Chi[1,2], Kuo Li[4], Maiko Kofu[5], Kenji Nakajima[5], Yuan Wei[6], Wenliang Zhang[6], Daniel G. Mazzone[7], Zi Yang Meng[3] & Shiliang Li[1,2,8]

Model-Design and Numerical Simulations

- Magnetic phase transitions and Dynamical properties ✓
- Kagome models and Z2 quantum spin liquid (BFG) ✓
- Pyrochlore models and U1 quantum spin liquid (Quantum Spin ice)
- Dirac fermion/spinon coupled with U1 gauge field
- YCu3-Br/Cl and SCBO
- Polynomial Sign problem
- ……

Pyrochlore U1 spin ice

PHYSICAL REVIEW B **69**, 064404 (2004)

Pyrochlore photons: The $U(1)$ spin liquid in a $S=\frac{1}{2}$ three-dimensional frustrated magnet

Michael Hermele,[1] Matthew P. A. Fisher,[2] and Leon Balents[1]

PRL **108**, 037202 (2012) PHYSICAL REVIEW LETTERS week ending 20 JANUARY 2012

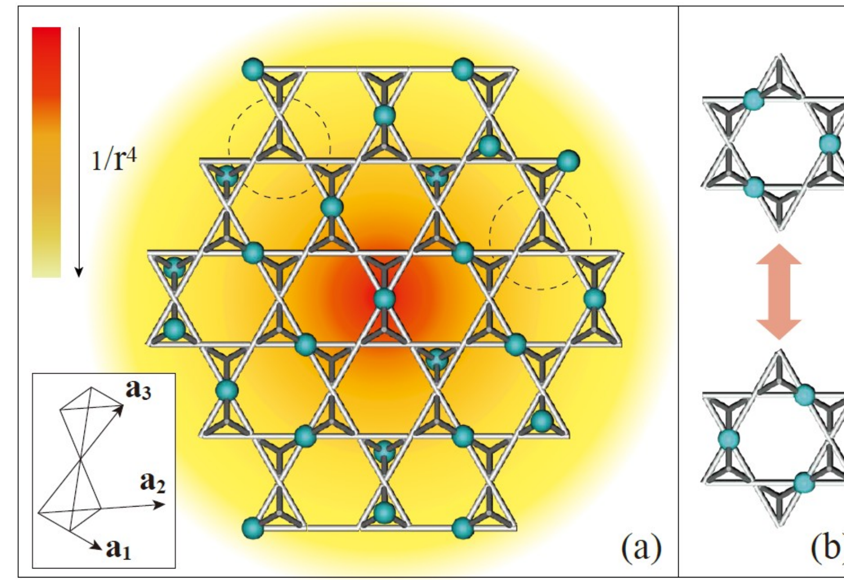
Coulombic Quantum Liquids in Spin-1/2 Pyrochlores

Lucile Savary[1,2] and Leon Balents[3]

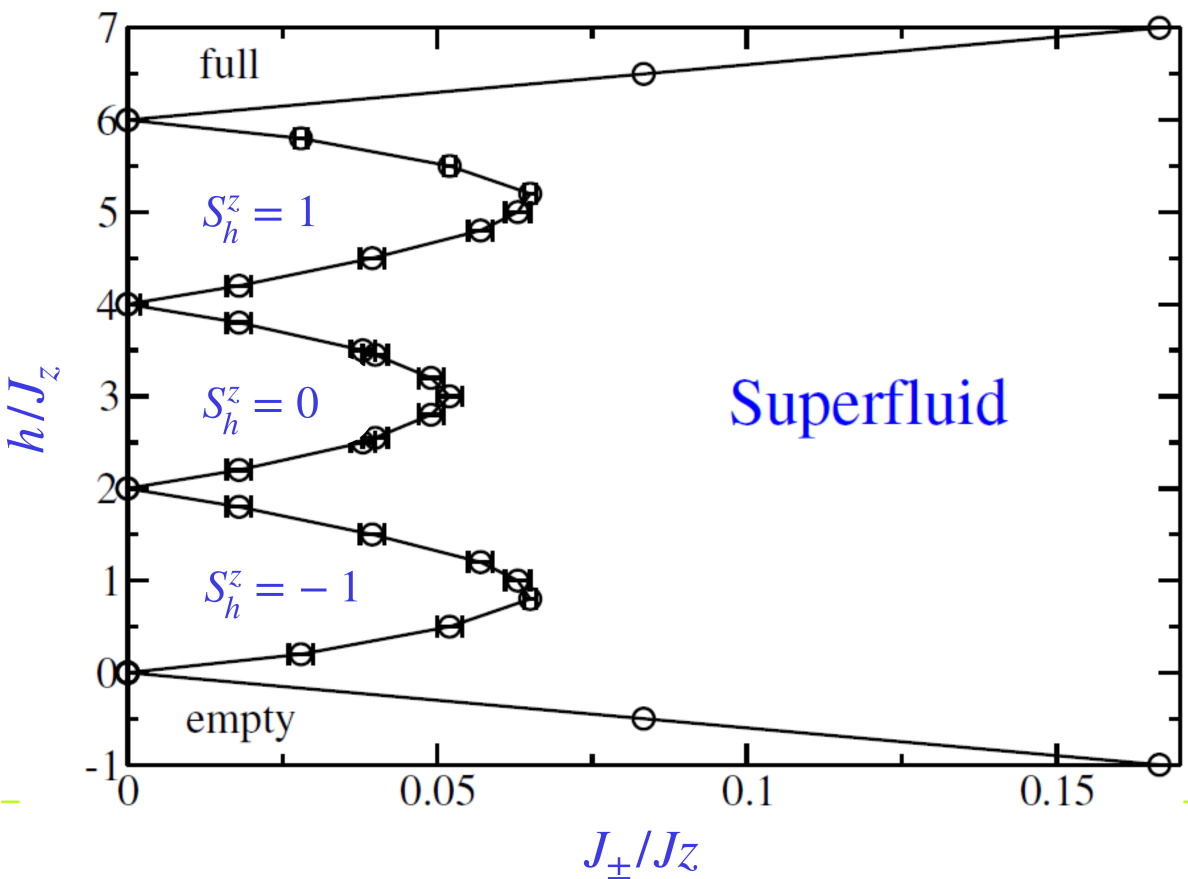
PHYSICAL REVIEW LETTERS **120**, 167202 (2018)

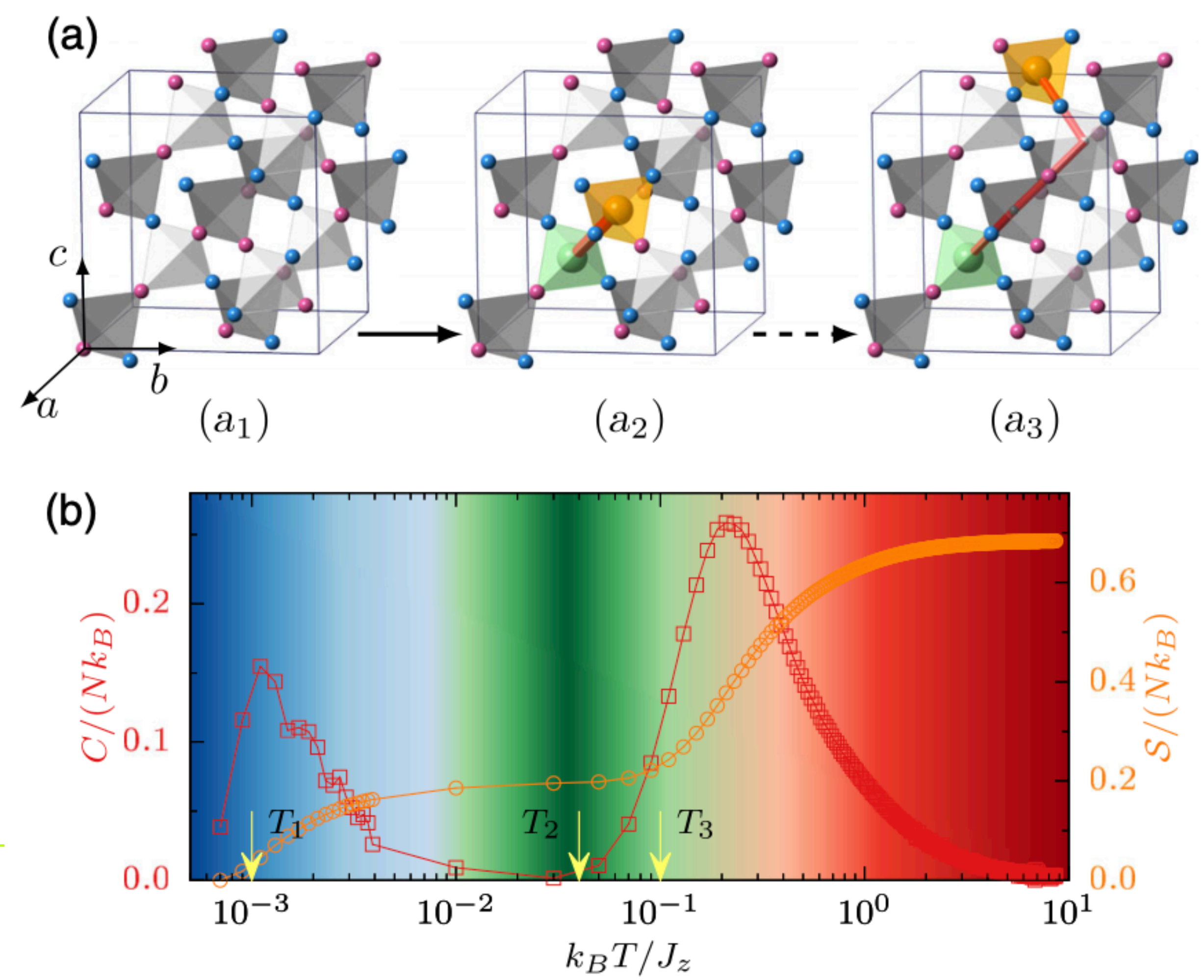
Dynamics of Topological Excitations in a Model Quantum Spin Ice

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



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





J.-P. Lv, G. Chen, Y. Deng, and Z. Y. Meng, Phys. Rev. Lett. 115, 037202 (2015).

Pyrochlore U1 spin ice

PHYSICAL REVIEW LETTERS **120,** 167202 (2018)

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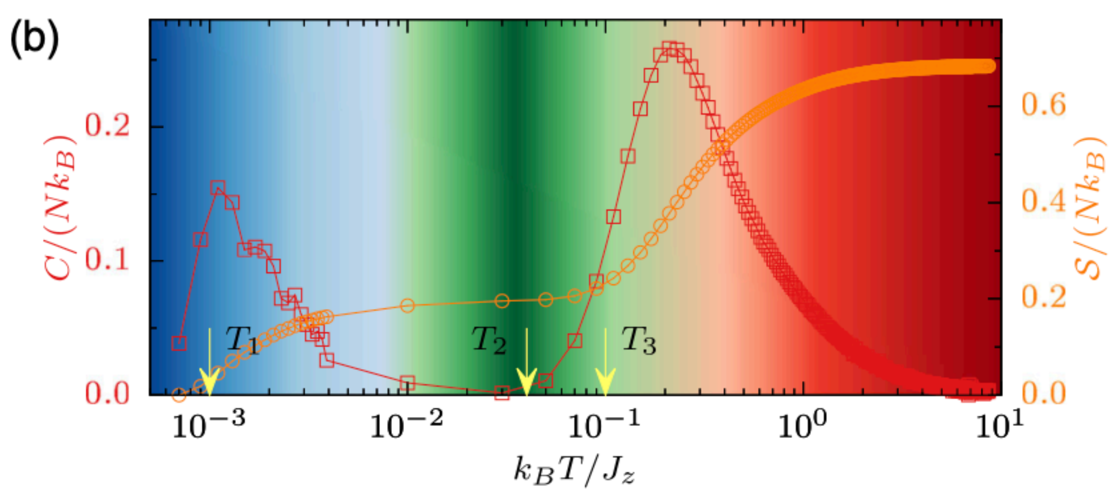
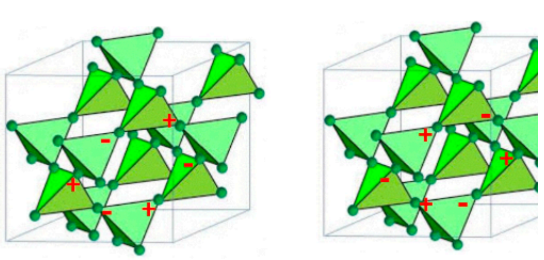
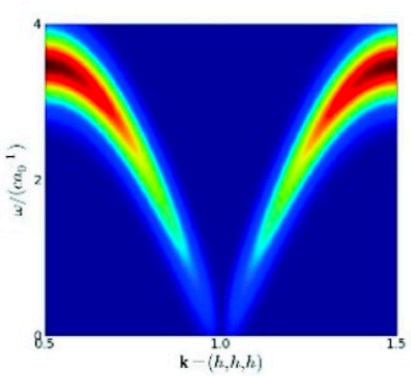
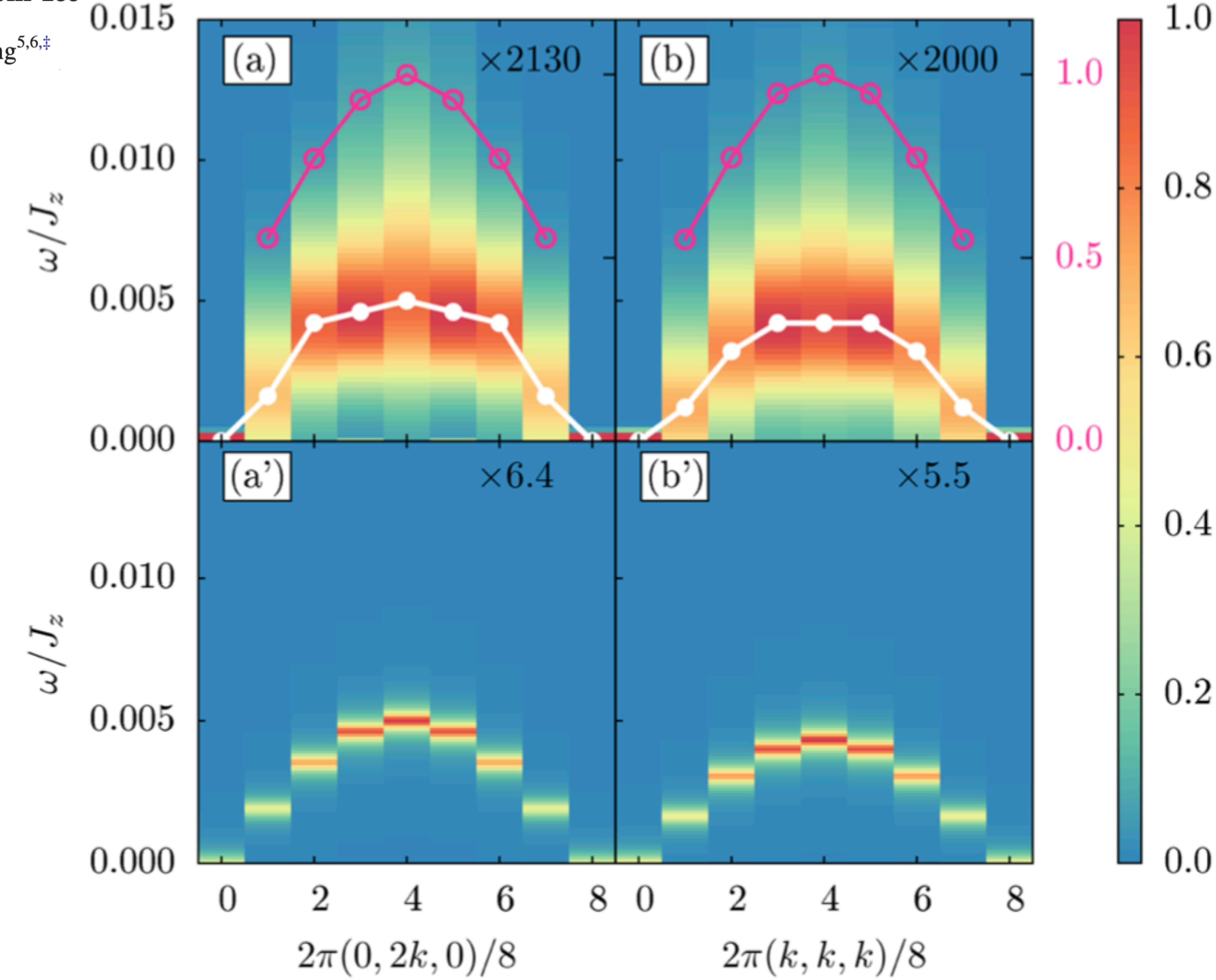






$$(\delta_{\mu,\nu} - k_\mu k_\nu / \mathbf{k}^2)\omega\delta(\omega - v|\mathbf{k}|)$$

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



- M. Hermele, M. P. A. Fisher, and L. Balents, Phys. Rev. B 69, 064404 (2004).
- A. Banerjee, S. V. Isakov, K. Damle, and Y. B. Kim, Phys. Rev. Lett. 100, 047208 (2008).
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Pyrochlore U1 spin ice

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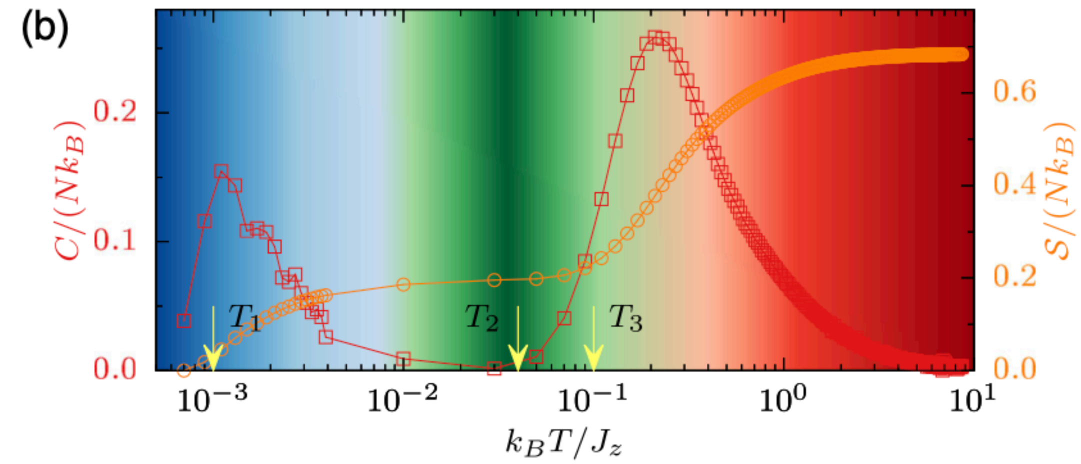
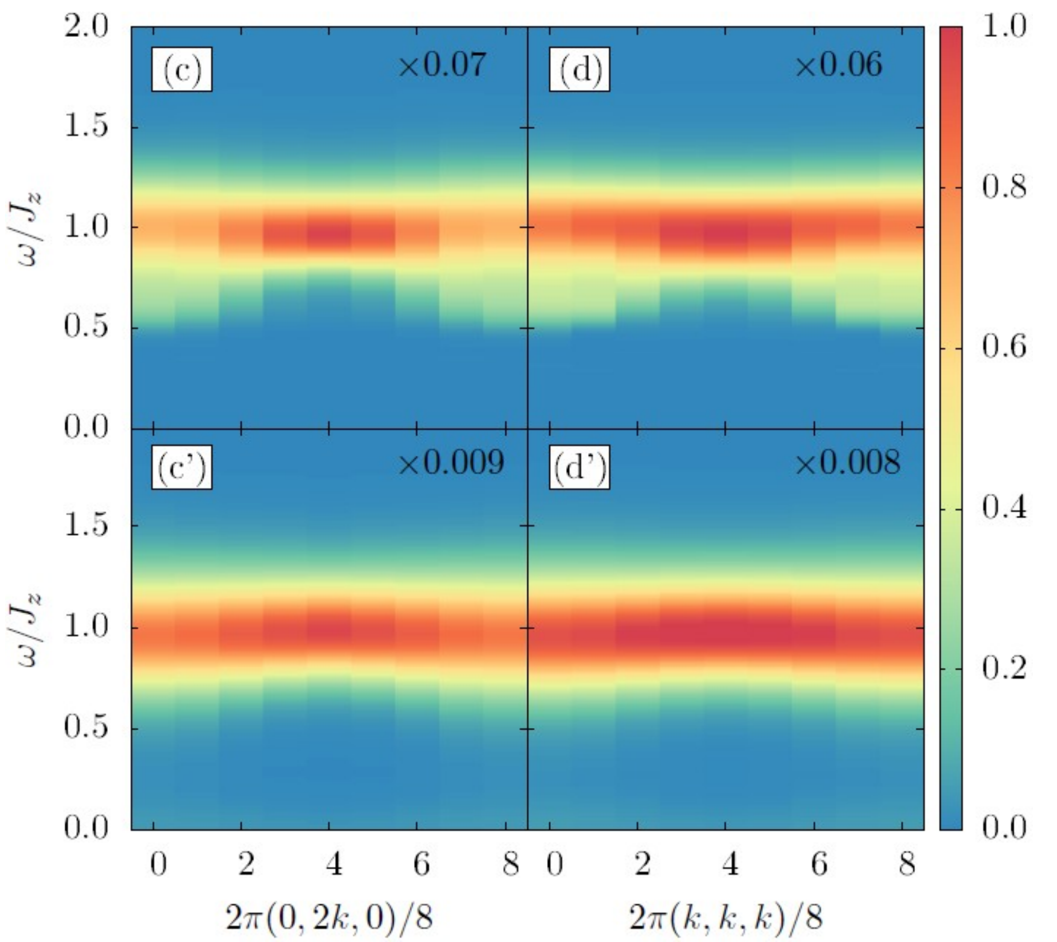
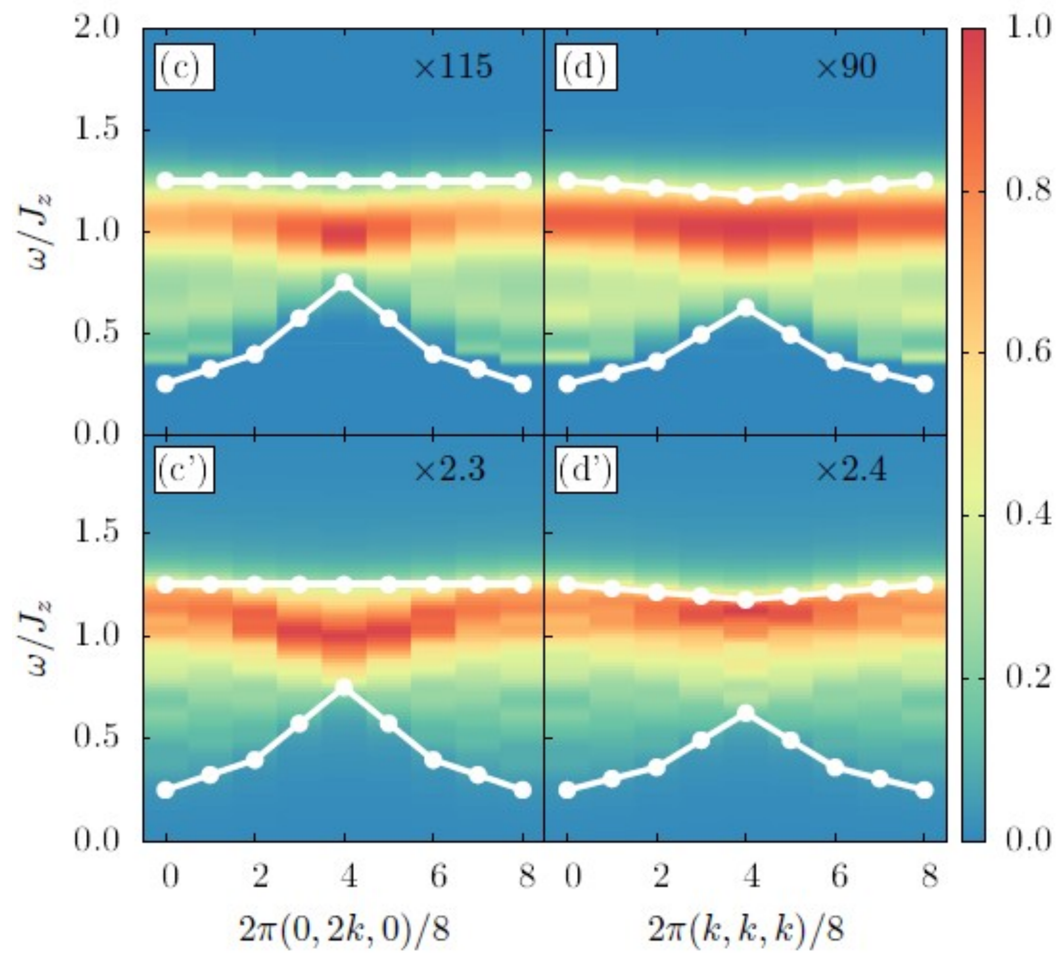


$$S_{\alpha\beta}^{+-}(\mathbf{q},\tau) = \langle S_{-\mathbf{q},\alpha}^{+}(\tau) S_{\mathbf{q},\beta}^{-}(0) \rangle,$$

Classical spin ice



Quantum spin ice



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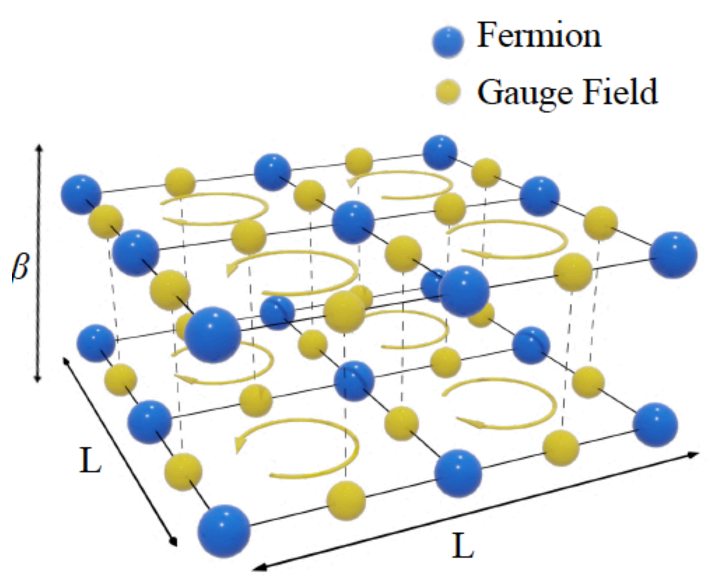
U1 Dirac spin liquid

PHYSICAL REVIEW X **9**, 021022 (2019)

Monte Carlo Study of Lattice Compact Quantum Electrodynamics with Fermionic Matter: The Parent State of Quantum Phases

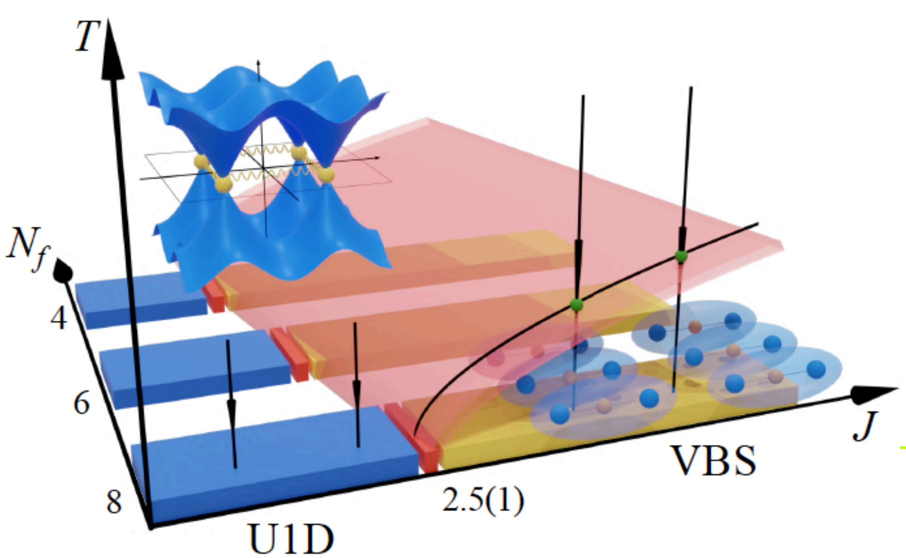
Xiao Yan Xu,[1,*] Yang Qi,[2–4,†] Long Zhang,[5] Fakher F. Assaad,[6] Cenke Xu,[7] and Zi Yang Meng[8,9,10,11,‡]



$$Z = \int D(\phi, \bar{\psi}, \psi) e^{-(S_\phi + S_F)} \quad S = S_F + S_\phi = \int_0^\beta d\tau (L_F + L_\phi)$$

$$L_F = \sum_{\langle i,j \rangle \alpha} \psi^\dagger_{i\alpha} \left[(\partial_\tau - \mu)\delta_{ij} - t e^{i\phi_{ij}} \right] \psi_{j\alpha} + \text{h.c.},$$

$$L_\phi = \frac{4}{J N_f \Delta\tau^2} \sum_{\langle i,j \rangle} (1 - \cos(\phi_{ij}(\tau+1) - \phi_{ij}(\tau))) + \frac{1}{2} K N_f \sum_{\square} \cos(\text{curl}\phi)$$



$$Z = \int D(\phi, \bar{\psi}, \psi) e^{-(S_\phi + S_F)} = \int D\phi e^{-S_\phi} \text{Tr}_\psi \left[e^{-S_F} \right]$$

$$\text{Tr}_\psi \left[e^{-S_F} \right] = \left[\det \left(I + \prod_{z=1}^{L_\tau} B_z \right) \right]^{N_f}$$

U1 Dirac spin liquid

PHYSICAL REVIEW X **9,** 021022 (2019)

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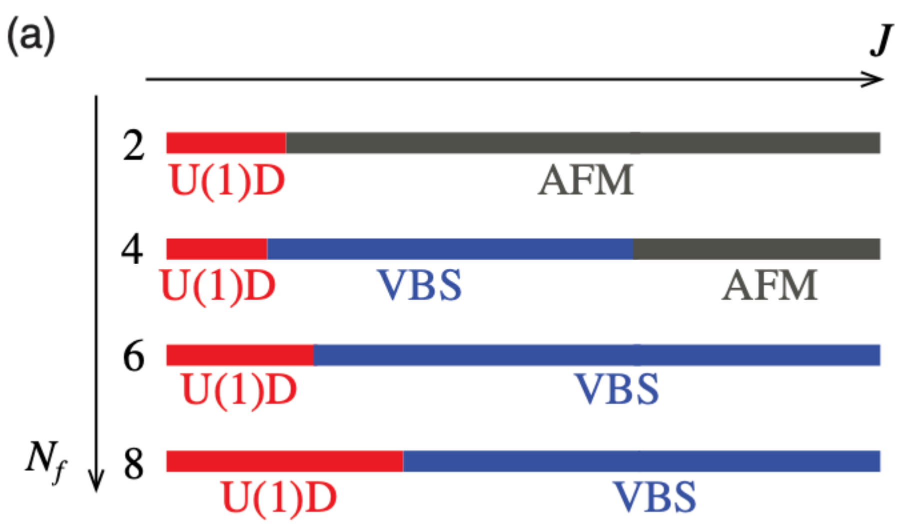
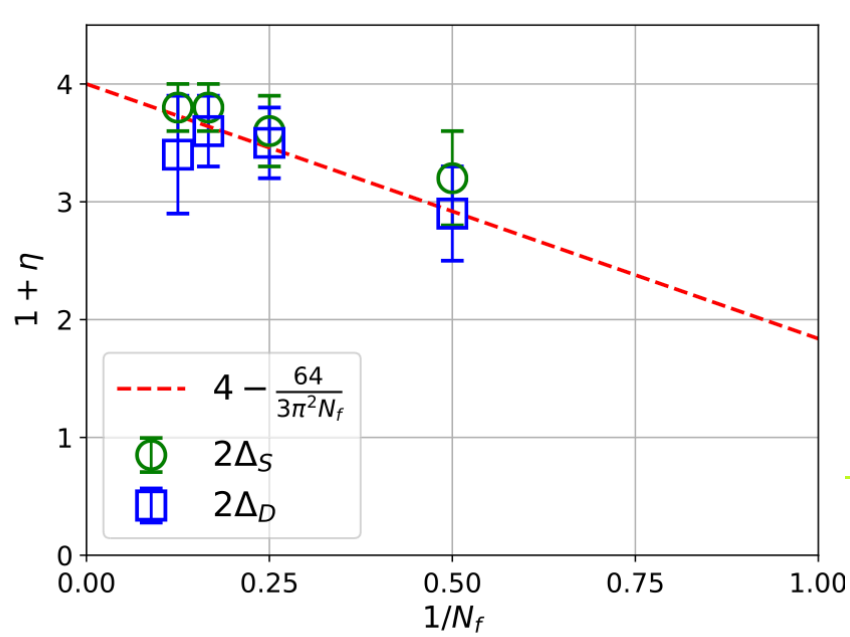
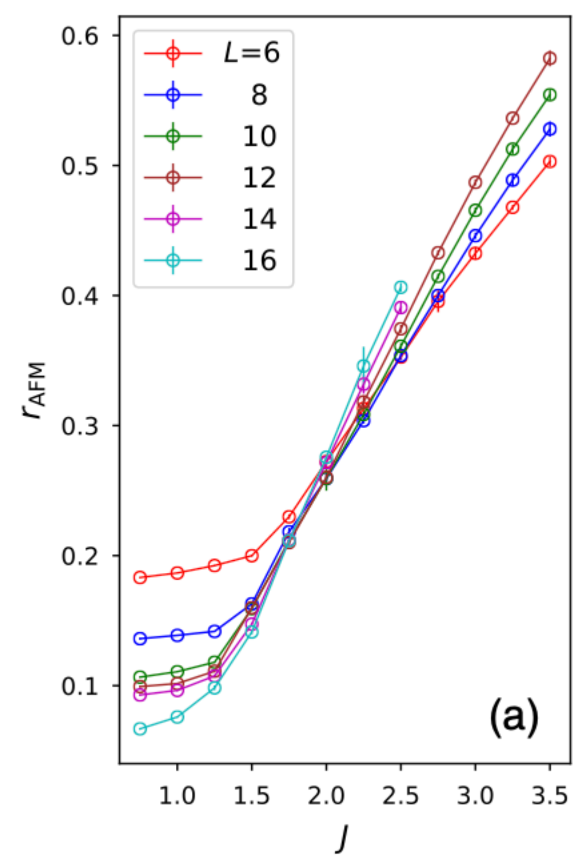
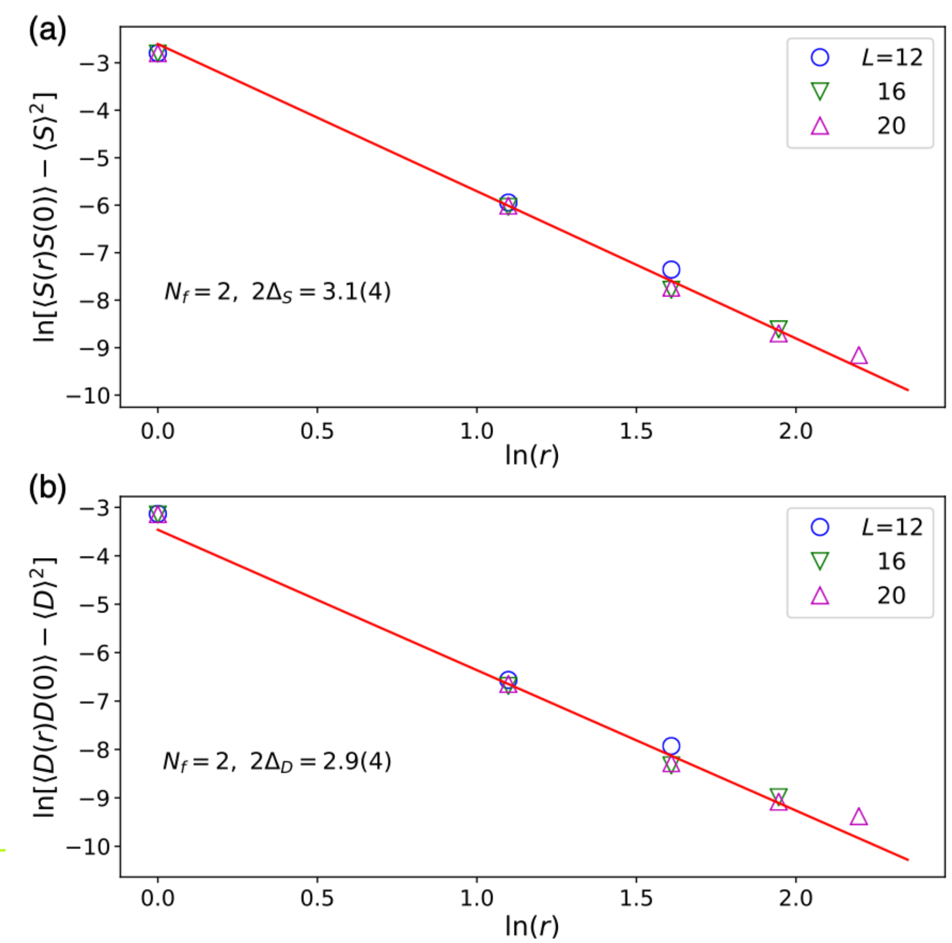
$$\chi_S(\mathbf{k}) = \frac{1}{L^4}\sum_{ij}\sum_{\alpha\beta}\langle S^\alpha_\beta(i)S^\beta_\alpha(j)\rangle e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}, \qquad S^\alpha_\beta(i) = c^\dagger_{i,\alpha}c_{i,\beta} - \frac{1}{N_f}\delta_{\alpha,\beta}\sum_\gamma c^\dagger_{i,\gamma}c_{i,\gamma}$$

$$\chi_D(\mathbf{k}) = \frac{1}{L^4}\sum(\langle D_iD_j\rangle - \langle D_i\rangle\langle D_j\rangle)e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}, \qquad D_i = \sum_{\alpha,\beta} S^\alpha_\beta(i)S^\beta_\alpha(i+\hat{x})$$









U1 Dirac spin liquid

PHYSICAL REVIEW X **9**, 021022 (2019)

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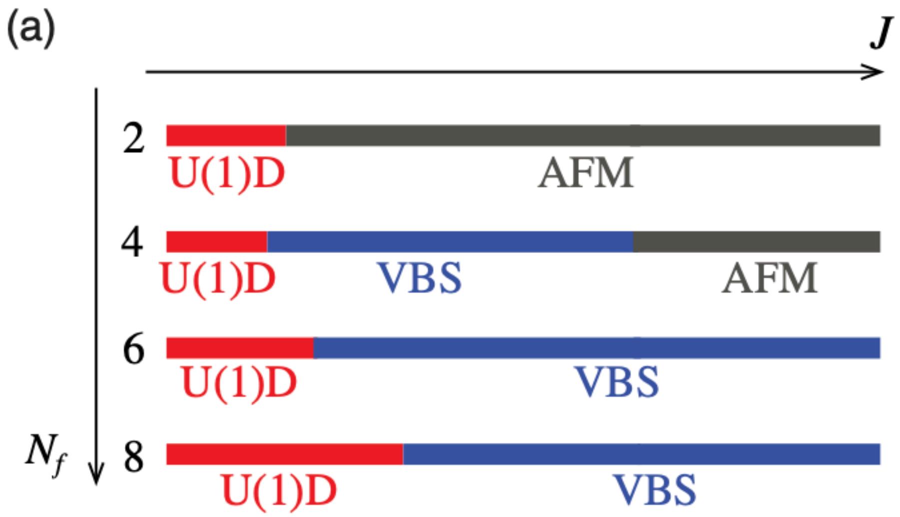

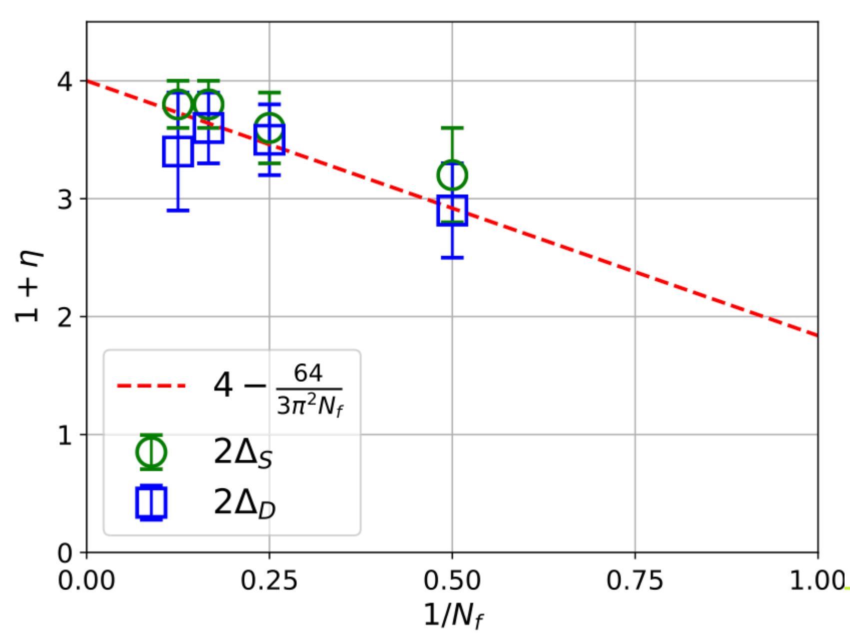

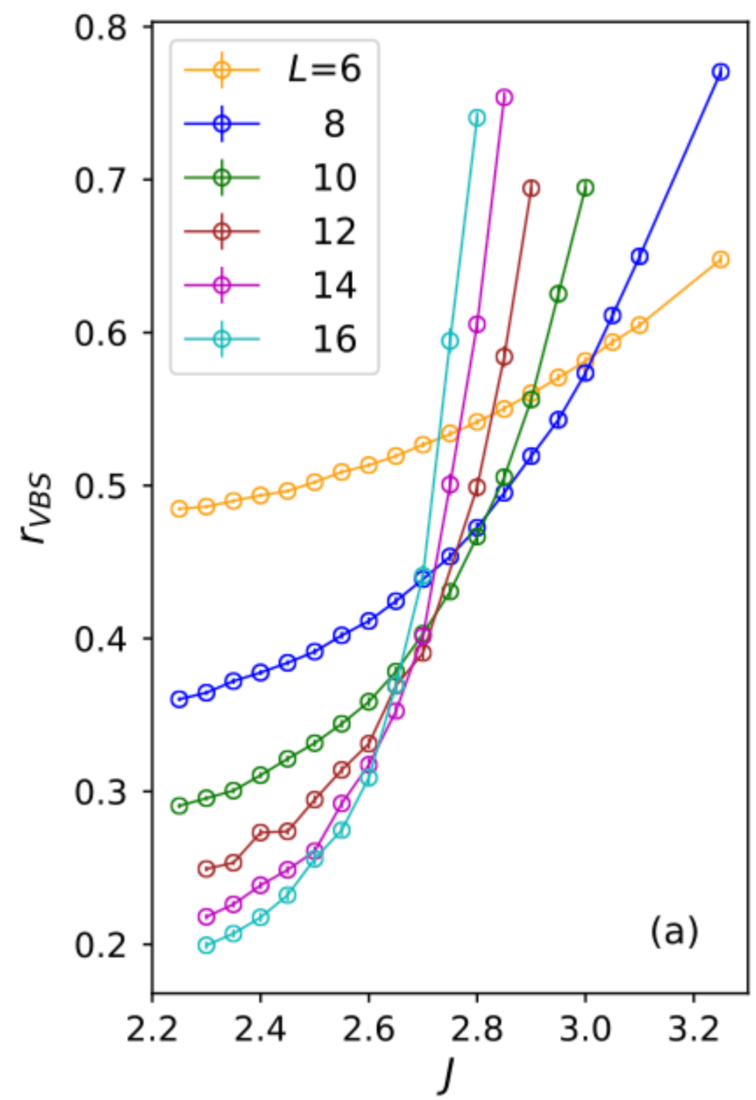

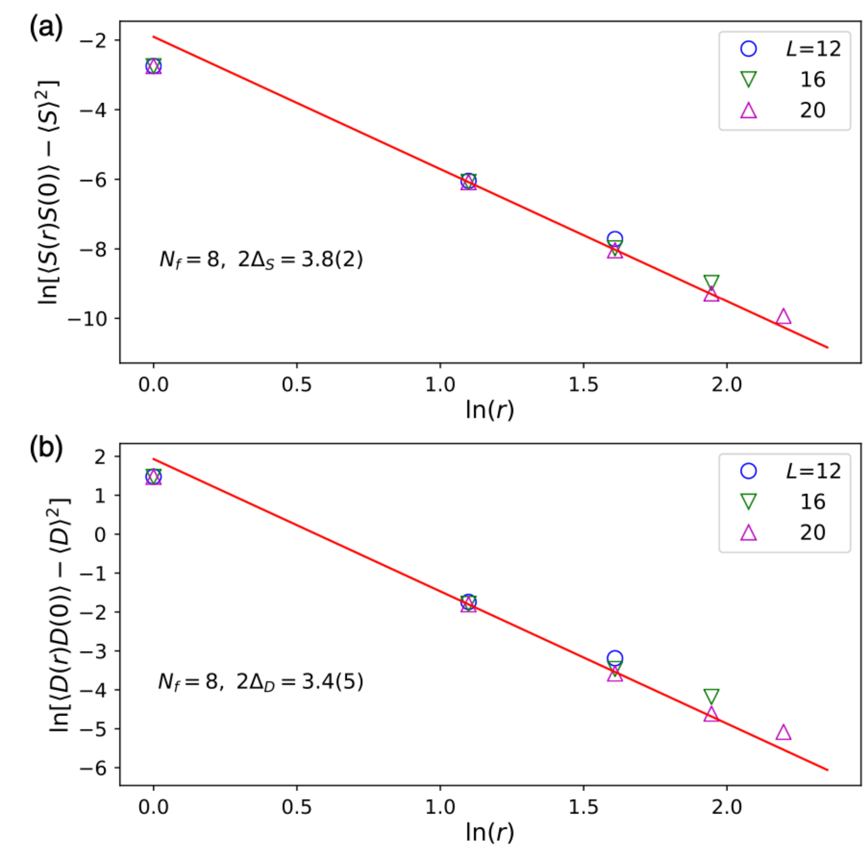

U1 Dirac spin liquid

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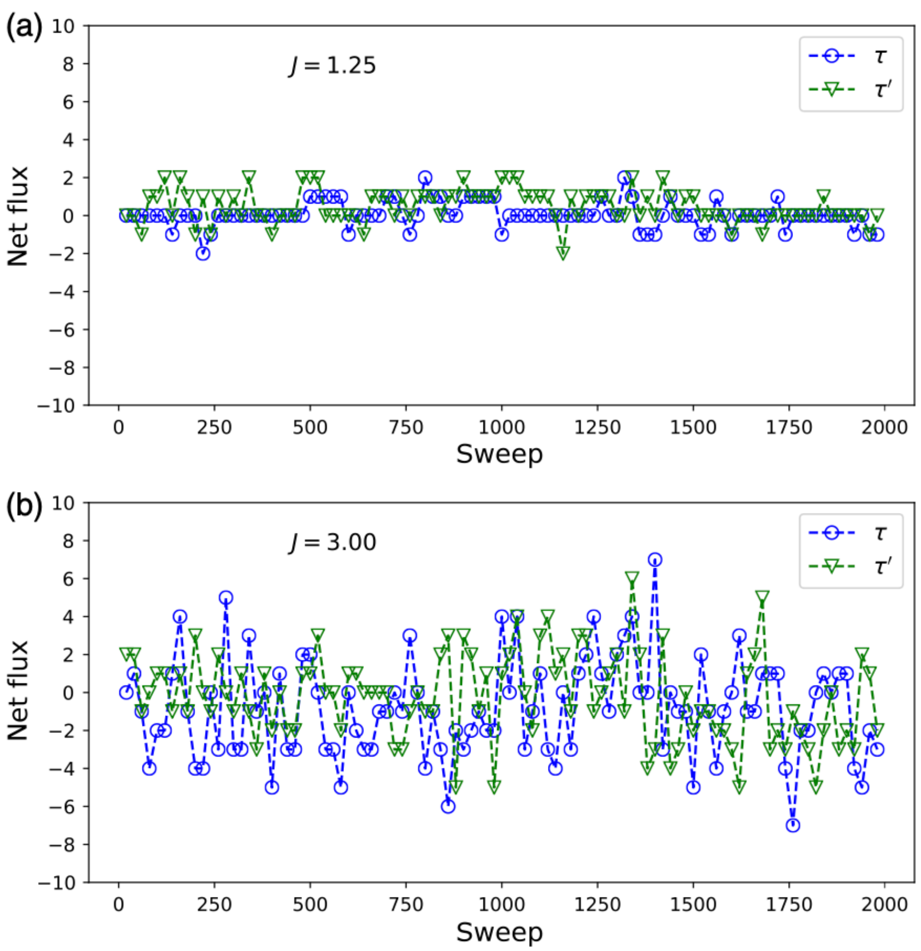
$N_f = 2$



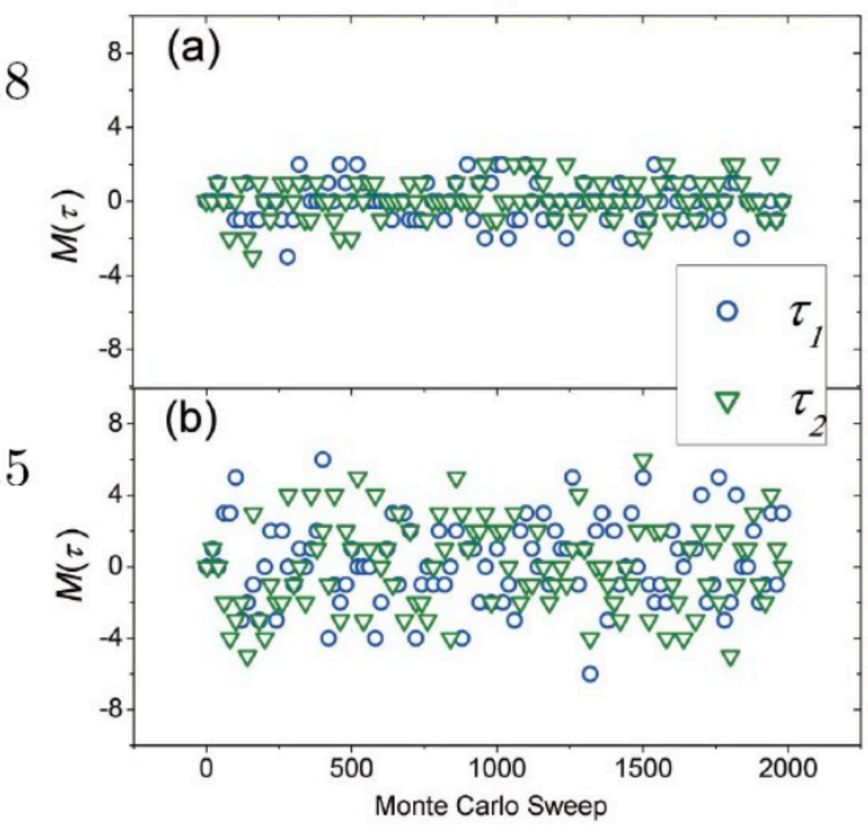
$N_f = 8$

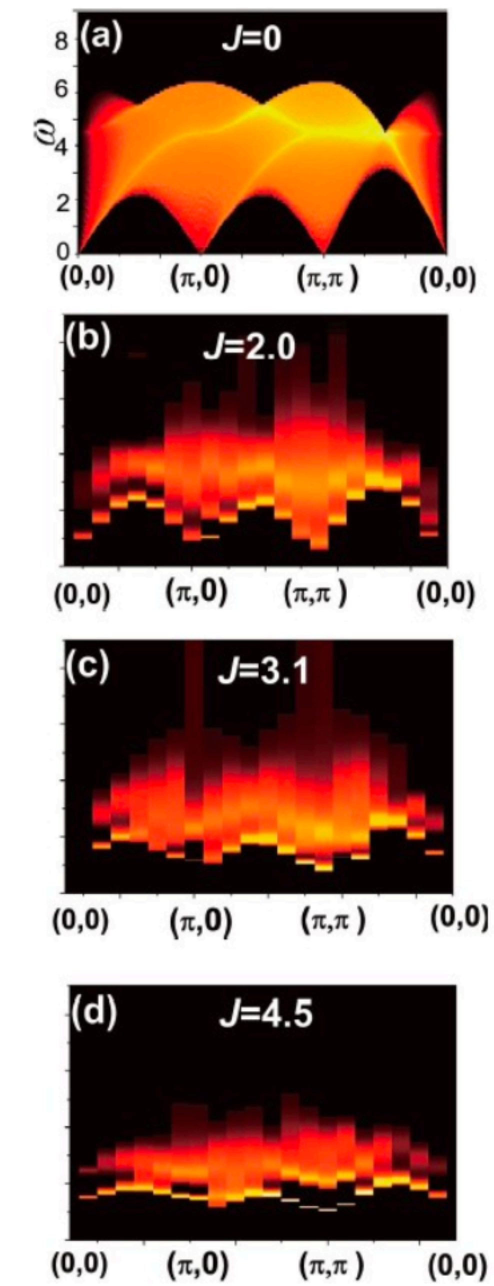
$$\sum_{b\in\Box} \phi_b = \Phi_\Box + 2\pi m_\Box \qquad M(\tau) = \sum_\Box m(\tau)$$

$L = 12, \beta = 2L$

$J = 1.8$

$J = 3.5$





Monopole proliferation leads to confinement of gauge field

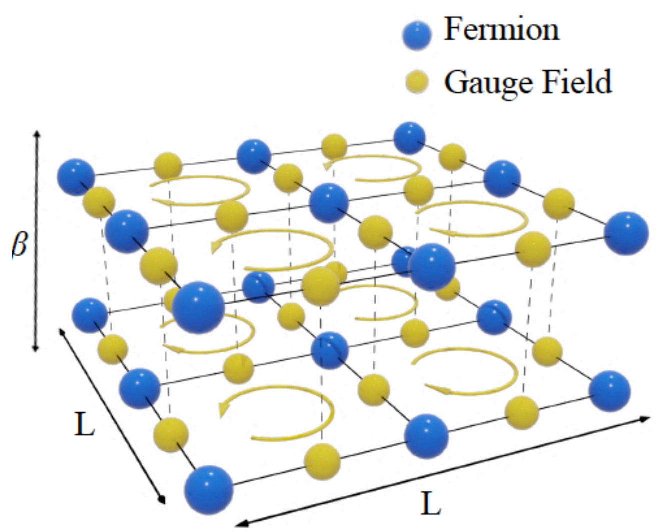
- Wei Wang, et. al. PRB 100, 085123 (2019)

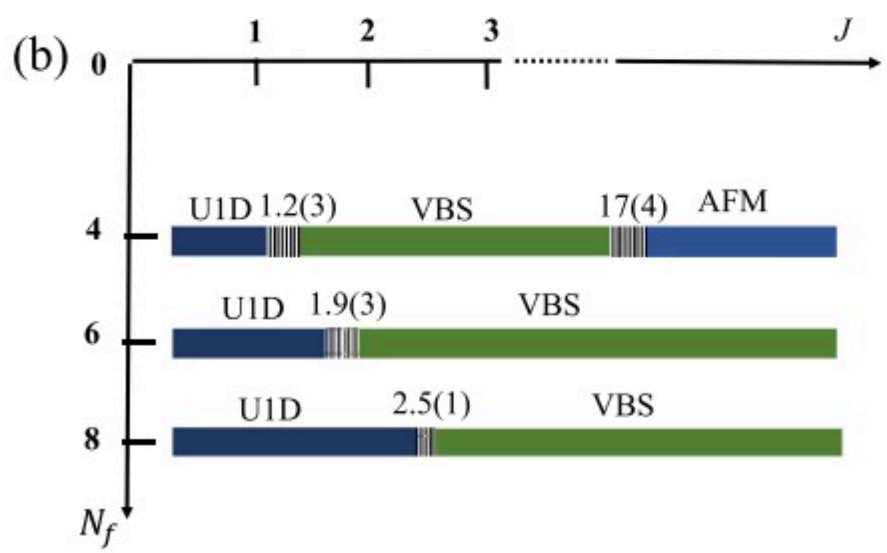
U1 Dirac spin liquid

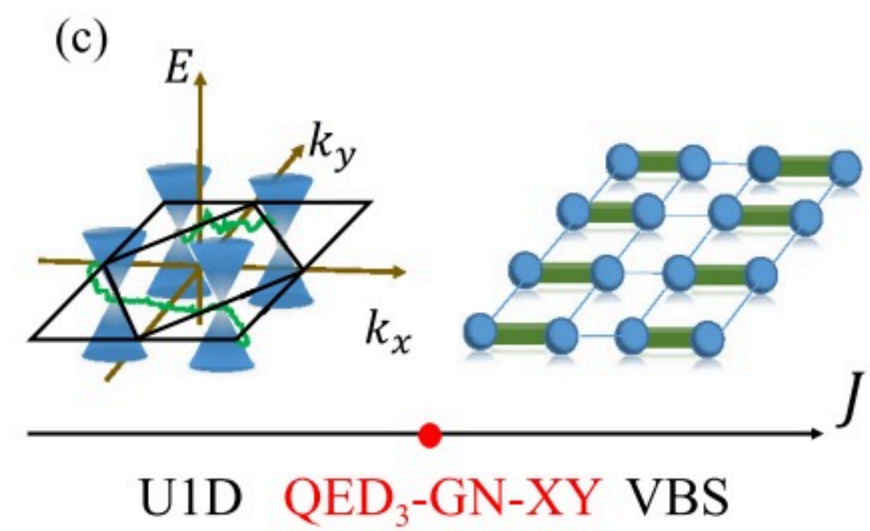
PHYSICAL REVIEW B **101**, 235118 (2020)

Confinement transition in the QED$_3$-Gross-Neveu-XY universality class

Lukas Janssen,[1] Wei Wang,[2,3] Michael M. Scherer,[4] Zi Yang Meng,[2,5,6] and Xiao Yan Xu[7]

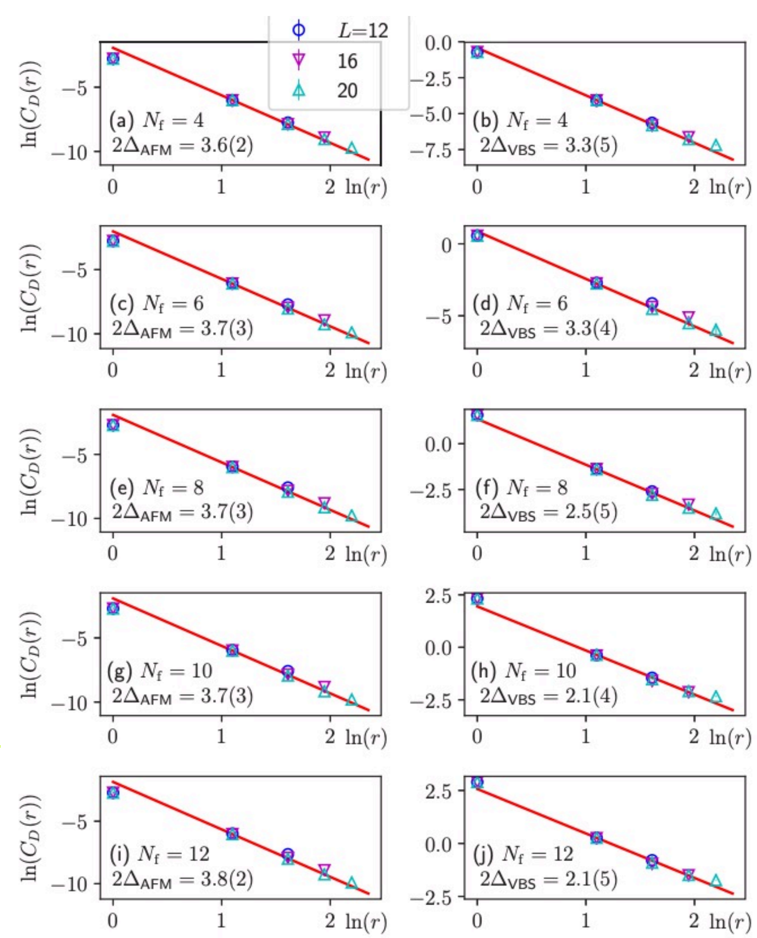


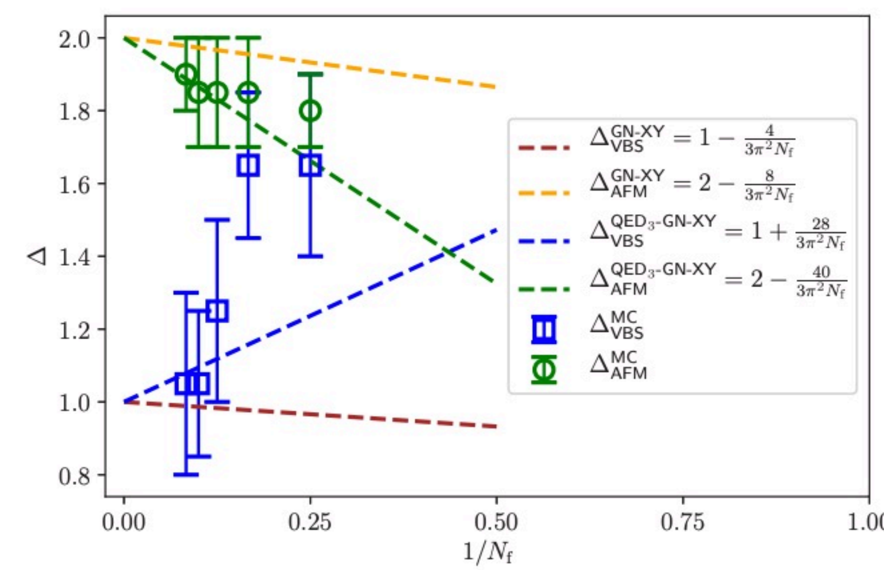




$$\Delta_{\mathrm{VBS}}\big|_{\mathrm{QED_3\text{-}GN\text{-}XY}} = 1 + \frac{28}{3\pi^2 N_f} + O(1/N_f^2),$$

$$\Delta_{\mathrm{AFM}}\big|_{\mathrm{QED_3\text{-}GN\text{-}XY}} = 2 - \frac{40}{3\pi^2 N_f} + O(1/N_f^2).$$





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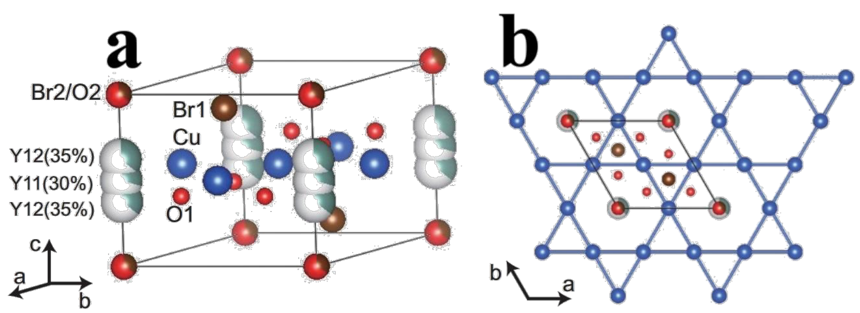
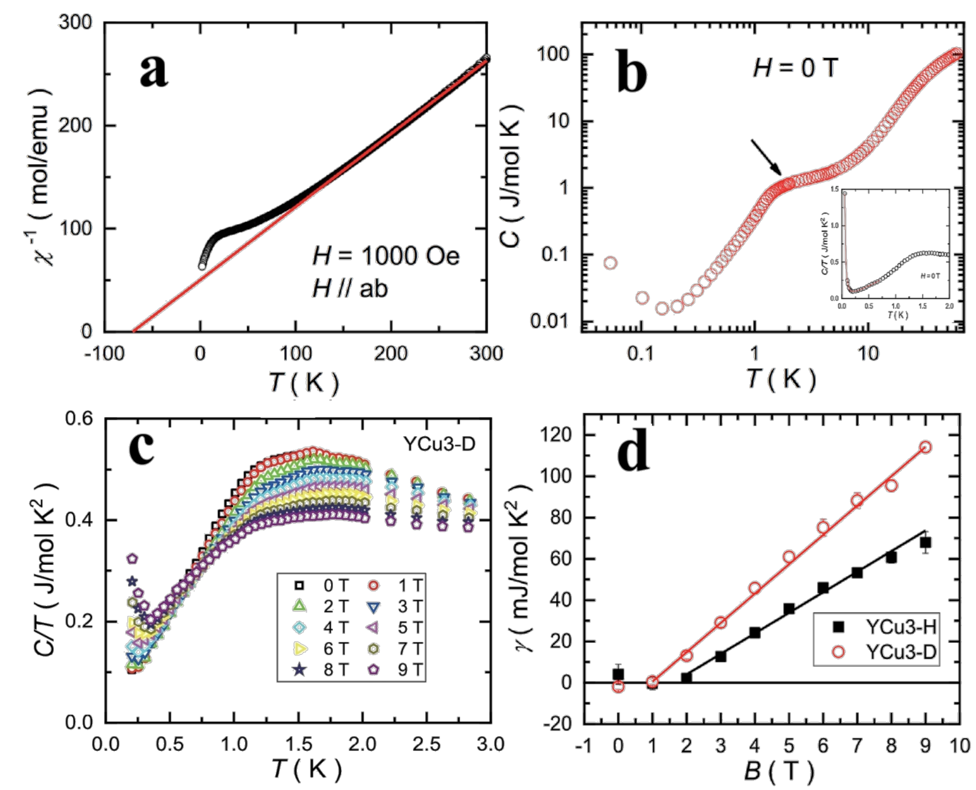
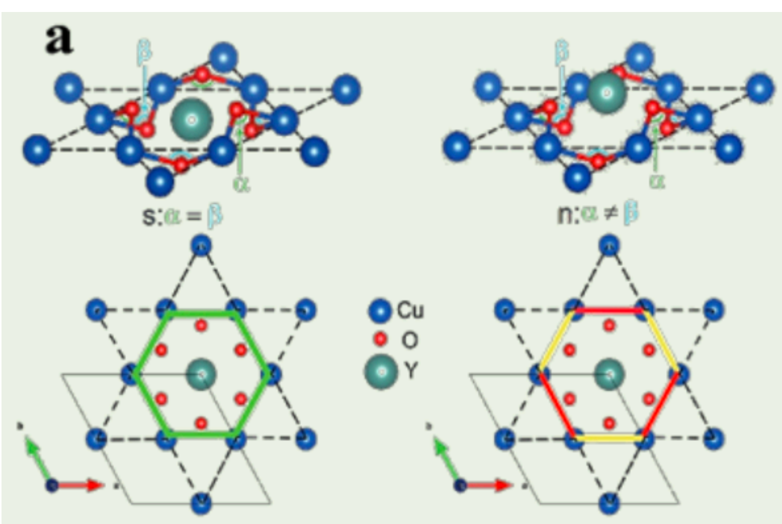
Kagome material YCu3-Br/Cl

$YCu_3(OH)_6Br_2[Br_{(1-x)}\ (OH)\ _x]$ (YCu_3-Br)

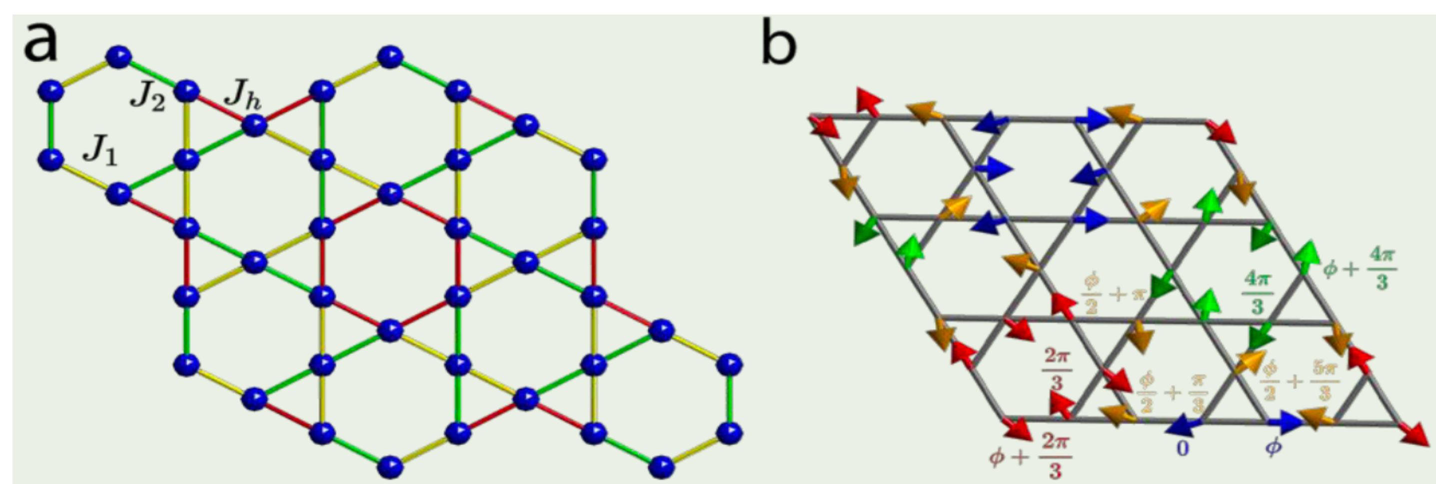




$YCu_3(OH)_6[(Cl_xBr_{1-x})_{3-y}\ (OH)_y]$ (YCu_3-Br/Cl)

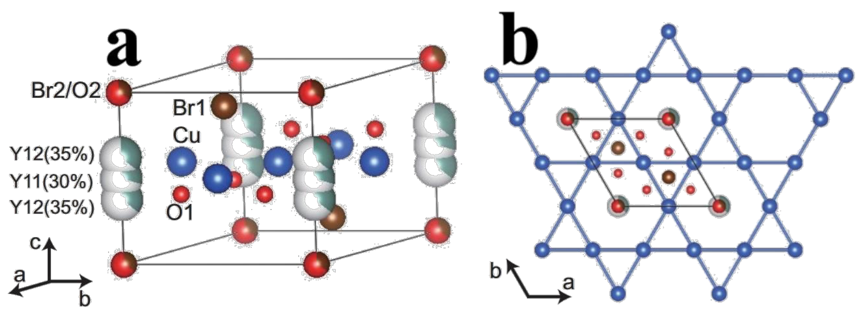


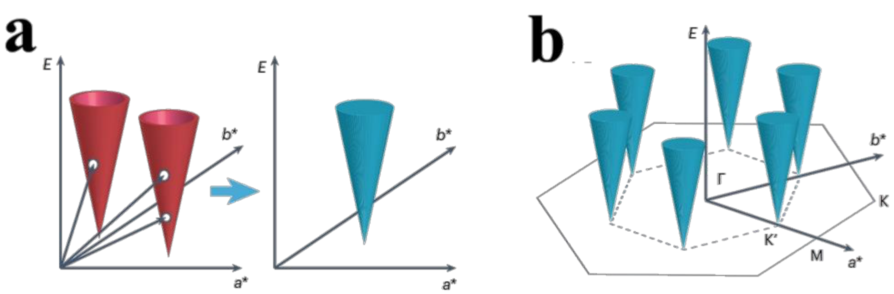
YCu3-Cl YCu3-Br

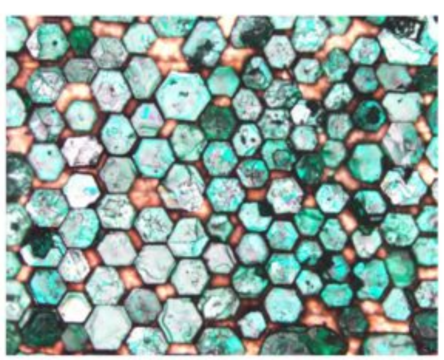


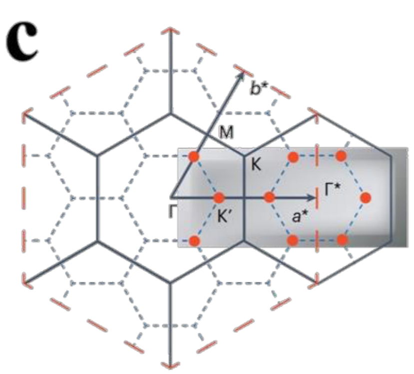
Kagome material YCu3-Br

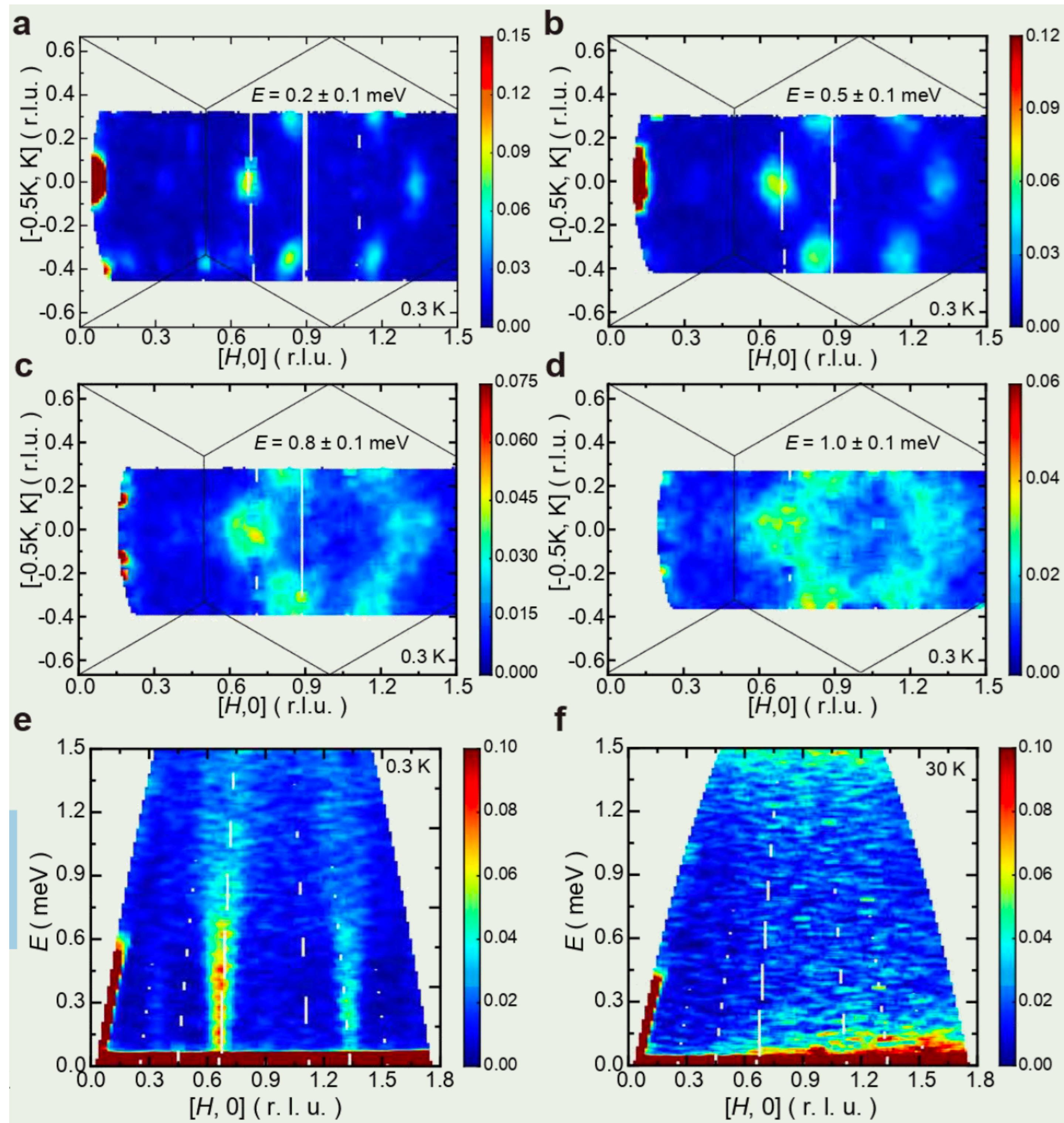
$YCu_3(OH)_6Br_2[Br_{(1-x)}(OH)_x]$ (YCu_3-Br)











nature physics

Article

https://doi.org/10.1038/s41567-024-02495-z

Spectral evidence for Dirac spinons in a kagome lattice antiferromagnet

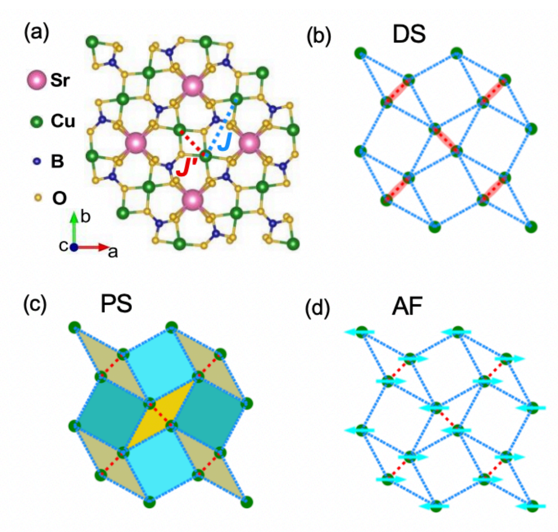
Zhenyuan Zeng[1,2], Chengkang Zhou[3], Honglin Zhou[1,2], Lankun Han[1,2], Runze Chi[1,2], Kuo Li[4], Maiko Kofu[5], Kenji Nakajima[5], Yuan Wei[6], Wenliang Zhang[6], Daniel G. Mazzone[7], Zi Yang Meng[3] & Shiliang Li[1,2,8]

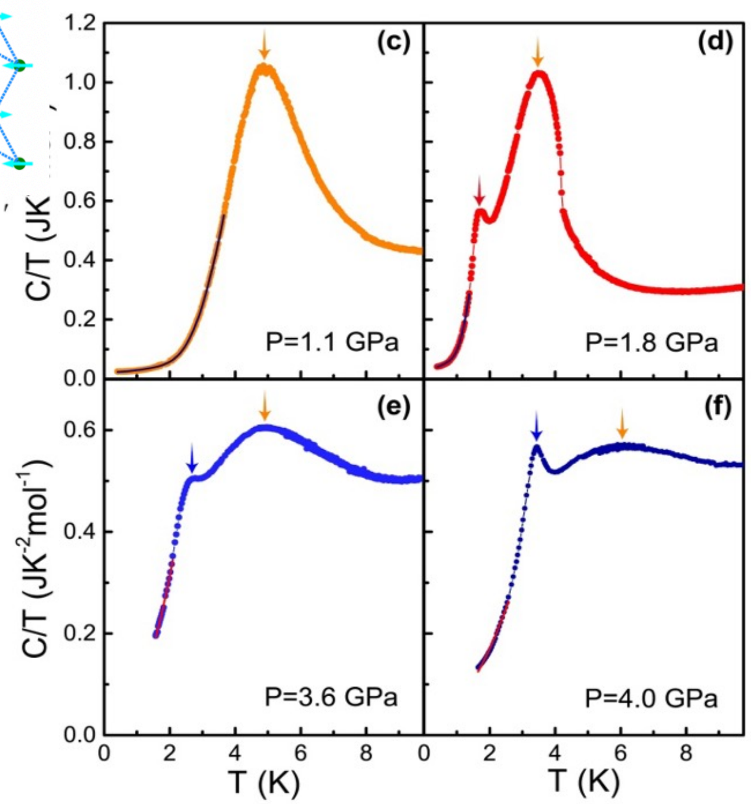
SCBO Experiment

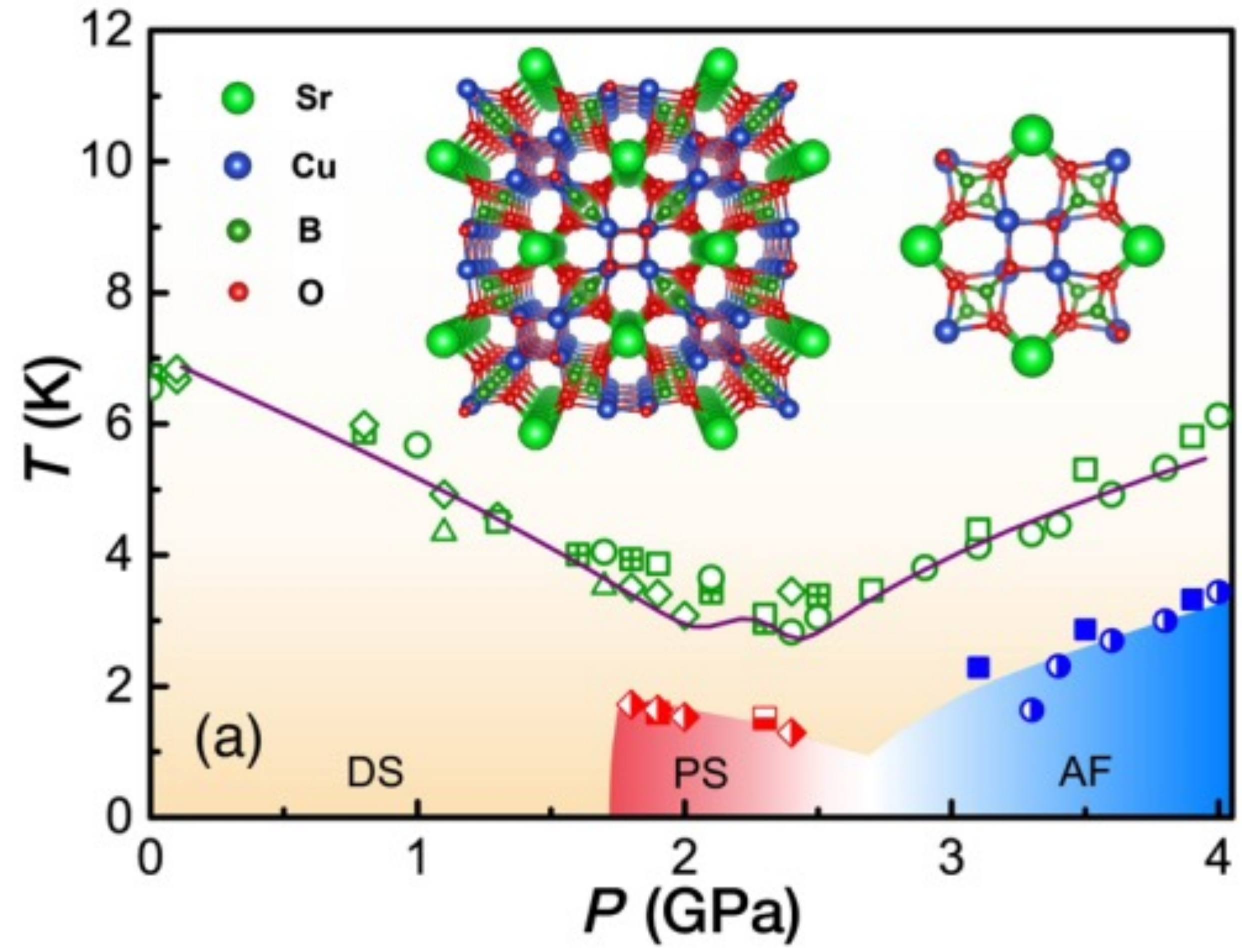
PHYSICAL REVIEW LETTERS **124**, 206602 (2020)

Quantum Phases of $SrCu_2(BO_3)_2$ from High-Pressure Thermodynamics

Jing Guo,[1] Guangyu Sun,[1,2] Bowen Zhao,[3] Ling Wang,[4,5] Wenshan Hong,[1,2] Vladimir A. Sidorov,[6] Nvsen Ma,[1] Qi Wu,[1] Shiliang Li,[1,2,7] Zi Yang Meng,[1,8,7,*] Anders W. Sandvik,[3,1,†] and Liling Sun[1,2,7,‡]







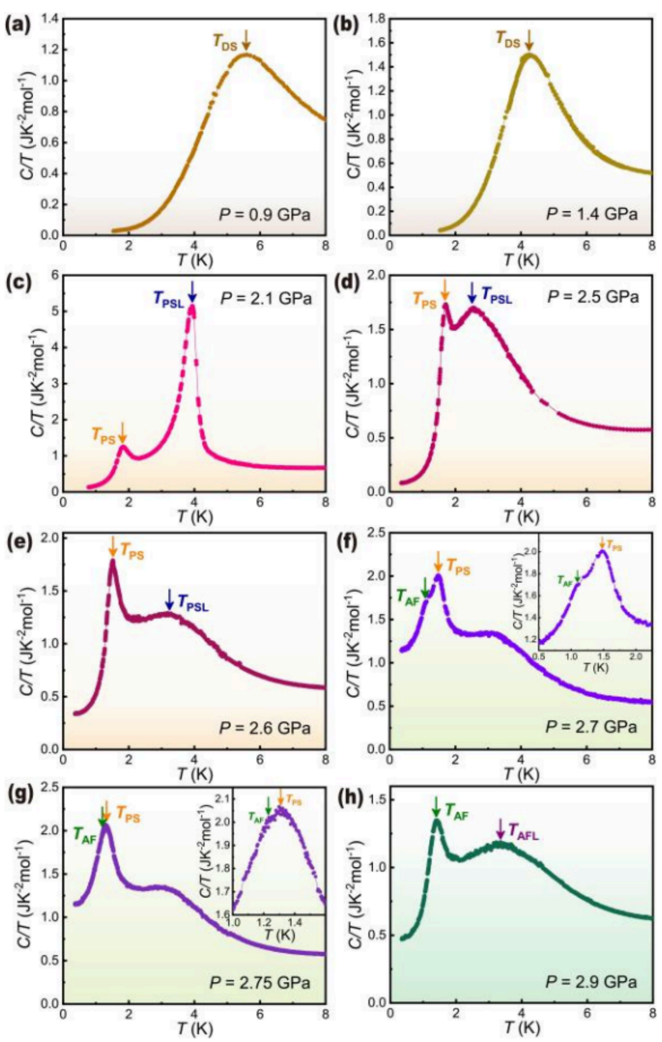
- P < 1.8 GPa: Dimer-singlet state
- P < 2.5GPa: Plaquette-singlet state
- 3 GPa < P < 4 GPa: AF state

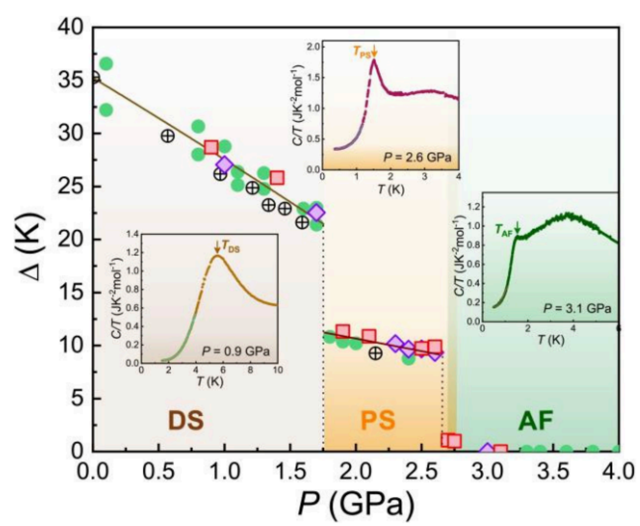
SCBO Experiments

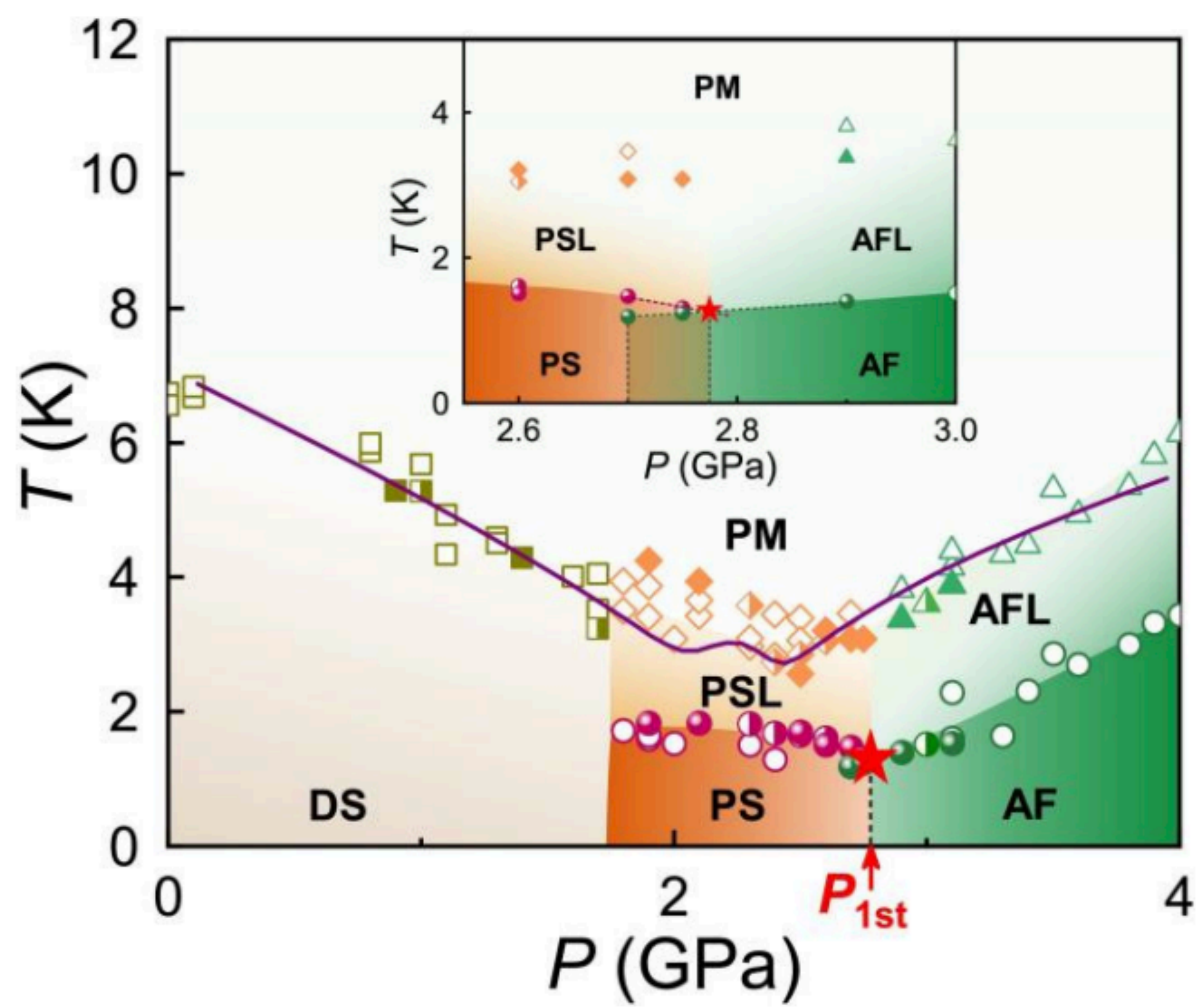
arXiv:2310.20128

Deconfined quantum critical point lost in pressurized $SrCu_2(BO_3)_2$

Jing Guo,[1,5,*] Pengyu Wang,[1,2,*] Cheng Huang,[3,*] Bin-Bin Chen,[3] Wenshan Hong,[1,2] Shu Cai,[4] Jinyu Zhao,[1,2] Jinyu Han,[1,2] Xintian Chen,[1,2] Yazhou Zhou,[1] Shiliang Li,[1,2,5] Qi Wu,[1] Zi Yang Meng,[3,†] and Liling Sun[1,2,4,5,‡]







Simulation

PHYSICAL REVIEW LETTERS **124**, 206602 (2020)

Jing Guo,[1] Guangyu Sun,[1,2] Bowen Zhao,[3] Ling Wang,[4,5] Wenshan Hong,[1,2] Vladimir A. Sidorov,[6] Nvsen Ma,[1]
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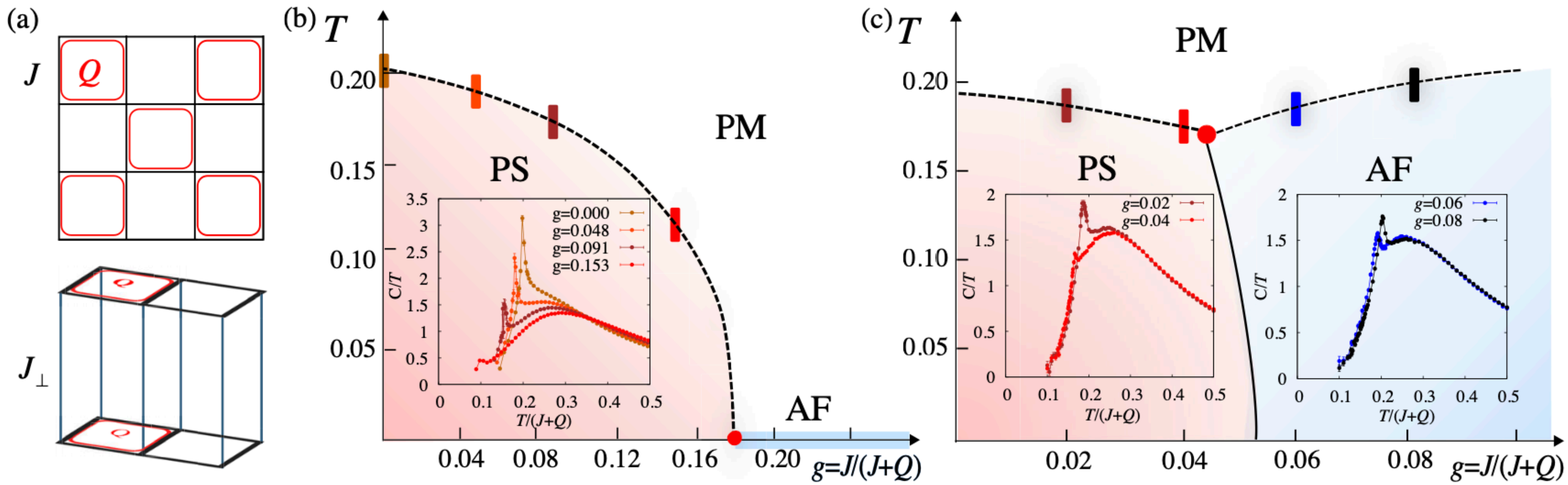
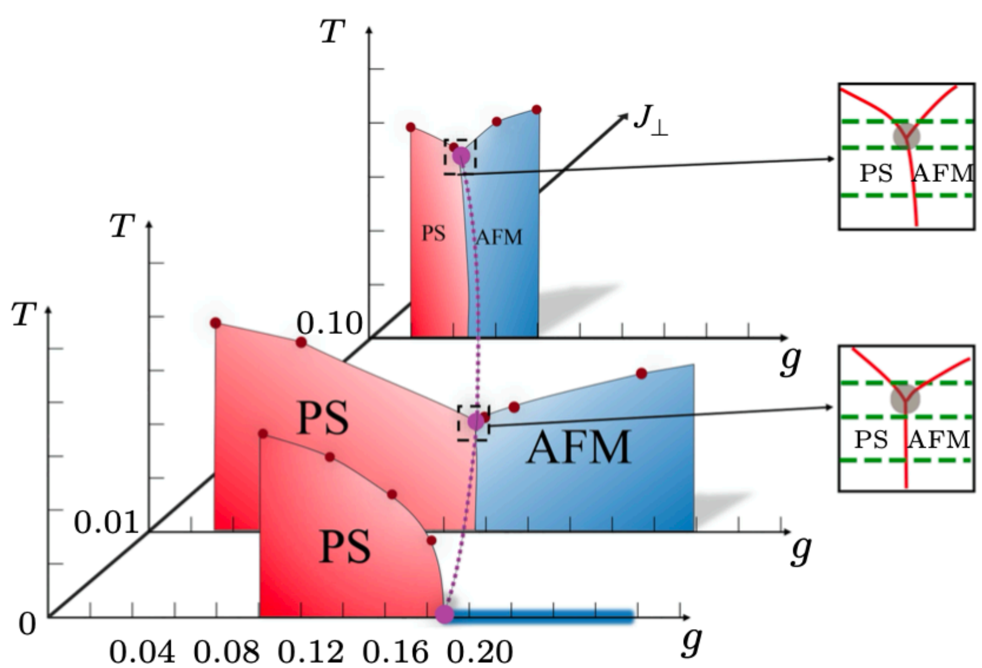
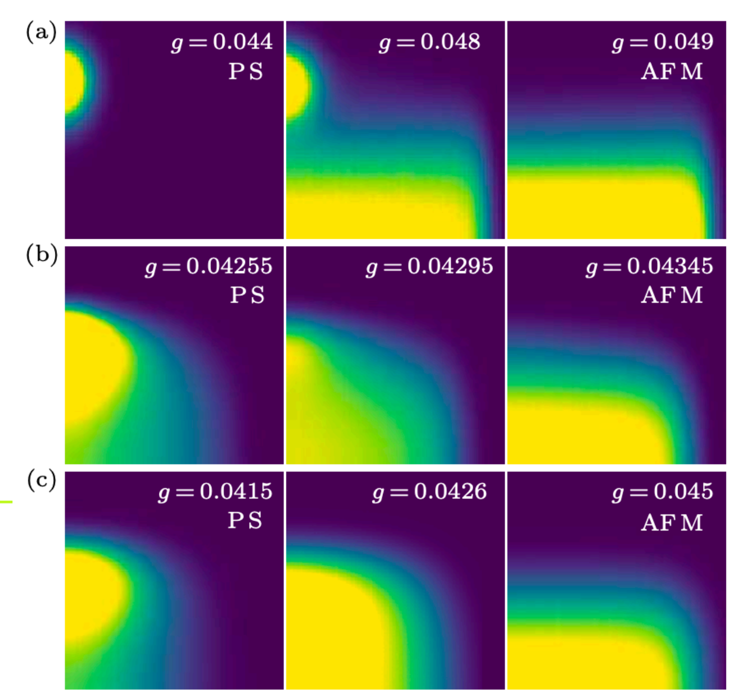


Chin. Phys. B Vol. 30, No. 6 (2021) 067505

Guangyu Sun(孙光宇)[1,2], Nvsen Ma(马女森)[3,1], Bowen Zhao(赵博文)[4],
Anders W. Sandvik[4,1,†], and Zi Yang Meng(孟子杨)[1,5,‡]





Model-Design and Numerical Simulations

- Magnetic phase transitions and Dynamical properties ✔
- Kagome models and Z2 quantum spin liquid (BFG) ✔
- Pyrochlore models and U1 quantum spin liquid (Quantum Spin ice) ✔
- Dirac fermion/spinon coupled with U1 gauge field ✔
- YCu3-Br/Cl and SCBO ✔
- Polynomial Sign problem in TBG
- ……

Auxiliary field quantum Monte Carlo for frustrated spin systems

Julius-Maximilians-UNIVERSITÄT WÜRZBURG

Fakher F. Assaad, Exotic quantum matter from quantum spin liquids to novel field theories, Pollica 26 June 2024

PHYSICAL REVIEW B **104**, L081106 (2021)

Letter

Quantum Monte Carlo simulation of generalized Kitaev models

Toshihiro Sato[1] and Fakher F. Assaad[1,2]

[1]*Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*

[2]*Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany*

arXiv:2312.03080v1

Scale-invariant magnetic anisotropy in α-$RuCl_3$: A quantum Monte Carlo study

Toshihiro Sato,[1,2] B. J. Ramshaw,[3,4] K. A. Modic,[5] and Fakher F. Assaad[1,6]

T. Sato

K. Modic

B. Ramshaw

DFG

SFB1170 ToCoTronics

Center of excellence – complexity and topology in quantum matter

NIC

lrz Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften

GCS Gauss Centre for Supercomputing

KONWIHR

Fermion QMC

Let $\hat{H} = \hat{H}_0 - \lambda \sum_n \left(\hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}} \right)^2$ with $O^{(n)} = O^{(n),\dagger}$

$$Z = \int D\left\{ \Phi(n,\tau) \right\} \; e^{-S(\Phi(n,\tau))}$$

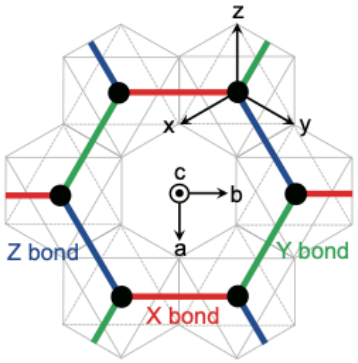
$$S(\Phi(n,\tau)) = \sum_{n,\tau} \Phi^2(n,\tau)/2 - \log \underbrace{\prod_{\tau=1}^{L_\tau} \left(e^{-\Delta\tau \hat{H}_0} \prod_n e^{\sqrt{2\Delta\tau\lambda}\Phi(n,\tau)\hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}}} \right)}_{\det[M(\Phi(n,\tau))]} \qquad L_\tau \Delta\tau = \beta$$

<u>Is the determinant positive ?</u>

C. Wu and S.-C. Zhang. Phys. Rev. B, 71, 155115, (2005).
E. Huffman and S. Chandrasekharan, Phys. Rev. B 89 (2014), 111101.
Zi-Xiang Li, Yi-Fan Jiang, and H. Yao Phys. Rev. Lett. 117 (2016), 267002.
Z. C. Wei, C. Wu, Yi Li, Shiwei Zhang, and T. Xiang. Phys. Rev. Lett. 116 (2016), 250601.
Z. C. Wei, arXiv:1712.09412
.....

R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24 (1981), 2278
J. E. Hirsch, Phys. Rev. B 31 (1985), 4403
White, D. Scalapino, R. Sugar, E. Loh, J. Gubernatis, and R. Scalettar, Phys. Rev. B 40 (1989), 506
....

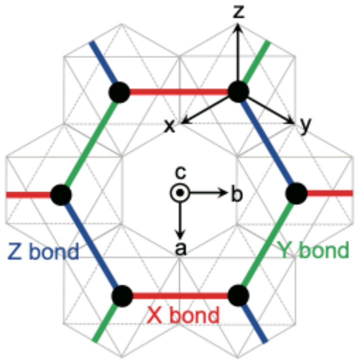
Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi), \ \ J = A\cos(\varphi), \ \ A = \sqrt{K^2 + J^2}$$

Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi), \;\; J = A\cos(\varphi), \;\; A = \sqrt{K^2 + J^2}$$

Simulating spins with fermions.

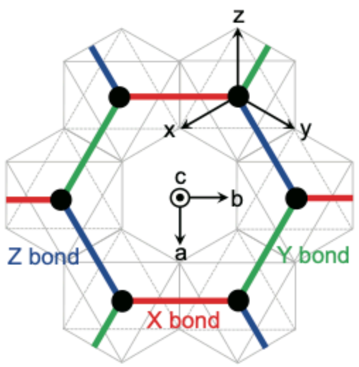
$$\hat{S}_i^{\delta} = \frac{1}{2} \sum_{s,s'} \hat{f}_{i,s}^{\dagger} \sigma_{s,s'}^{\delta} \hat{f}_{i,s'} \qquad \sum_s \hat{f}_{i,s}^{\dagger} \hat{f}_{i,s} \equiv \hat{n}_i = 1$$

$$\hat{H}_{QMC} = |K| \sum_{i \in A, \delta} s_\delta \left(s_\delta \hat{S}_i^{\delta} + \frac{K}{|K|} \hat{S}_{i+\delta}^{\delta} \right)^2 - \frac{J}{8} \sum_{i \in A, \delta} \left(\left[\hat{D}_{i,\delta}^{\dagger} + \hat{D}_{i,\delta} \right]^2 + \left[i\hat{D}_{i,\delta} - i\hat{D}_{i,\delta}^{\dagger} \right]^2 \right) + U \sum_i (\hat{n}_i - 1)^2$$

$$\hat{D}_{i,\delta}^{\dagger} = \sum_s \hat{f}_{i,s}^{\dagger} \hat{f}_{i+\delta,s} \qquad s_\delta = \pm 1$$

Constraint commutes with Hamiltonian dynamics $\left[\hat{H}_{QMC}, (-1)^{\hat{n}_i} \right] = 0$

Auxiliary field quantum Monte Carlo for frustrated spin systems

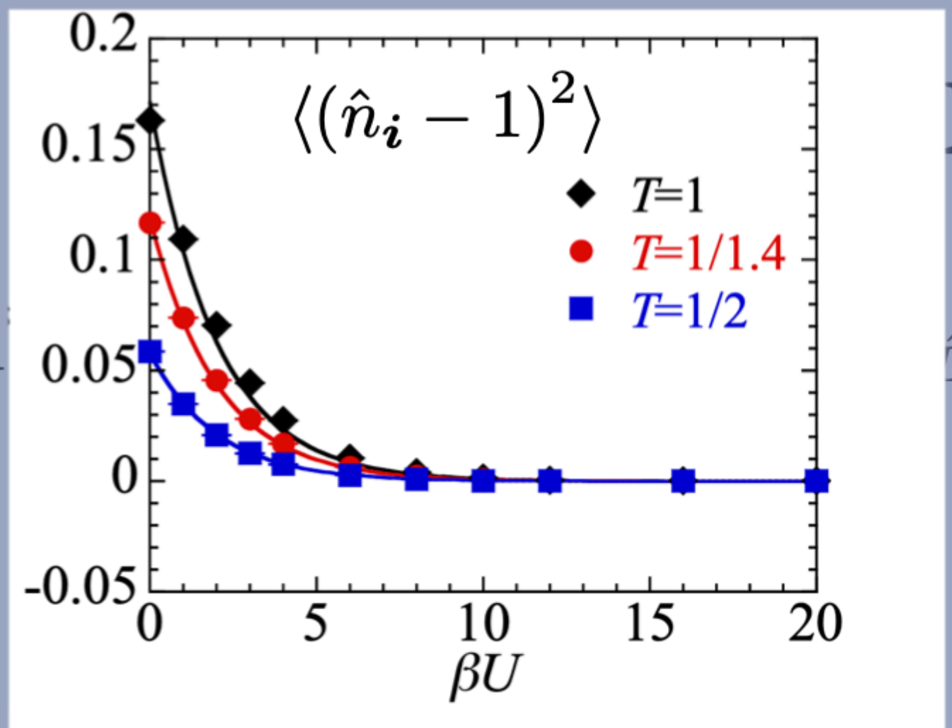


$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi), \;\; J = A\cos(\varphi), \;\; A = \sqrt{K^2 + J^2}$$

Simulating spins with fermions.

$$\hat{f}_{i,s}^{\dagger}\hat{f}_{i,s} \equiv \hat{n}_i = 1$$



$$\hat{H}_{QMC} = |K| \sum_{i \in A, \delta} s_\delta \Big(s_\delta \hat{S}_i^{\delta} + \quad \hat{D}_{i,\delta} - i\hat{D}_{i,\delta}^{\dagger} \Big]^2 \Big) + U \sum_i (\hat{n}_i - 1)^2$$

$$\hat{D}_{i,\delta}^{\dagger} = \sum_s \hat{f}_{i,s}^{\dagger} \hat{f}_{i+\delta,s} \qquad s_\delta$$

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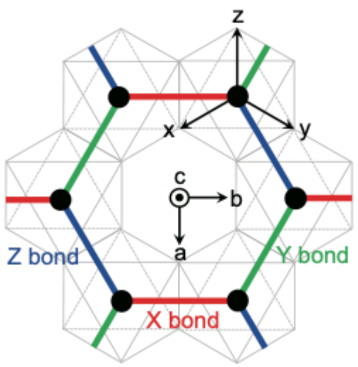
Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

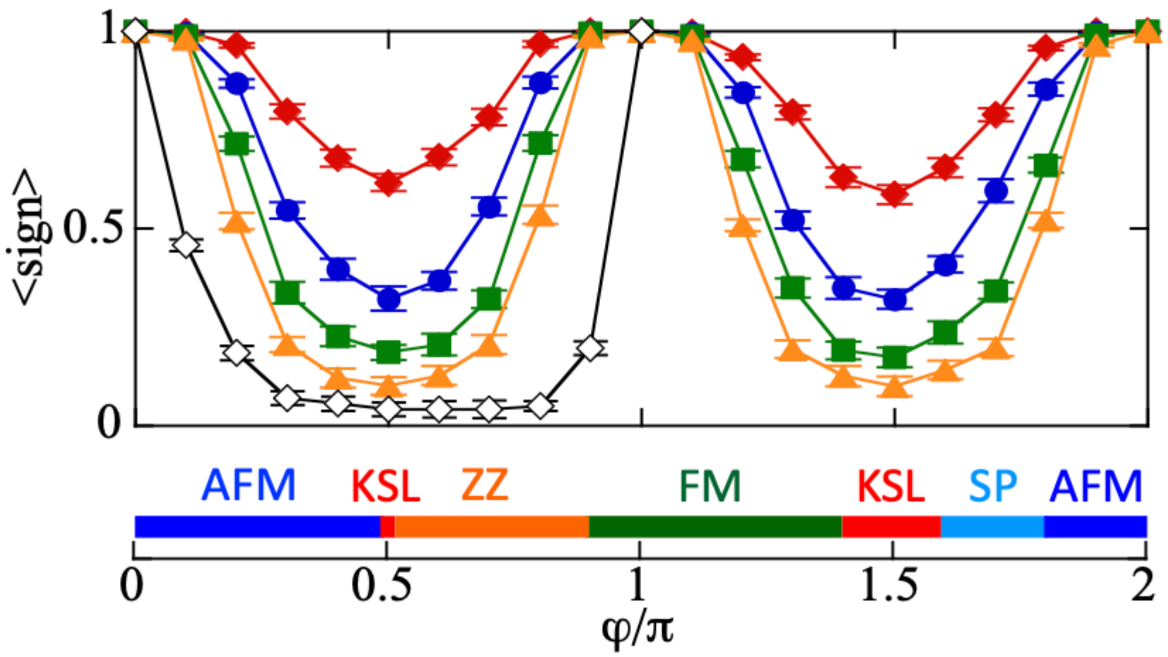
$$K = A\sin(\varphi), \; J = A\cos(\varphi), \; A = \sqrt{K^2 + J^2}$$

$T/A = 1$

◆ V=18 ▲ V=72 Filled symbols $s_x = 1, s_y = s_z = -1$

● V=32 ○ V=18 ○ $s_x = s_y = s_z = 1$

■ V=50



Possible to reach temperatures down to $\beta A \simeq 3$

$A \simeq 10meV \simeq 100K$

→ Experimentally relevant energy scales are accessible

J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.

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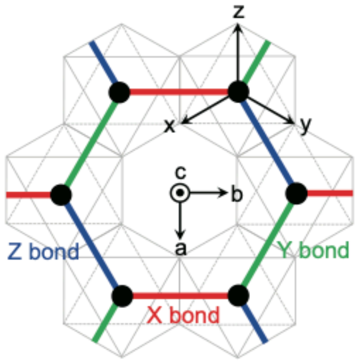
Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = 2K \sum_{i\in A,\delta} \hat{S}_i^\delta \hat{S}_{i+\delta}^\delta + J \sum_{i\in A,\boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

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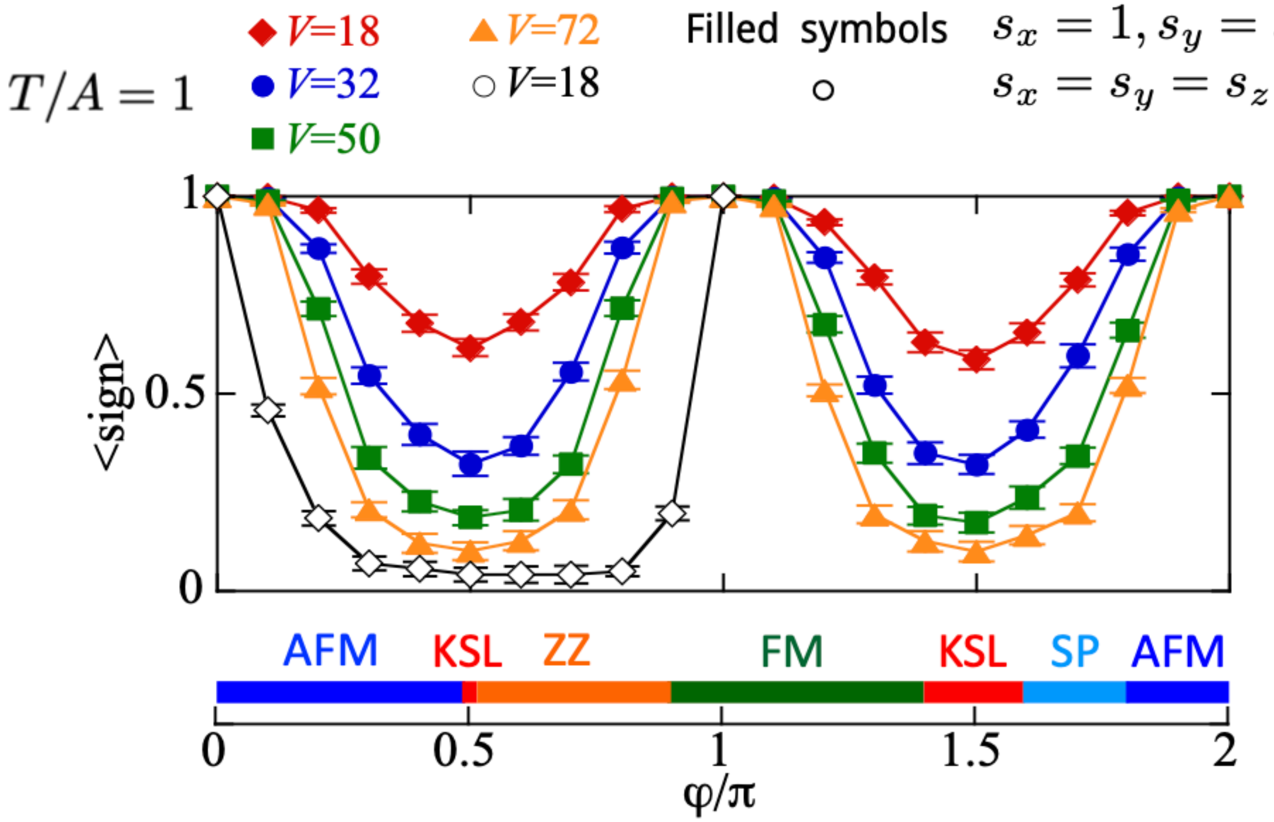
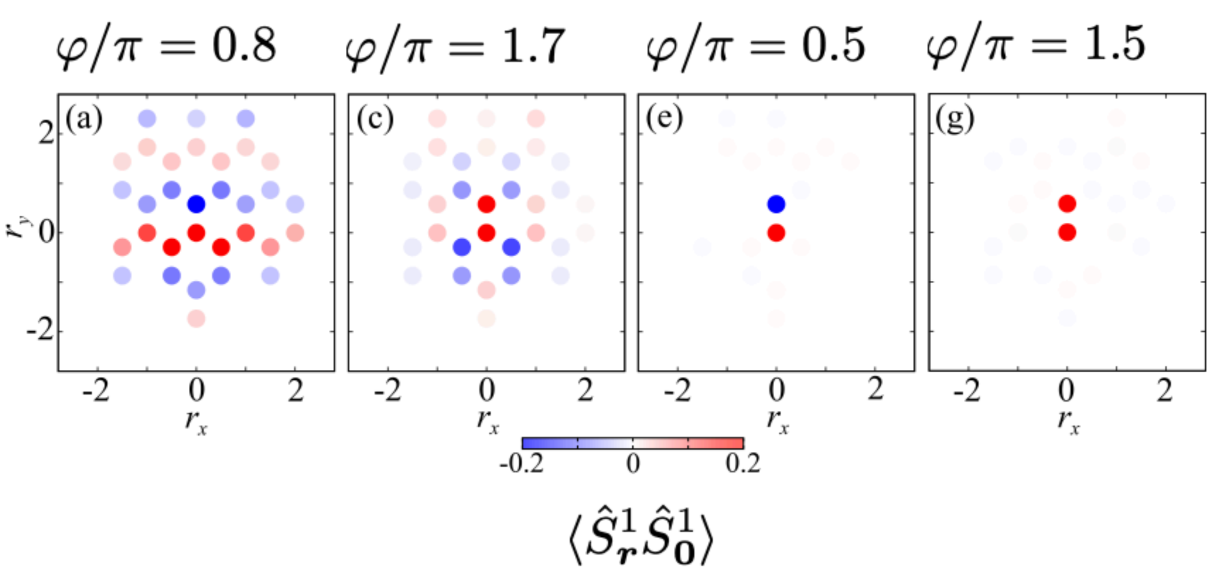
○ $s_x = s_y = s_z = 1$





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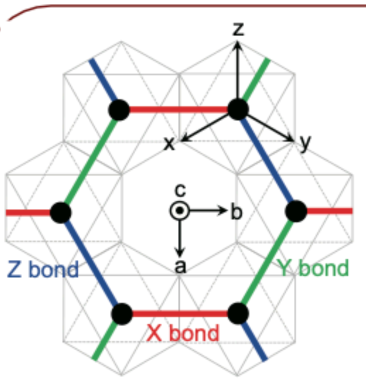
Auxiliary field quantum Monte Carlo for frustrated spin systems



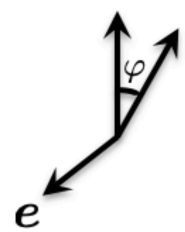
$RuCl_3$

$$\hat{H}(\varphi) = \sum_{\langle i,j \rangle} \left[K \hat{S}_i^\gamma \hat{S}_j^\gamma + \Gamma \hat{S}_i^\alpha \hat{S}_j^\beta + J_1 \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \right] + J_3 \sum_{\langle\langle i,j \rangle\rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j - \mu_B \sum_i \boldsymbol{B}(\varphi) \cdot \boldsymbol{g} \hat{\boldsymbol{S}}_i$$

$$(J_1, J_3, K, \Gamma) = (-0.5, 0.5, -5.0, 2.5) \ [\mathrm{meV}] \qquad \boldsymbol{g} = \mathrm{diag}\,[2.3, 2.3, 1.3]$$

Winter et al. Nat. Comm. 8 (2017), PRL. 120 (2018)

Magnetic rigidity: magnetotropic susceptibility



$$e^{i\varphi \boldsymbol{K}\cdot\boldsymbol{e}} \boldsymbol{B} \equiv \boldsymbol{B}(\varphi)$$

$$k \equiv \left. \frac{\partial^2 F(\varphi)}{\partial \varphi^2} \right|_{\varphi=0} = \mu_B \boldsymbol{g} \langle \hat{\boldsymbol{S}}_{tot} \rangle \cdot \boldsymbol{e} \times (\boldsymbol{e} \times \boldsymbol{B})$$

$$-\mu_B^2 \int_0^\beta d\tau \left[\left\langle \left(\boldsymbol{g}\hat{\boldsymbol{S}}_{tot}(\tau) \cdot \boldsymbol{e} \times \boldsymbol{B} \right) \left(\boldsymbol{g}\hat{\boldsymbol{S}}_{tot}(0) \cdot \boldsymbol{e} \times \boldsymbol{B} \right) \right\rangle - \left(\langle \boldsymbol{g}\hat{\boldsymbol{S}}_{tot}(0) \cdot \boldsymbol{e} \times \boldsymbol{B} \rangle \right)^2 \right]$$

A. Shekhter et al. PRB 2023

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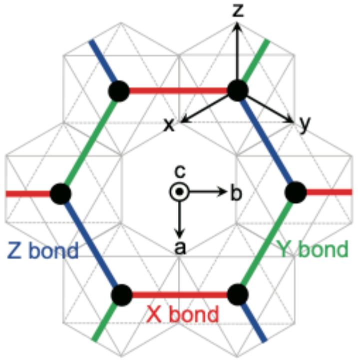
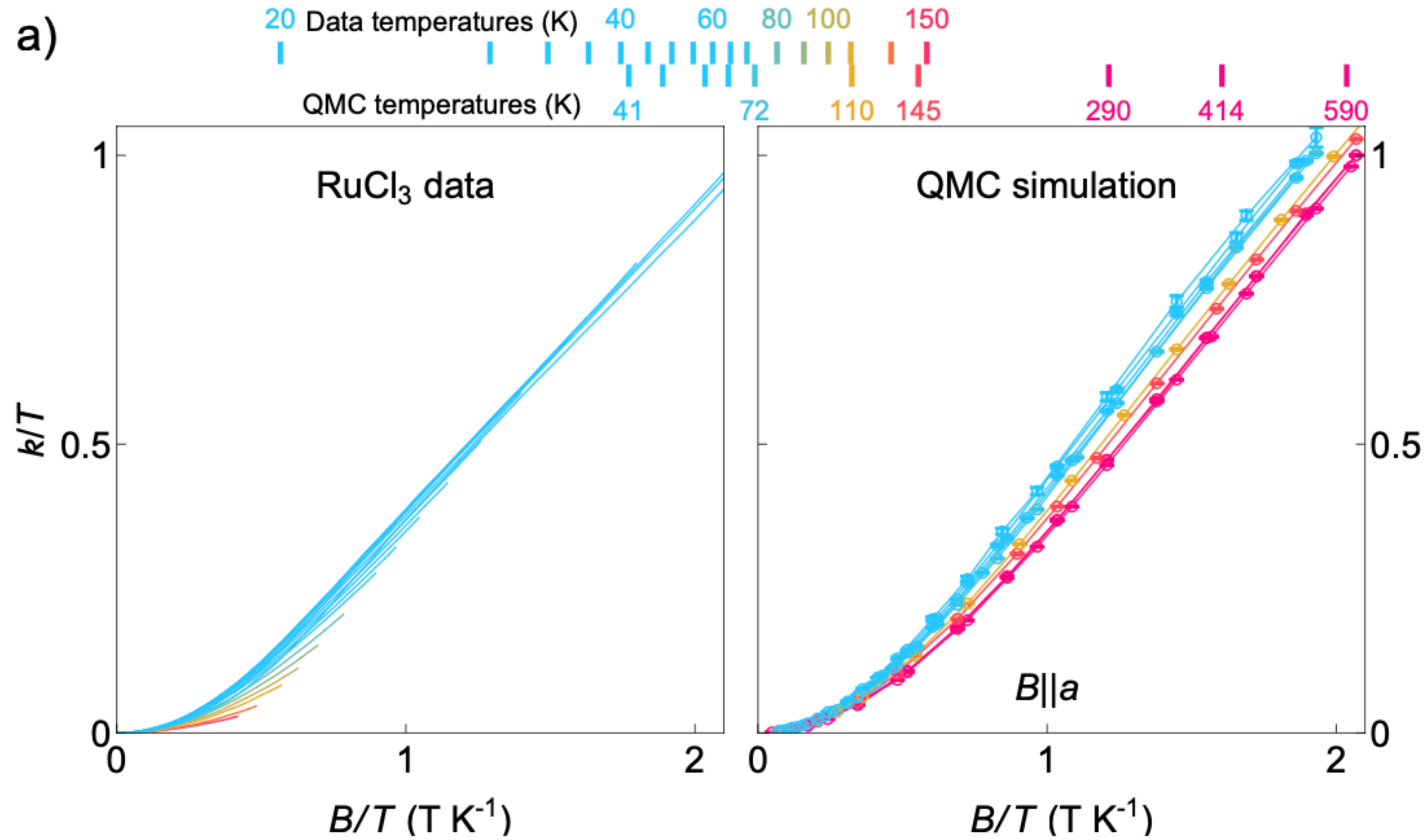
Auxiliary field quantum Monte Carlo for frustrated spin systems



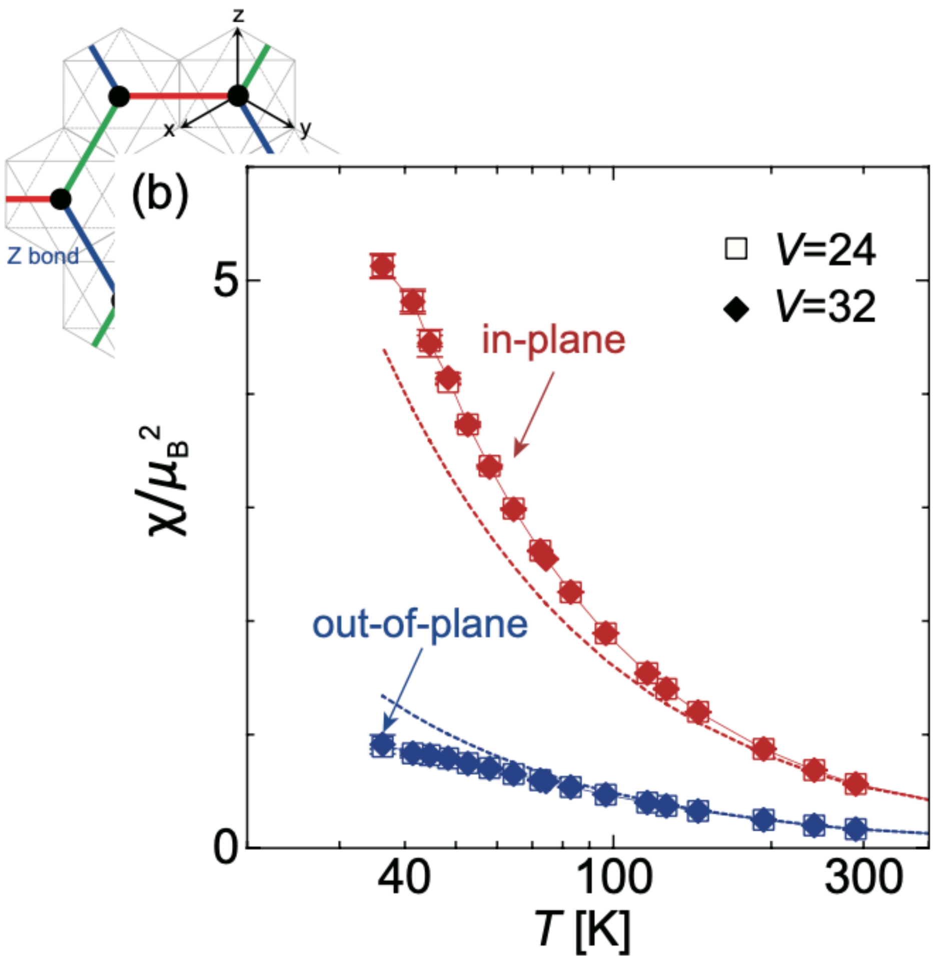


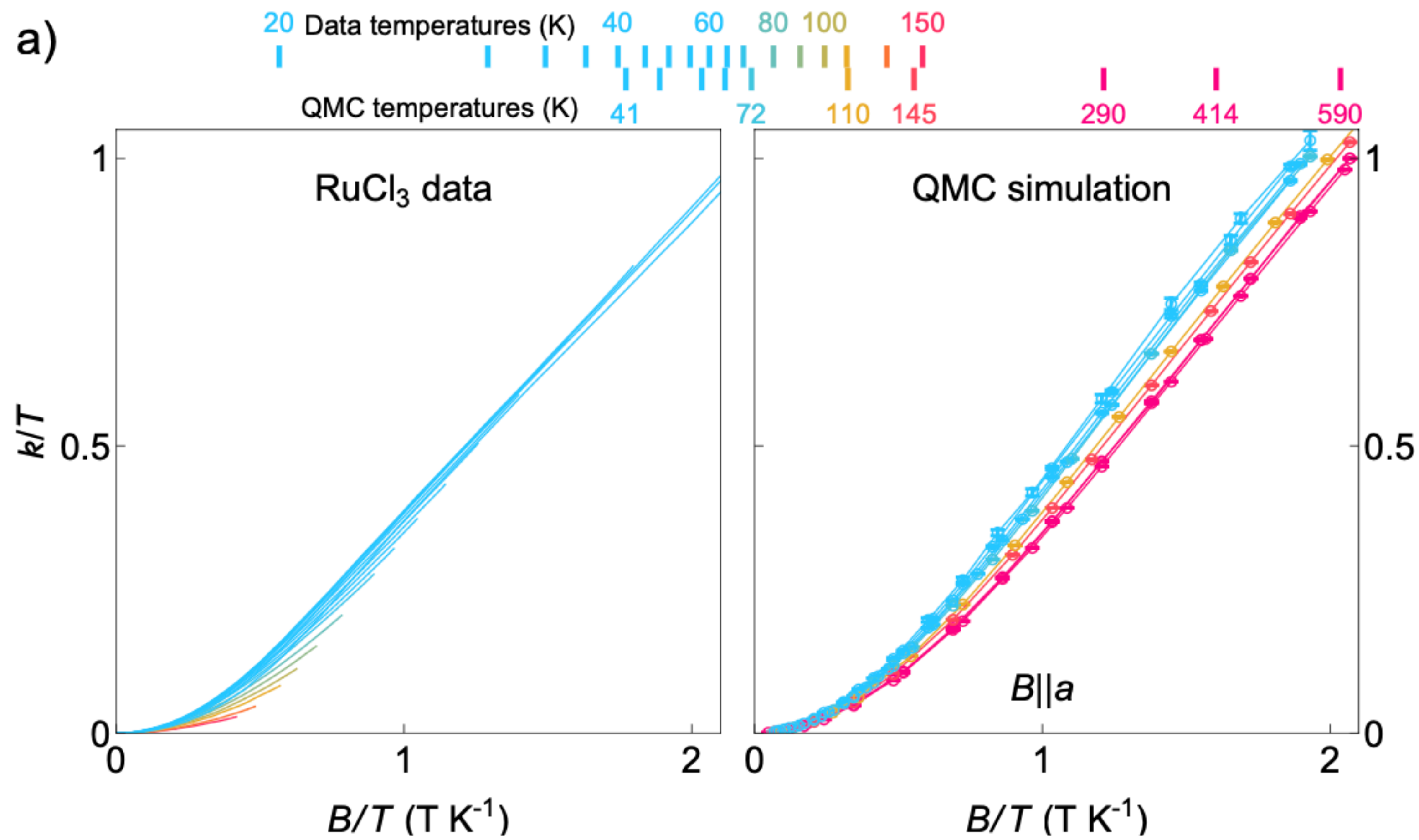
ARTICLES
https://doi.org/10.1038/s41567-020-1028-0
nature physics

Scale-invariant magnetic anisotropy in $RuCl_3$ at high magnetic fields

K. A. Modic[1,2], Ross D. McDonald[3], J. P. C. Ruff[4], Maja D. Bachmann[2,5], You Lai[3,6,7], Johanna C. Palmstrom[5], David Graf[7], Mun K. Chan[3], F. F. Balakirev[3], J. B. Betts[3], G. S. Boebinger[6,7], Marcus Schmidt[2], Michael J. Lawler[8], D. A. Sokolov[2], Philip J. W. Moll[2,9], B. J. Ramshaw[8] and Arkady Shekhter[7]

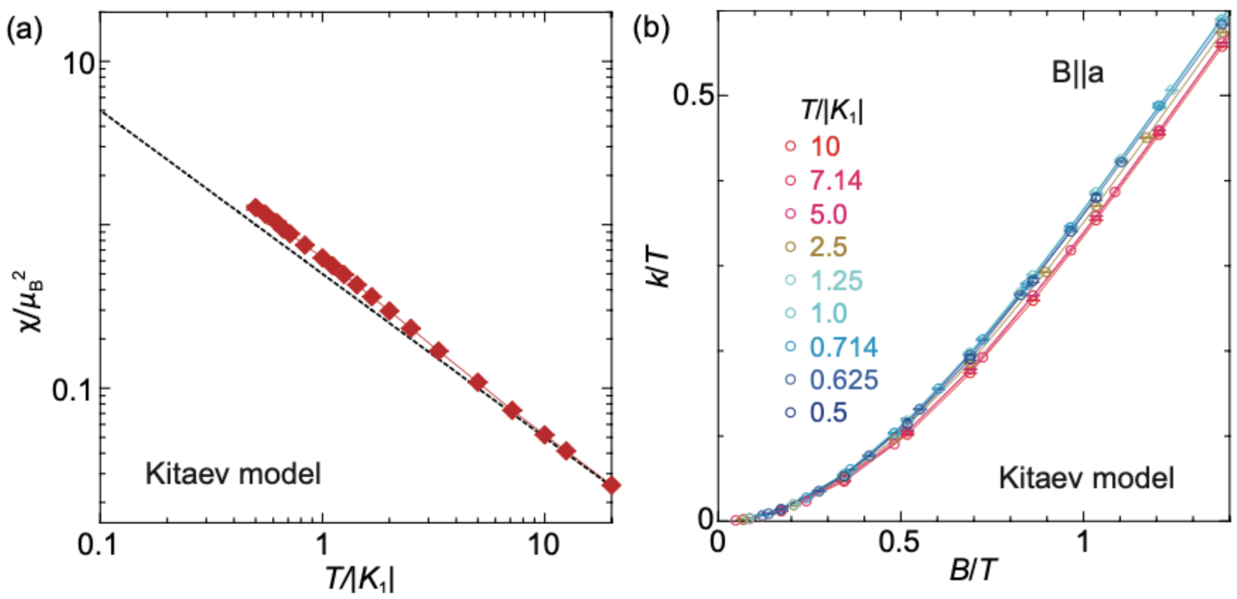
Auxiliary field quantum Monte Carlo for frustrated spin systems





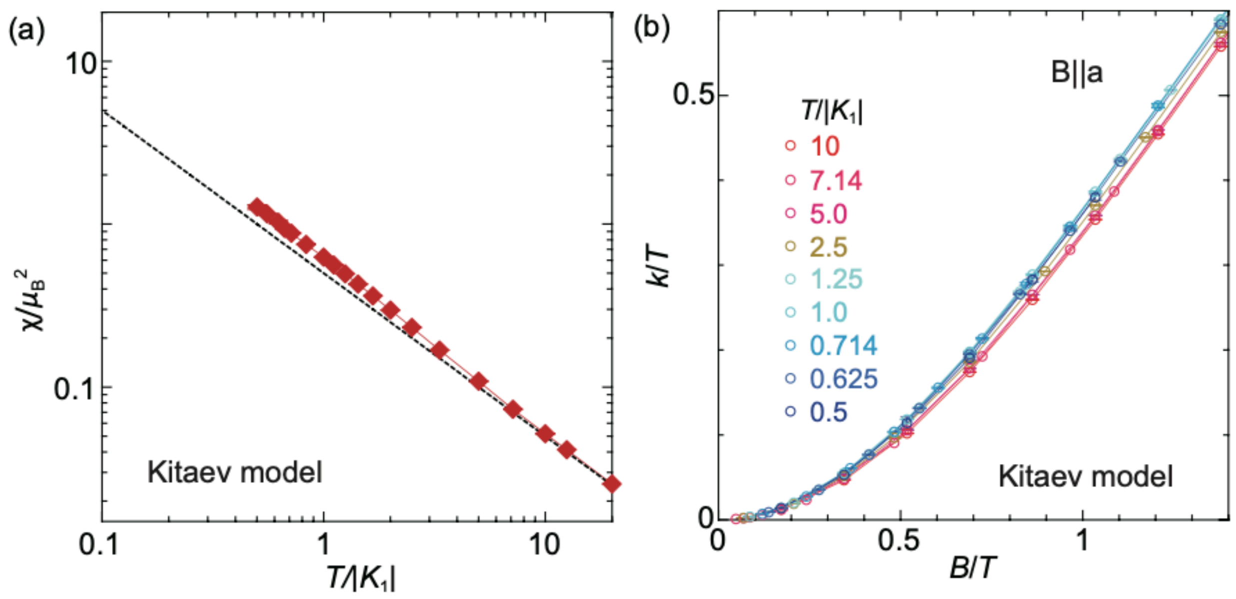
Local moment (no scale): $$k/T = f(|\boldsymbol{B}|/T)$$

Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = K \sum_{\langle i,j \rangle} \hat{S}_i^{\gamma} \hat{S}_j^{\gamma}$$

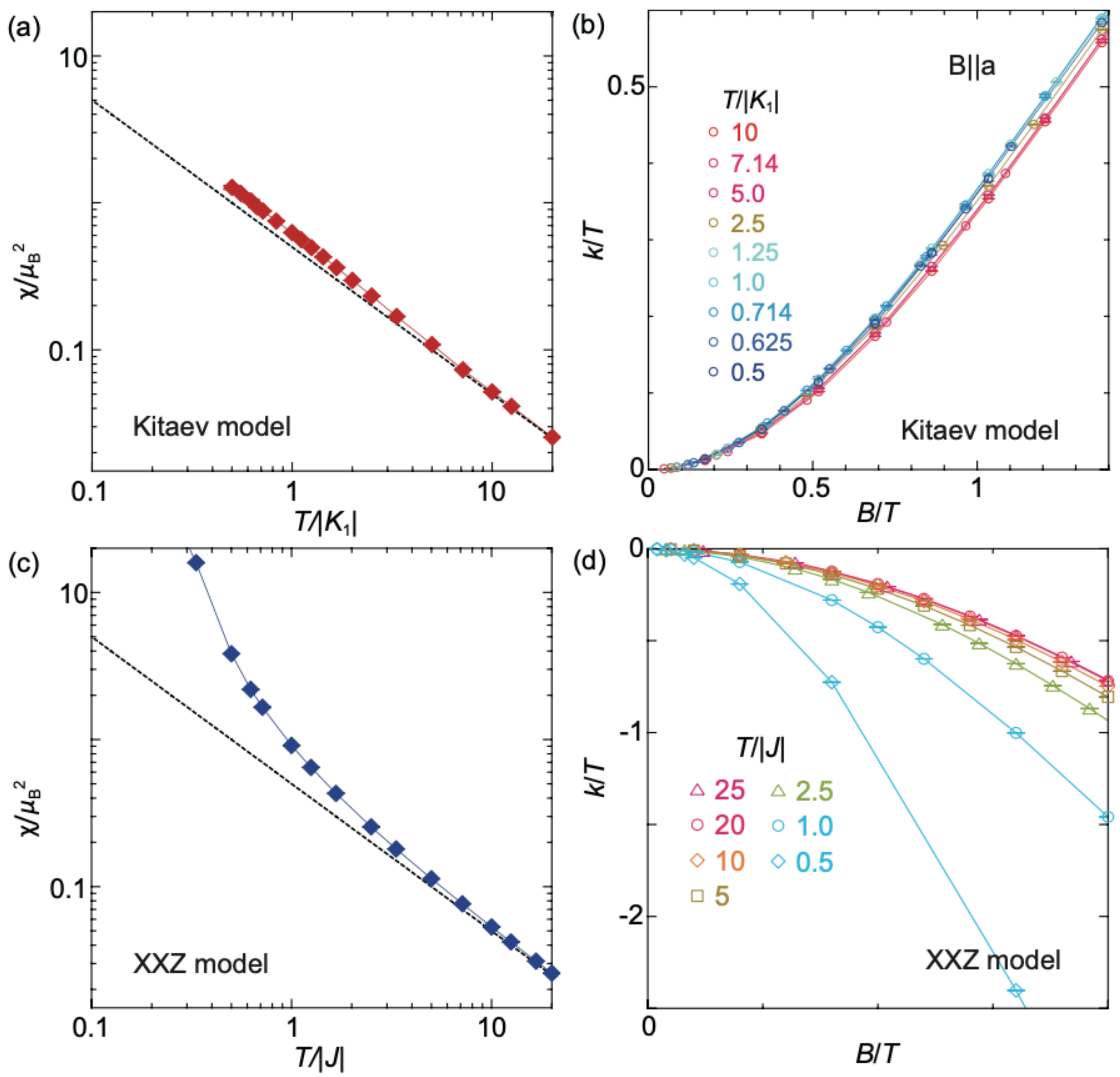
Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = K \sum_{\langle i,j \rangle} \hat{S}_i^{\gamma} \hat{S}_j^{\gamma}$$

$RuCl_3$ is proximate to the Kitaev model

Auxiliary field quantum Monte Carlo for frustrated spin systems

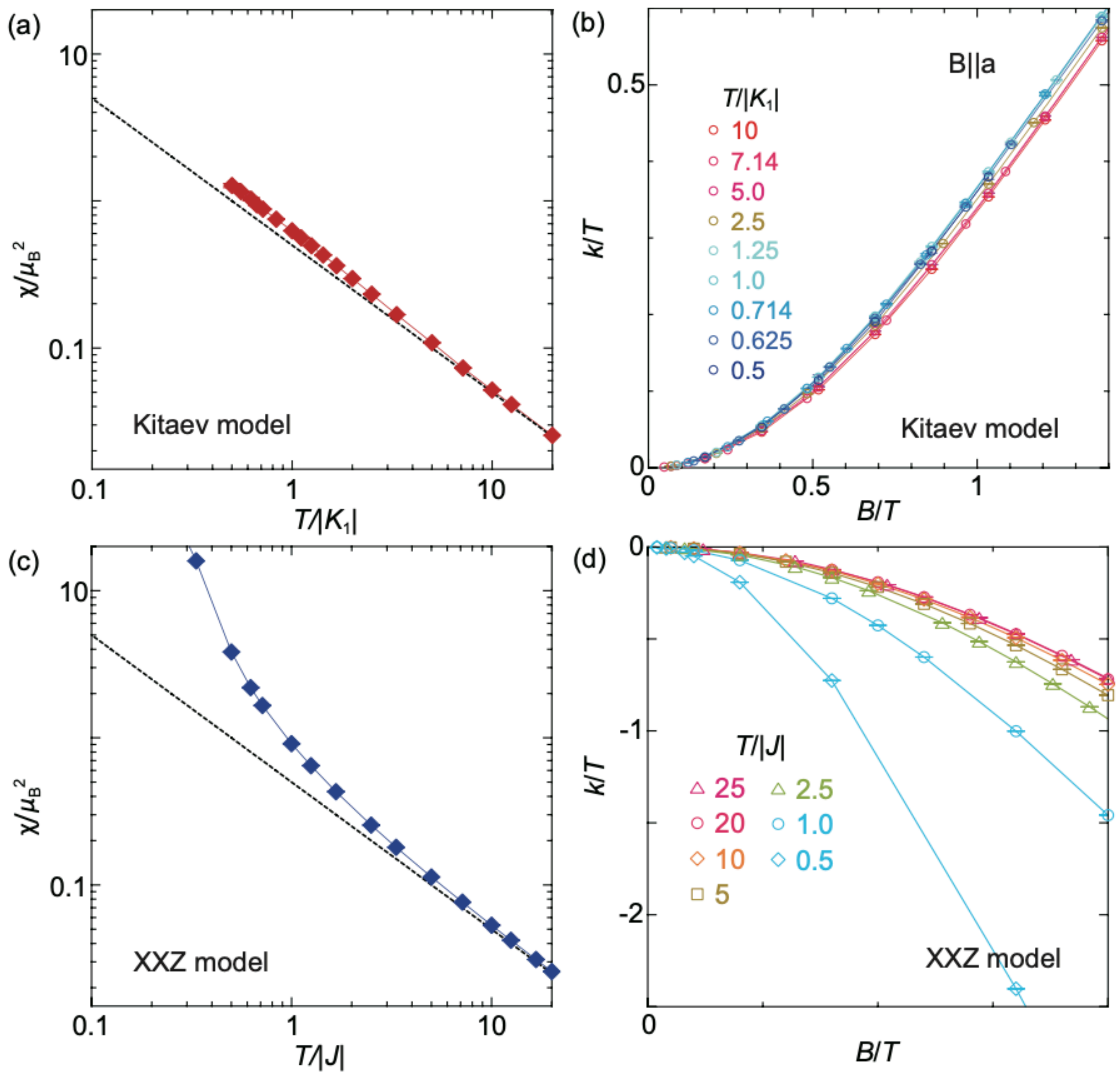


$$\hat{H} = K \sum_{\langle i,j \rangle} \hat{S}_i^\gamma \hat{S}_j^\gamma$$

$RuCl_3$ is proximate to the Kitaev model

$$\hat{H}_{XXZ} = \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} J \left[\hat{S}_{\boldsymbol{i}}^x \cdot \hat{S}_{\boldsymbol{j}}^x + \hat{S}_{\boldsymbol{i}}^y \cdot \hat{S}_{\boldsymbol{j}}^y \right] + [J + J_z] \, \hat{S}_{\boldsymbol{i}}^z \hat{S}_{\boldsymbol{j}}^z$$

Auxiliary field quantum Monte Carlo for frustrated spin systems



$$\hat{H} = K \sum_{\langle i,j \rangle} \hat{S}_i^\gamma \hat{S}_j^\gamma$$

$RuCl_3$ is proximate to the Kitaev model

$$\hat{H}_{XXZ} = \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} J \left[\hat{S}_{\boldsymbol{i}}^x \cdot \hat{S}_{\boldsymbol{j}}^x + \hat{S}_{\boldsymbol{i}}^y \cdot \hat{S}_{\boldsymbol{j}}^y \right] + [J + J_z] \, \hat{S}_{\boldsymbol{i}}^z \hat{S}_{\boldsymbol{j}}^z$$

Low-T scaling is not generic

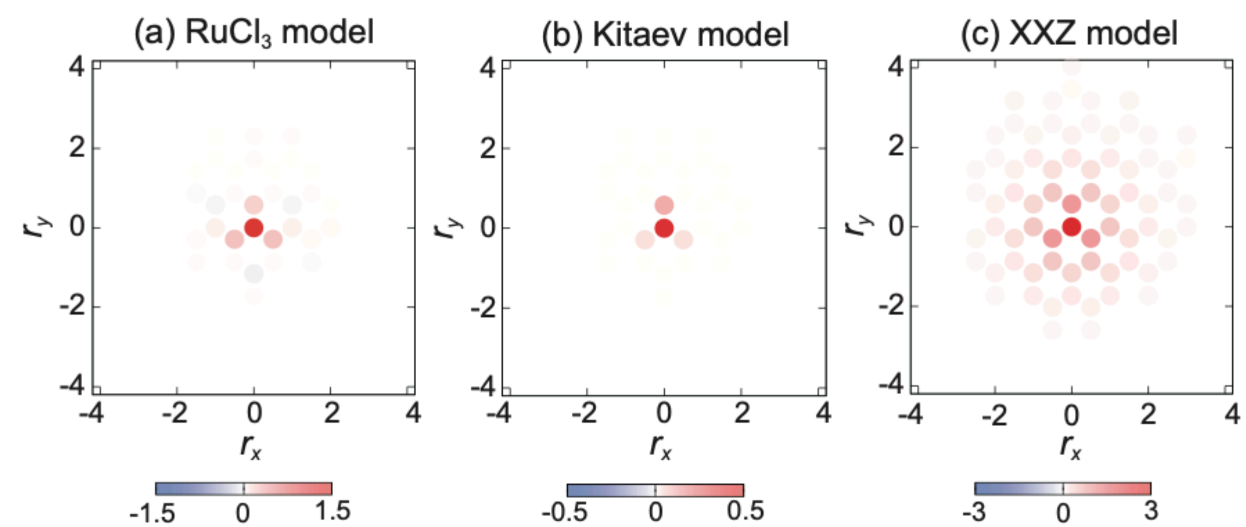
Auxiliary field quantum Monte Carlo for frustrated spin systems

Torque fluctuations

$$\frac{\partial F}{\partial \varphi} = \mu_B \sum_{\boldsymbol{i}} \hat{t}_{\boldsymbol{i}} \quad \text{with} \quad \hat{t}_{\boldsymbol{i}} = (\boldsymbol{e} \times \boldsymbol{B}) \cdot \boldsymbol{g} \hat{\boldsymbol{S}}_{\boldsymbol{i}}$$

$$\langle \hat{t}_{\boldsymbol{r}} \hat{t}_{\boldsymbol{0}} \rangle - \langle \hat{t}_{\boldsymbol{r}} \rangle \langle \hat{t}_{\boldsymbol{0}} \rangle = \sum_{\alpha,\beta} b_\alpha b_\beta \left(\hat{S}^{\alpha}_{\boldsymbol{r}} \hat{S}^{\beta}_{\boldsymbol{0}} \rangle - \langle \hat{S}^{\alpha}_{\boldsymbol{r}} \rangle \langle \hat{S}^{\beta}_{\boldsymbol{0}} \rangle \right)$$

$$\boldsymbol{b} = (\boldsymbol{e} \times \boldsymbol{B}) \cdot \hat{g}$$



Low temperature magnetic anisotropy is that of a renormalized local magnetic moment

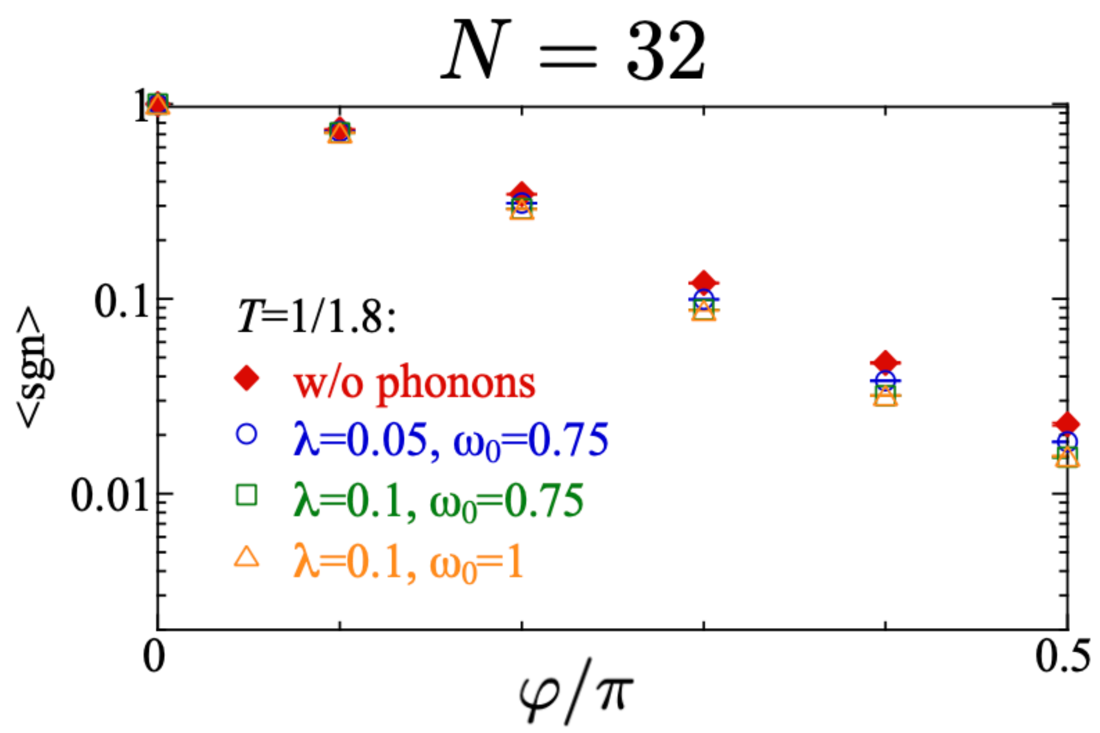
Low lying excitations do not contribute to the magnetotropic susceptibility

Auxiliary field quantum Monte Carlo for frustrated spin systems

Next steps? Debye temperature ~ 200K Magnetic energy scale ~ 100K

$$\hat{H} = \sum_{b=[i\in A,\delta]} \frac{\hat{P}_b^2}{2m} + \frac{k}{2}\hat{Q}_b + 2K(1+\hat{Q}_b)\hat{S}_i^{\delta}\hat{S}_{i+\delta}^{\delta} + J(1+\hat{Q}_b)\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+\delta}$$

$$\omega_0 = \sqrt{\frac{k}{m}},\ \lambda = \frac{1}{2k}$$



Coupling to phonons does not lead to a more severe sign problem!

$$K = A\sin(\varphi),\ J = A\cos(\varphi),\ A = \sqrt{K^2+J^2}$$

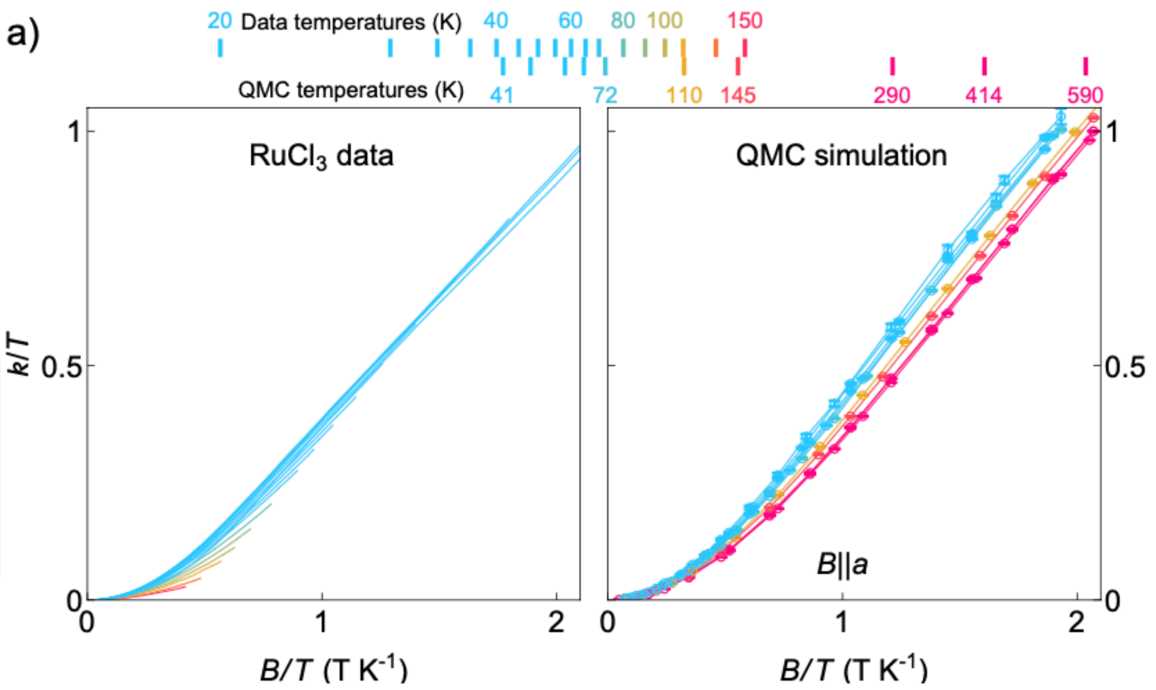
Auxiliary field quantum Monte Carlo for frustrated spin systems

Summary I

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(i,\tau)\right\} e^{-S\left\{\Phi(i,\tau)\right\}}$$

We can simulate frustrated spin models down to experimentally relevant energy scales.

Coupling to phonons does not render the sign problem more severe.

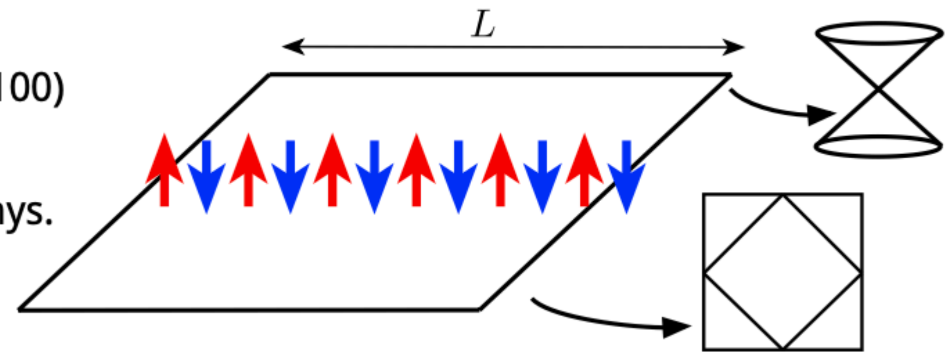


Dimensional mismatch Kondo systems

Toy models to realize **metallic** phases and phase transitions in Kondo systems (FL*, FL, LRO) without confronting the sign problem.

Co atoms
on $Cu_2N/Cu(100)$

R. Toskovic
et al. Nat. Phys.
2016



Kondo breakdown transitions and phases

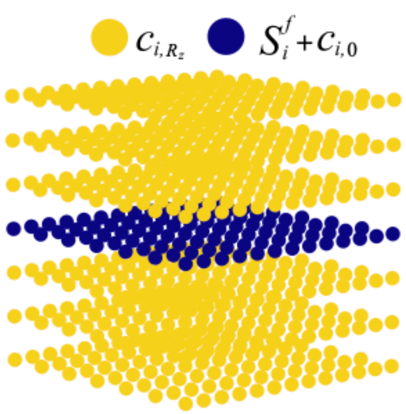
B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.

Dissipation induced magnetic order-disorder transitions

B. Danu, M. Vojta, T. Grover FFA, Phys. Rev. B 106 (2022), L161103.
M. Weber, D. J. Luitz, and FFA, Phys. Rev. Lett. 129 (2022), 056402.

$LaIn_3/CeIn_3$

H. Shishido et al.
Science 2010



Marginal Fermi liquid at magnetic quantum criticality from dimensional confinement

Zi Hong Liu, B. Frank, L. Janssen, M. Vojta, FFA, Phys. Rev. B 107, 165104 (2023)
B. Frank, Zi Hong Liu, FFA, M. Vojta, and L. Janssen, Phys. Rev. B 108 (2023), L100405.

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Dimensional mismatch Kondo systems

Many thanks to...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B. Frank (TUD)


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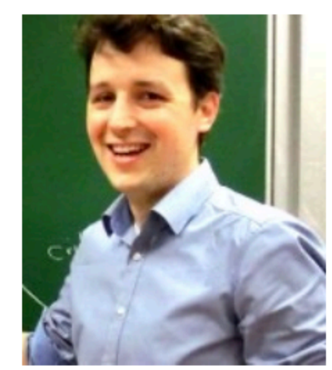
M. Raczkowski (Wü)


S. Biswas (Wü)


T. Grover (UCSD)


M. Vojta (TUD)


L. Janssen (TUD)


D. Luitz (Bonn)

DFG

SFB1170
ToCoTronics

Center of excellence –
complexity and topology in quantum matter

NIC

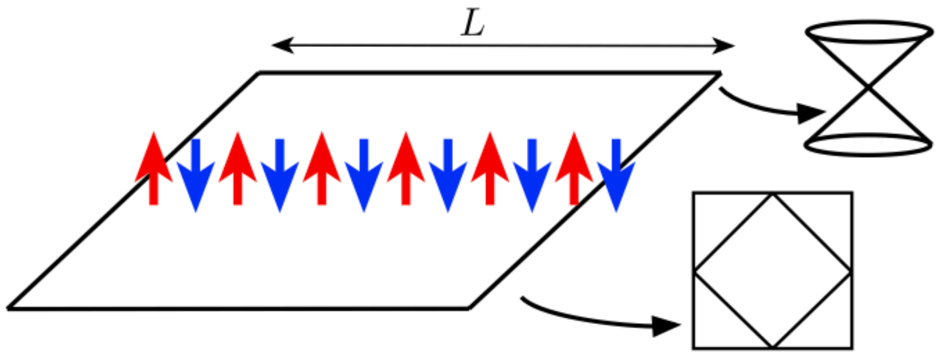
lrz Leibniz-Rechenzentrum
der Bayerischen Akademie der Wissenschaften

GCS
Gauss Centre for Supercomputing

KONWIHR

Kondo phase $J_k >> t$

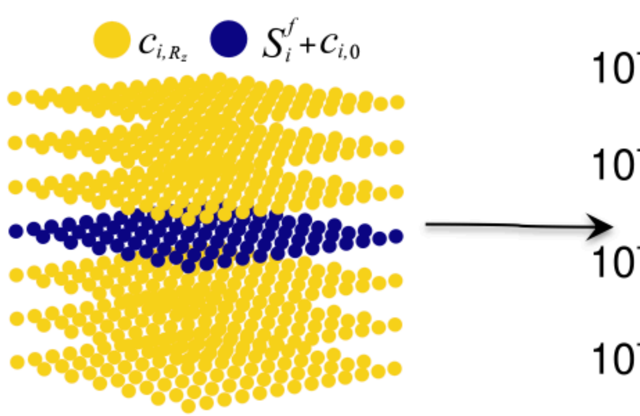
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

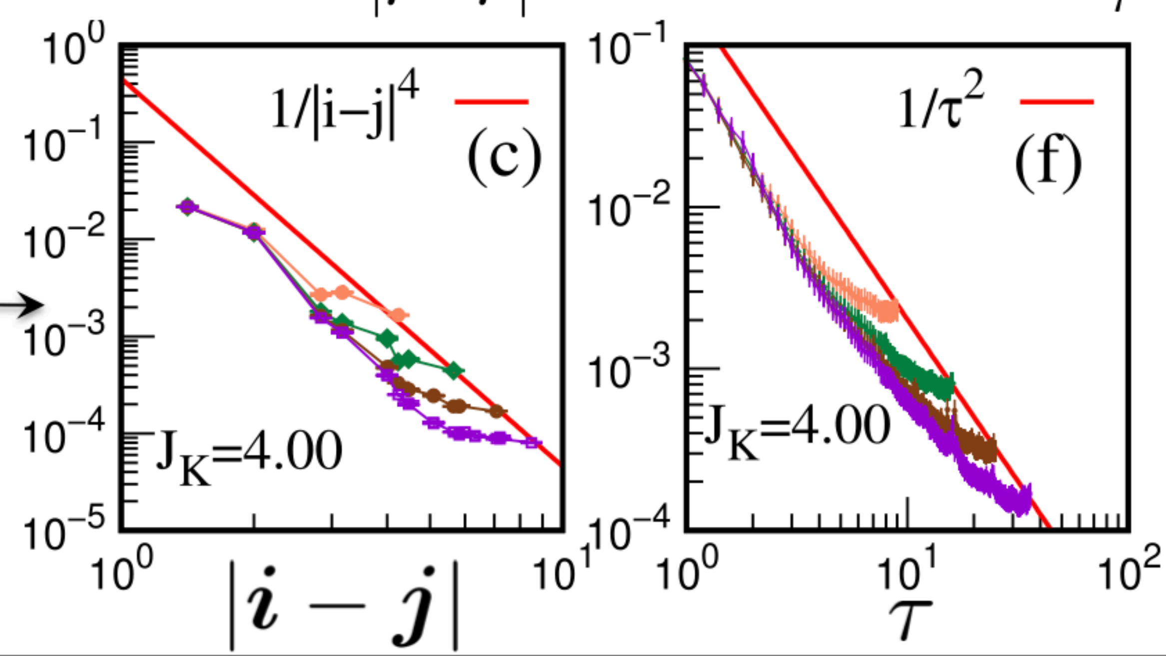


$\hat{\boldsymbol{\Psi}}_i = \hat{\boldsymbol{S}}_i \cdot \boldsymbol{\sigma} \hat{\boldsymbol{c}}_i$ Emergent composite fermion that participates in Luttinger count

Spin-spin correlations inherit power-law of conduction electrons.

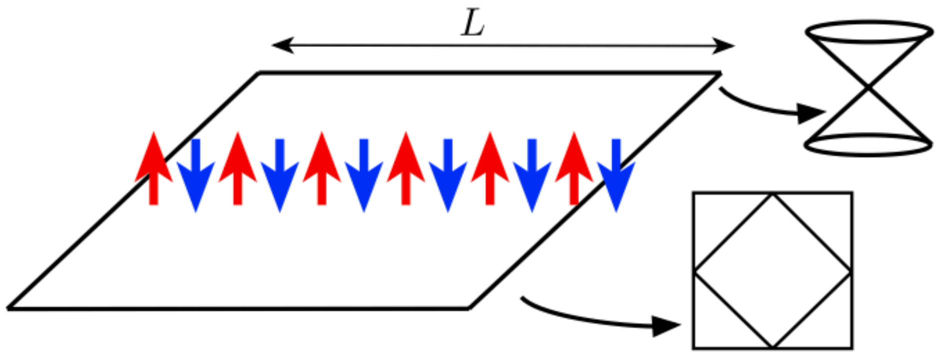
$$\langle \hat{\boldsymbol{S}}_{\boldsymbol{r}} \hat{\boldsymbol{S}}_{\boldsymbol{r}'} \rangle \propto \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|^4} \qquad \langle \hat{\boldsymbol{S}}_{\boldsymbol{r}}(\tau) \hat{\boldsymbol{S}}_{\boldsymbol{r}}(0) \rangle \propto \frac{1}{\tau^2}$$





$$\langle \boldsymbol{f}_{\boldsymbol{i}}^{\dagger}(\tau) \boldsymbol{\sigma} \boldsymbol{f}_{\boldsymbol{i}}(\tau) \cdot \boldsymbol{f}_{\boldsymbol{j}}^{\dagger}(0) \boldsymbol{\sigma} \boldsymbol{f}_{\boldsymbol{j}}(0) \rangle = \langle \tilde{\boldsymbol{f}}_{\boldsymbol{i}}^{\dagger}(\tau) \boldsymbol{\sigma} \tilde{\boldsymbol{f}}_{\boldsymbol{i}}(\tau) \cdot \tilde{\boldsymbol{f}}_{\boldsymbol{j}}^{\dagger}(0) \boldsymbol{\sigma} \tilde{\boldsymbol{f}}_{\boldsymbol{j}}(0) \rangle$$

Weak-coupling $J_k << t$

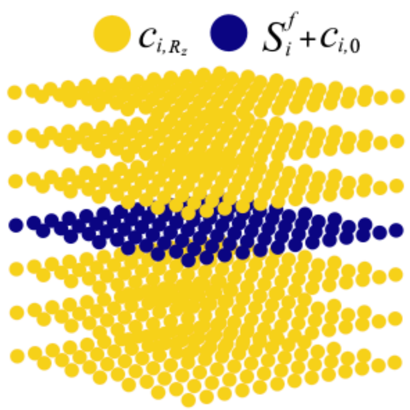


$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Integrate out electrons à la Hertz-Millis

$$\mathcal{S}(\boldsymbol{n}) = \mathcal{S}_{\text{spin}}(\boldsymbol{n}) + \mathcal{S}_{\text{diss}}(\boldsymbol{n}) + \cdots$$

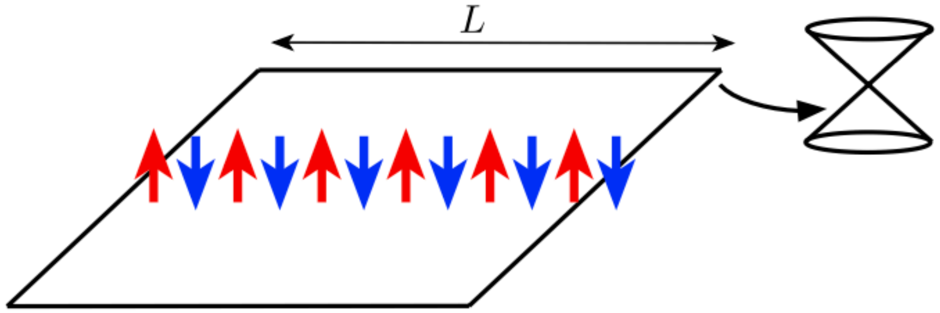
$$\mathcal{S}_{\text{diss}}(\boldsymbol{n}) = \frac{J_k^2}{8} \int d\tau d\tau' \sum_{\boldsymbol{r},\boldsymbol{r}'} \boldsymbol{n}_{\boldsymbol{r}}(\tau) \chi^0(\boldsymbol{r}-\boldsymbol{r}', \tau-\tau') \boldsymbol{n}_{\boldsymbol{r}'}(\tau').$$



Spin susceptibility of the host metal

Spin chain on semi-metal

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.



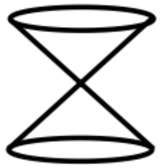
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Integrate out electrons à la Hertz-Millis

$$\mathcal{S}(\boldsymbol{n}) = \mathcal{S}_{\text{spin}}(\boldsymbol{n}) + \mathcal{S}_{\text{diss}}(\boldsymbol{n}) + \cdots$$

$$\mathcal{S}_{\text{diss}}(\boldsymbol{n}) = \frac{J_k^2}{8} \int d\tau d\tau' \sum_{\boldsymbol{r},\boldsymbol{r}'} \boldsymbol{n}_{\boldsymbol{r}}(\tau) \chi^0(\boldsymbol{r} - \boldsymbol{r}', \tau - \tau') \boldsymbol{n}_{\boldsymbol{r}'}(\tau').$$

$$\Delta_n = \frac{1}{2}$$



$$\chi^0(\boldsymbol{0}, \tau - \tau') \propto \frac{1}{v_F^2 (\tau - \tau')^4}$$

$$\chi^0(r\boldsymbol{e}_x, 0) \propto \frac{1}{r^4}$$

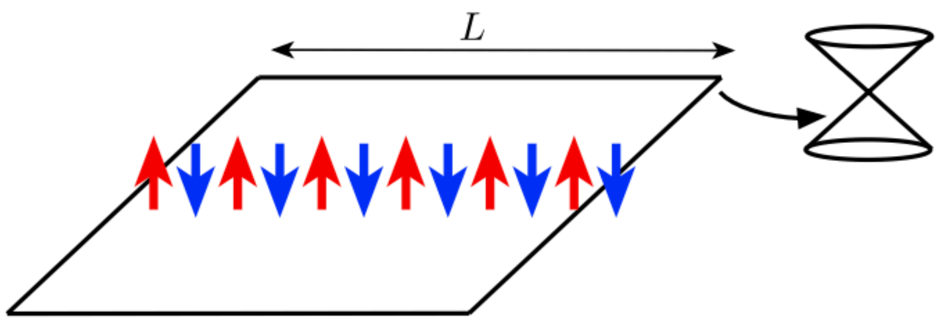
Kondo is irrelevant

For: $\boldsymbol{r} \rightarrow \lambda \boldsymbol{r}, \ \tau \rightarrow \lambda \tau$,

$$\mathcal{S}_{\text{diss}}(\boldsymbol{n}) = \frac{J_k^2}{8} \int d\tau d\tau' d\boldsymbol{r} \, \boldsymbol{n}_{\boldsymbol{r}}(\tau) \chi^0(0, \tau - \tau') \boldsymbol{n}_{\boldsymbol{r}}(\tau') \rightarrow \lambda^{-2} \mathcal{S}_{\text{diss}}(\boldsymbol{n})$$

Spin chain on semi-metal

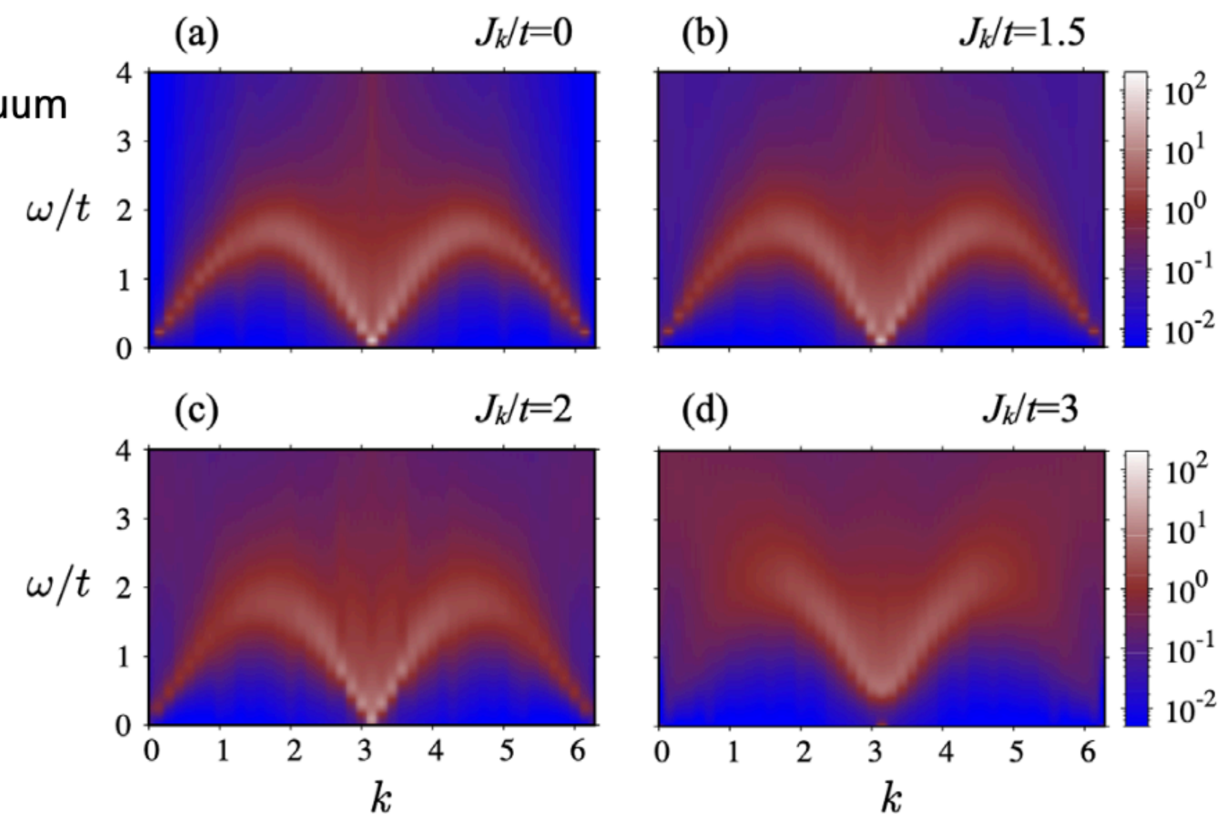
B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.



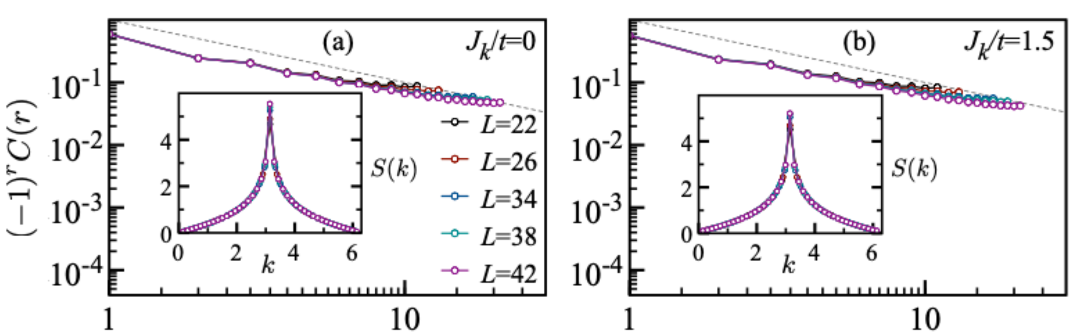
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

$$S(\boldsymbol{q},\omega) = \frac{\chi''(\boldsymbol{q},\omega)}{1 - e^{-\beta\omega}}$$

Two spinon continuum



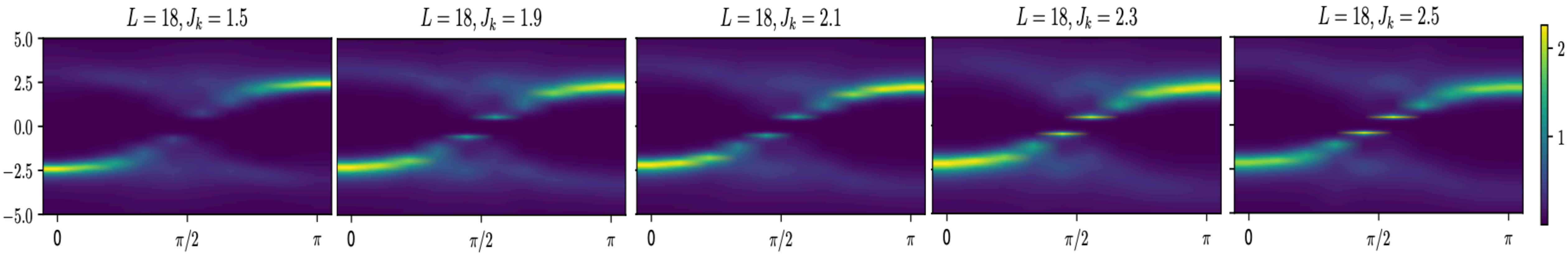
$S(\boldsymbol{q})$



Spin chain on semi-metal

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.

Composite fermion spectral function



$$A(\omega) = -\mathrm{Im}G^{\mathrm{ret}}(\omega), \quad G^{\mathrm{ret}}(\omega) = -i\int_0^\infty dt e^{i\omega t}\sum_\sigma \langle\{\hat{\psi}_\sigma(t), \hat{\psi}^\dagger_\sigma(0)\}\rangle$$

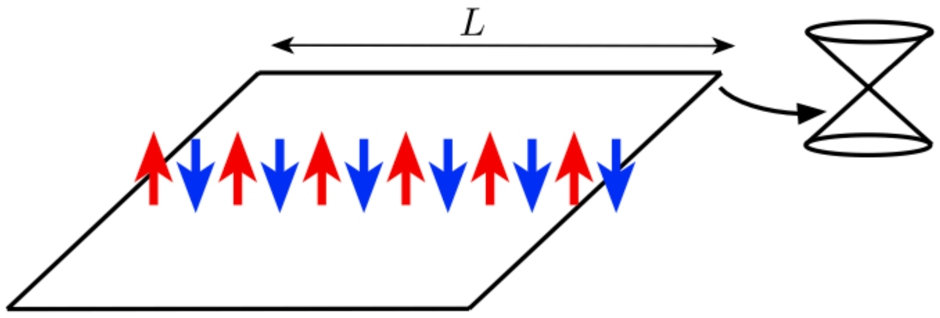
$$\hat{\boldsymbol{\psi}}^\dagger = e^{-S}\hat{\boldsymbol{d}}^\dagger e^S = \hat{\boldsymbol{c}}^\dagger_{\boldsymbol{r}=0}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{S}}$$

(S: Schrieffer Wolff transformation)

T.A. Costi, Phys. Rev. Lett. 85, 1504 (2000).

Spin chain on semi-metal

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.



$$\hat{H} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}(\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2}\sum_{\boldsymbol{r}}\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{r}}\boldsymbol{\sigma}\hat{\boldsymbol{c}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h\sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle}\hat{\boldsymbol{S}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

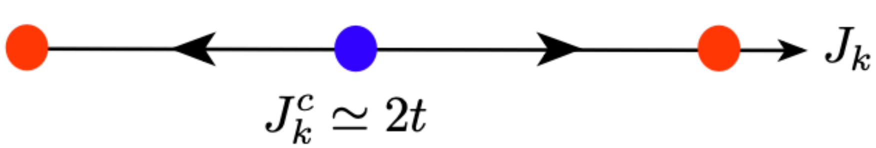
$$S(\boldsymbol{q},\omega) = \frac{\chi''(\boldsymbol{q},\omega)}{1-e^{-\beta\omega}}$$

FL*

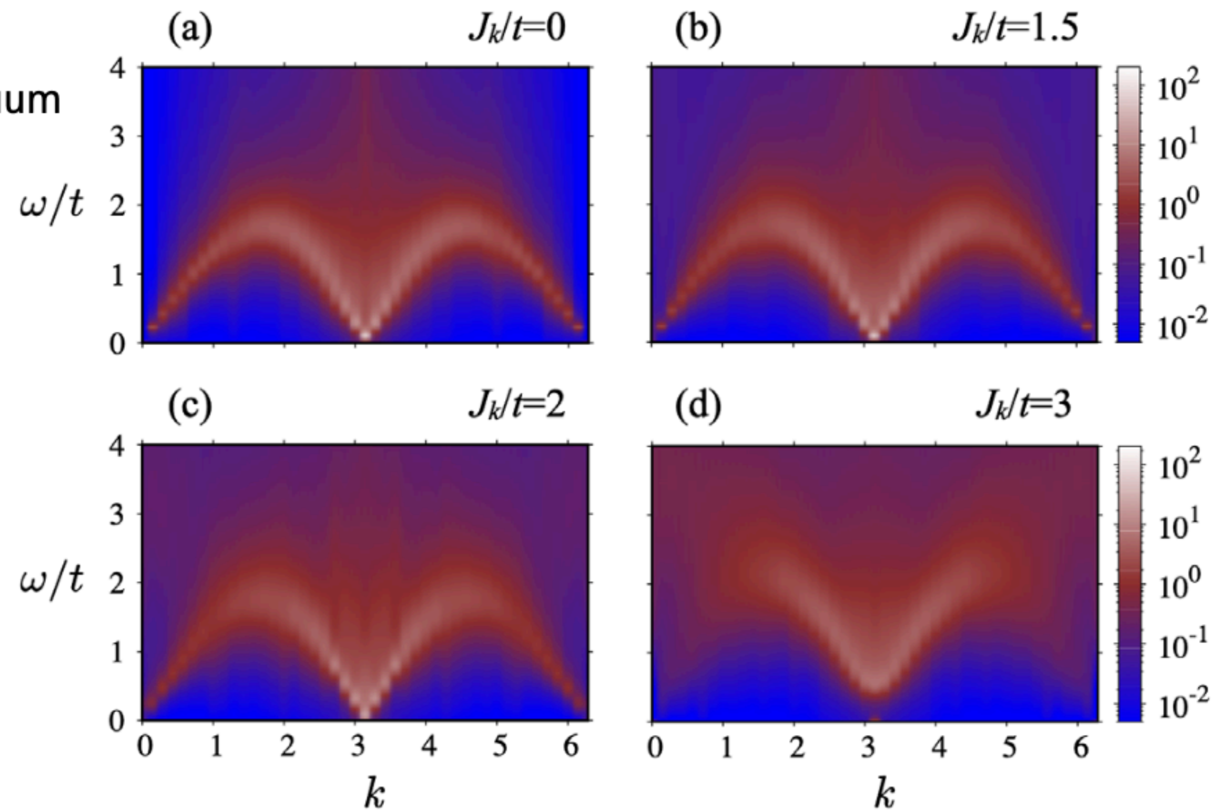
$\langle b\rangle = 0,\ \langle \boldsymbol{n}\rangle = 0$

Heavy fermion metal

$\langle b\rangle \neq 0,\ \langle \boldsymbol{n}\rangle = 0$



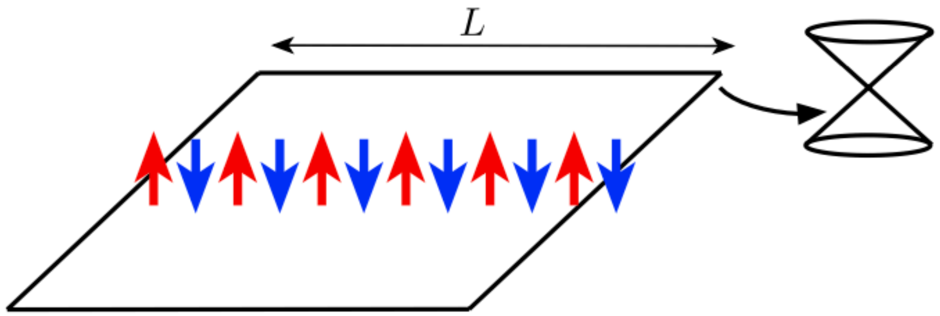
Two spinon continuum



Questions:

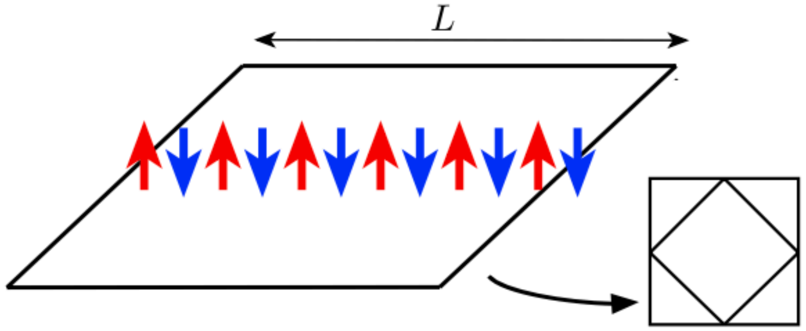
1) Critical exponents ?
2) Transport ?
3) Unique realization of Kondo Breakdown transition → playground to investigate various entanglement measures and witnesses. F. Mazza et al. arXiv:2403.12779.

Summary II



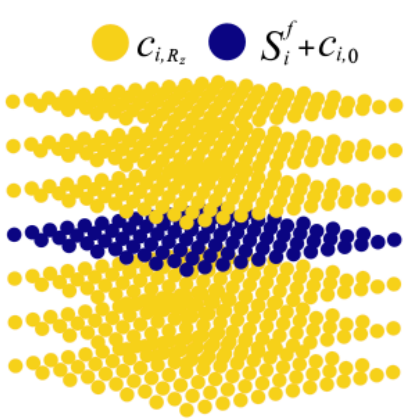
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Kondo breakdown transition



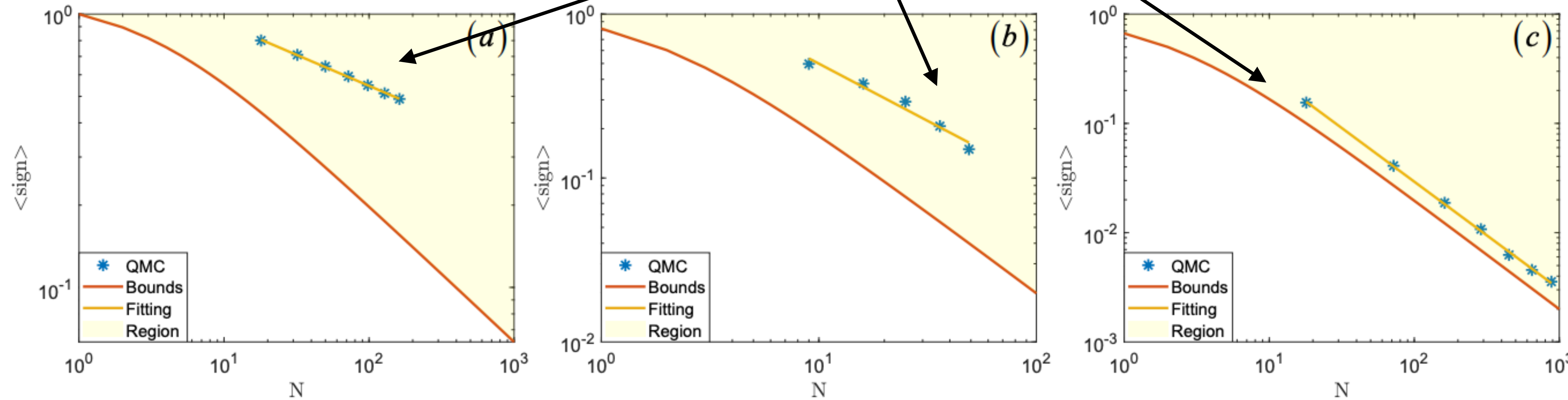
Dissipation induced long range order

QCP between antiferromagnetic heavy fermion metal and heavy fermion metal



Realization of marginal Fermi liquid at QCP between antiferromagnetic heavy fermion metal and heavy fermion metal

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



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

momentum space model

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

reference, two valley, charge neutrality point

real space model

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

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

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

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

$\nu = \pm 2$ target

$\nu = 0$ charge neutrality point, reference

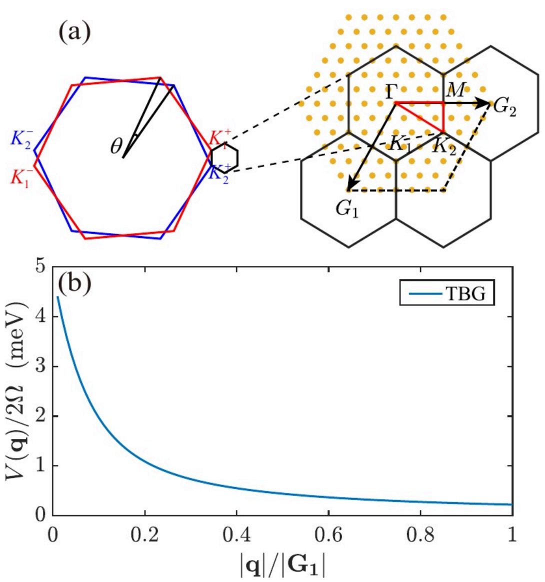
Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)

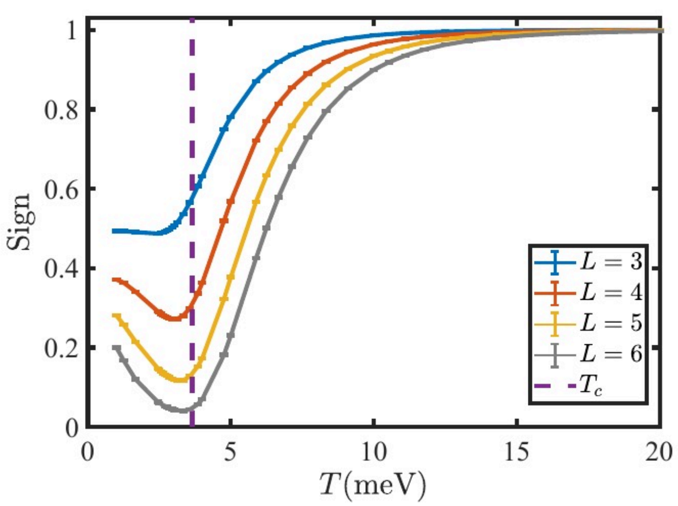
Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

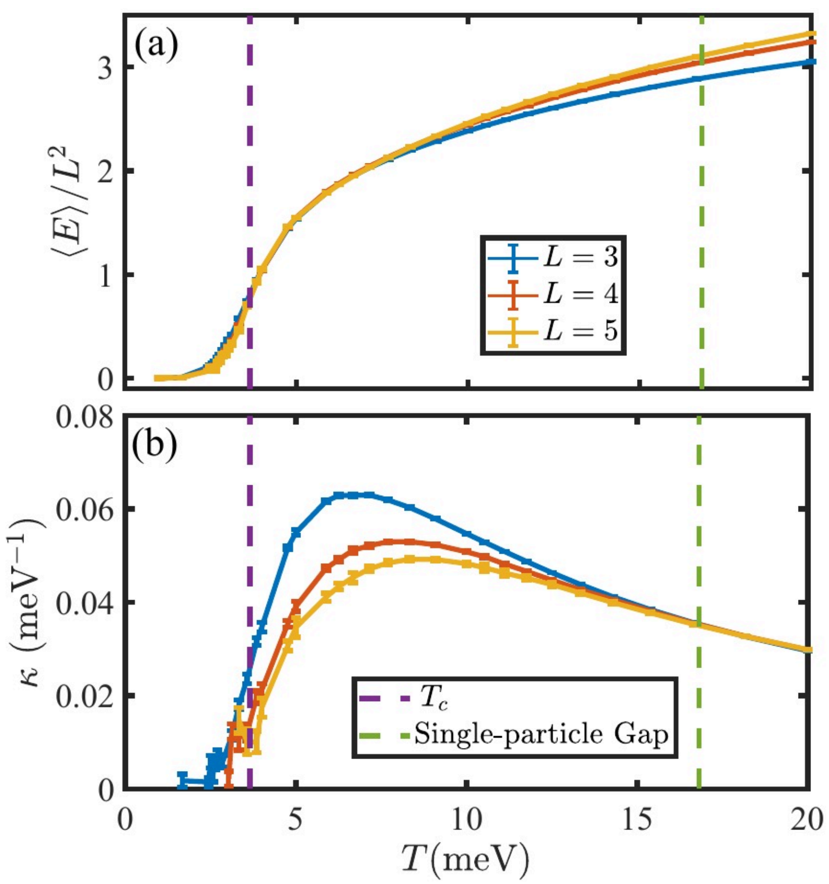
Gaopei Pan,[1,2] Xu Zhang,[3] Hongyu Lu,[3] Heqiu Li,[4] Bin-Bin Chen,[3] Kai Sun,[5,*] and Zi Yang Meng[3,†]

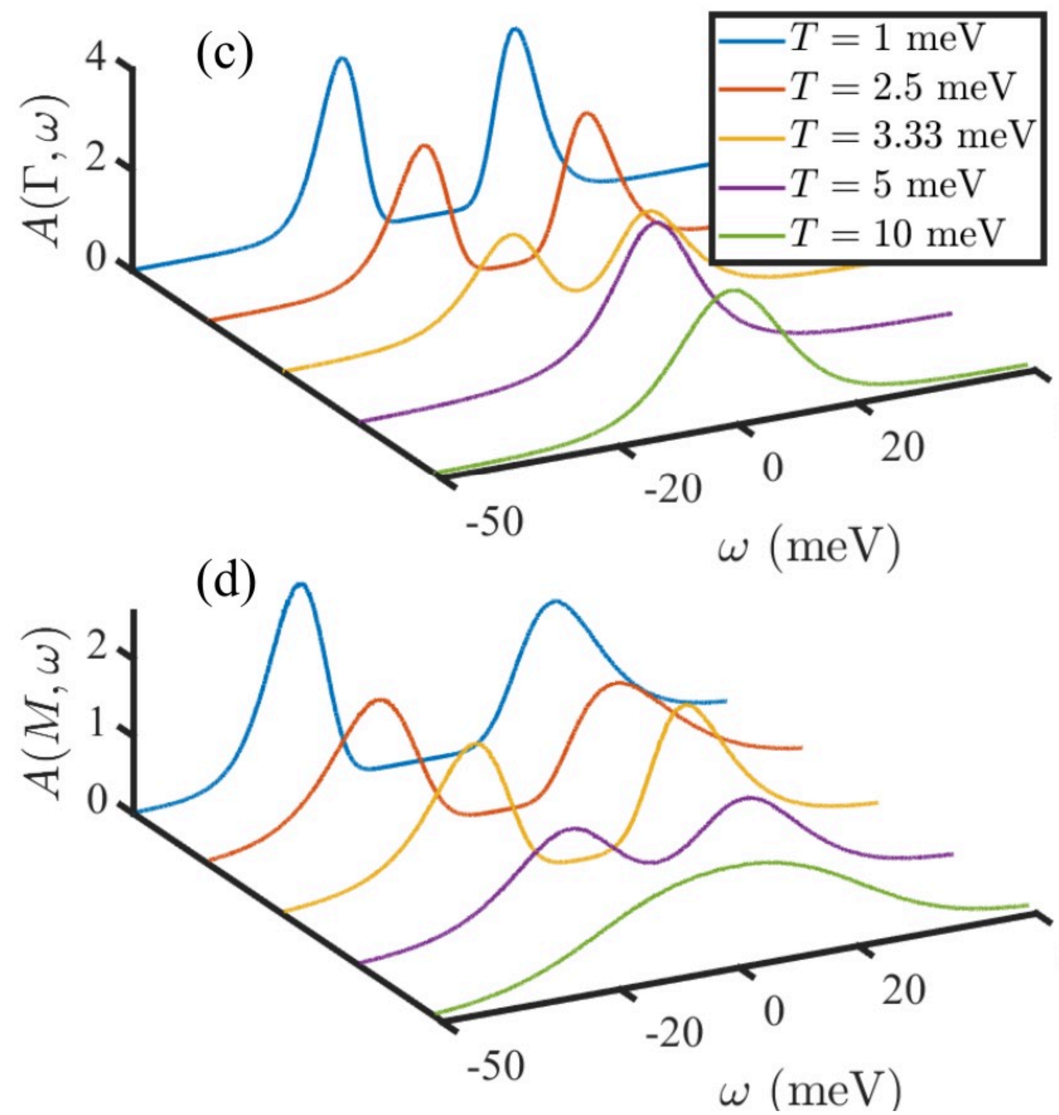
momentum-space QMC
Single valley and single spin

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

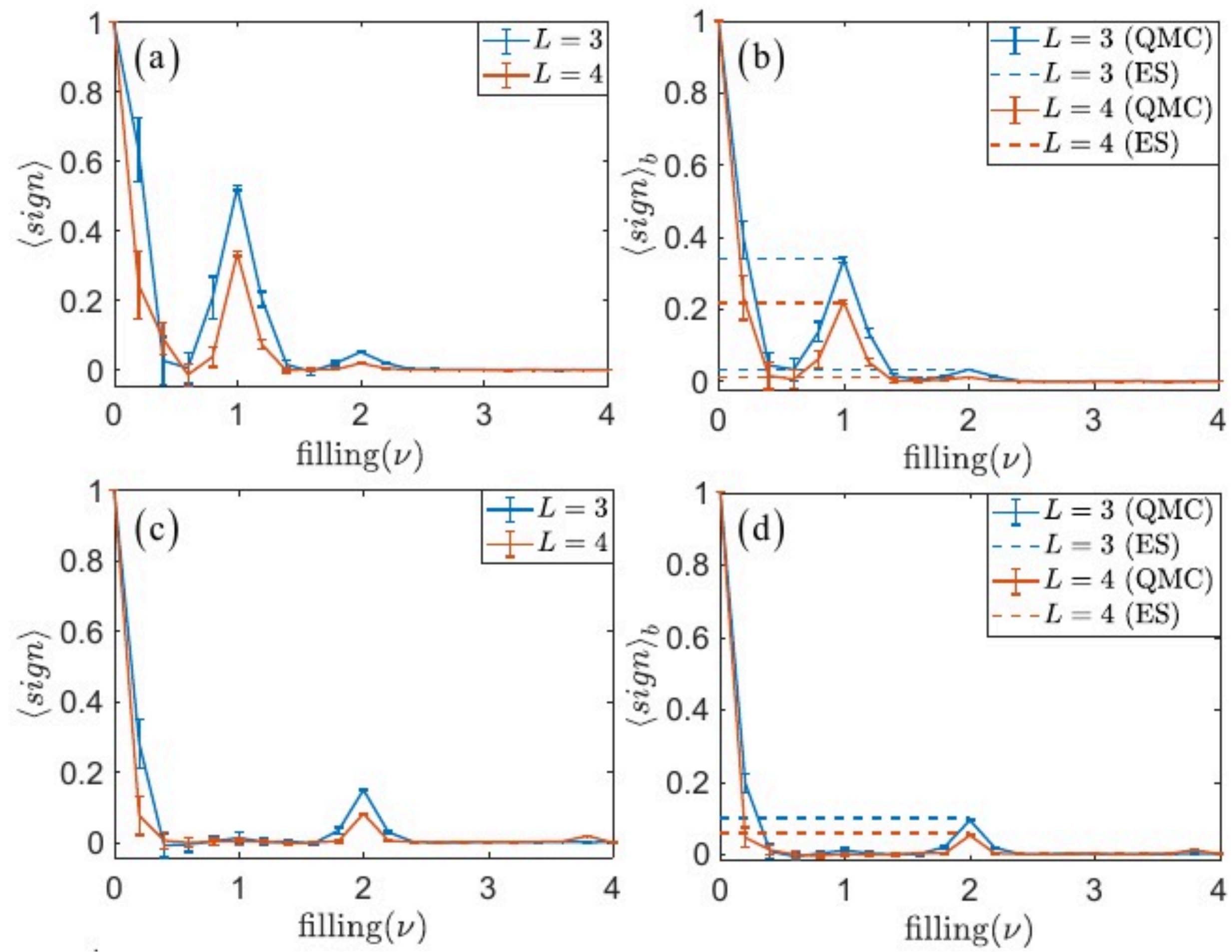
measured via STM

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}



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

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

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