TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Triple-q order and spin vestigial states in $Na_2Co_2TeO_6$

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Yuan Li

Quantum Critical Matter

JA 2306/4-1

Emmy Noether-Programm

DFG Deutsche Forschungsgemeinschaft

ct.qmat

Complexity and Topology in Quantum Matter

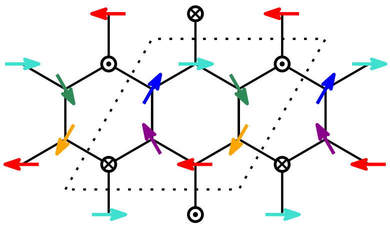
Würzburg-Dresden Cluster of Excellence

SFB 1143

Outline

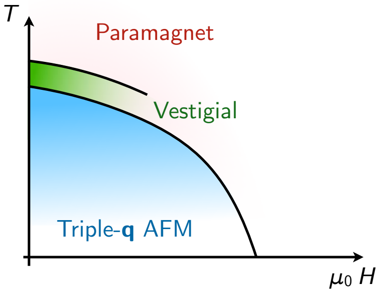
Message #1: $Na_2Co_2TeO_6$ features triple-$\mathbf{q}$ AFM order at low temperatures

[Krüger, Chen, Jin, Li, LJ, PRL '23]

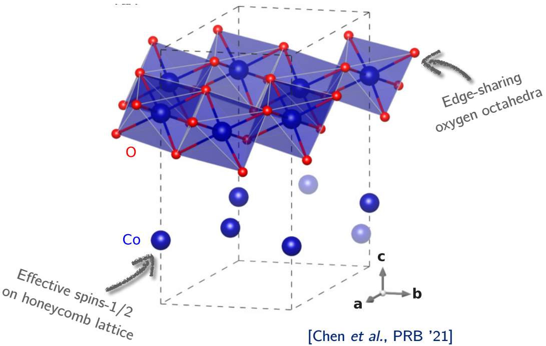


Message #2: Triple-$\mathbf{q}$ order can melt in two stages

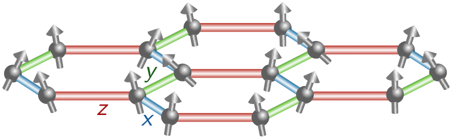
[Francini, LJ, arXiv:2311.08475]



Magnetic Mott insulator $Na_2Co_2TeO_6$



[Chen *et al.*, PRB '21]



Non-Kitaev terms

Effective spin-1/2 model:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + \dots$$

[Liu, Khaliullin, PRB '18]
[Sano, Kato, Motome, PRB '18]

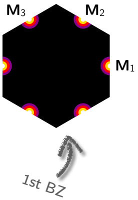
→ Talk by P. Mukharjee

Multi-q vs single-q order: Bragg peaks

Static spin structure factor:

... e.g., from neutron diffraction

[Chen *et al.*, PRB '21]



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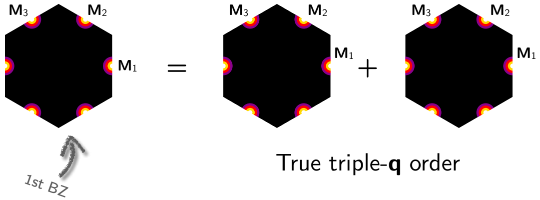

True triple-**q** order

Multi-q vs single-q order: Bragg peaks

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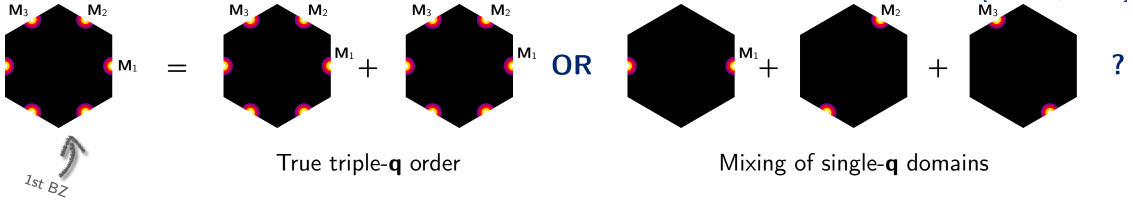

True triple-**q** order

Mixing of single-**q** domains

Multi-q vs single-q order: Bragg peaks

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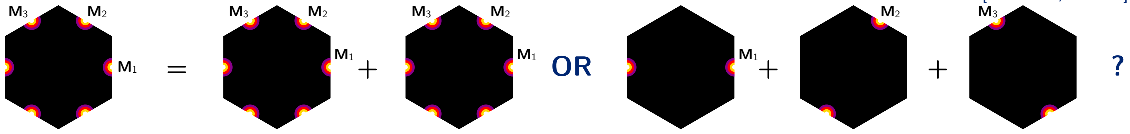
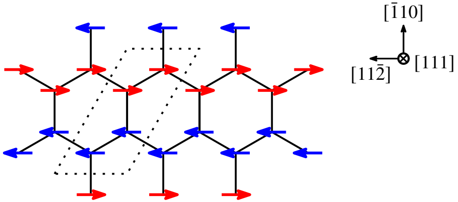


1st BZ

True triple-**q** order

Mixing of single-**q** domains

Real space:



α-$RuCl_3$, Na_2IrO_3, ...

[Choi *et al.*, PRL '12]
[Johnson *et al.*, PRB '15]
[Balz *et al.*, PRB '21]

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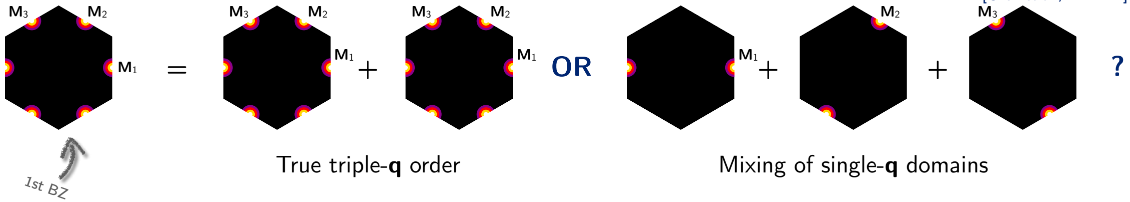

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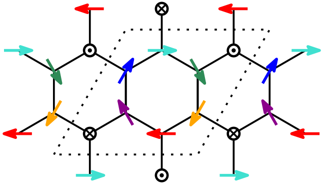
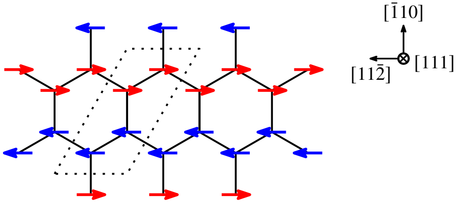


Kitaev-Heisenberg in field: [LJ, Andrade, Vojta, PRL '16]
Bilinear-Biquadratic Kitaev-Heisenberg: [Pohle, Shannon, Motome, PRB '23]

→ Talk by R. Pohle



α-$RuCl_3$, Na_2IrO_3, ...
[Choi *et al.*, PRL '12]
[Johnson *et al.*, PRB '15]
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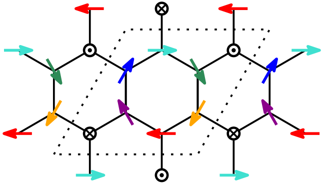
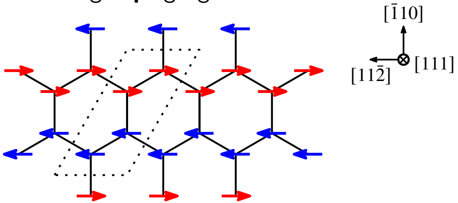
Multi-q vs single-q order: Symmetries

Triple-**q** AFM



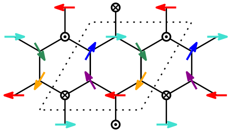
Single-**q** zigzag AFM



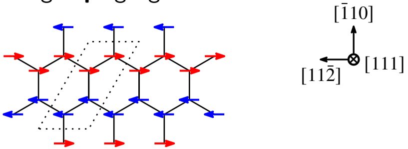
	Triple-**q** AFM	Single-**q** zigzag AFM
Time reversal:	✗	✗
Spin-lattice rotation C_3^*:	✓	✗
Translation $T_{\mathbf{a}_1}$:	✗	✗
Translation $T_{\mathbf{a}_2}$:	✗	✓

Multi-q vs single-q order: Magnetic excitation spectrum

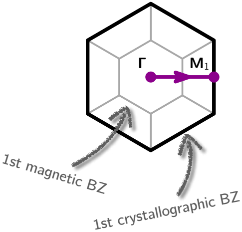
Triple-**q** AFM



Single-**q** zigzag AFM



Brillouin zone path:



Multi-q vs single-q order: Magnetic excitation spectrum

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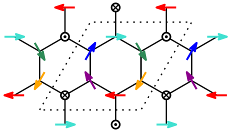
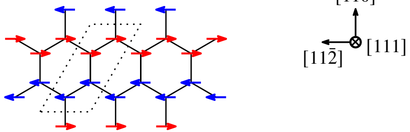


Single-**q** zigzag AFM



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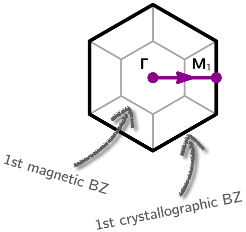
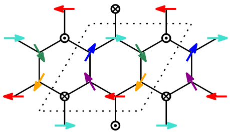


Spectrum necessarily symmetric

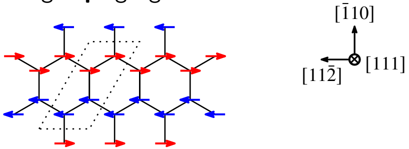
... independent of modeling

Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM



Single-**q** zigzag AFM



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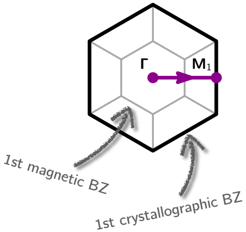

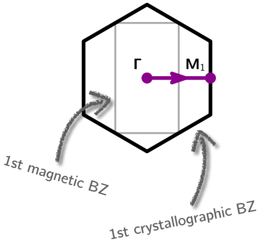

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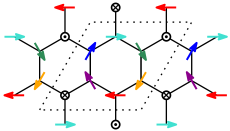
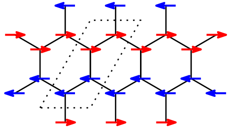
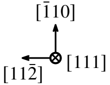
Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM



Single-**q** zigzag AFM





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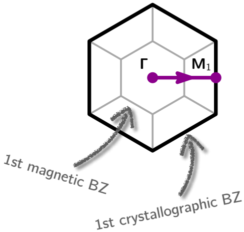

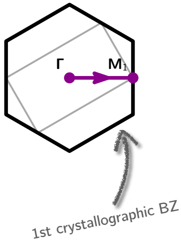

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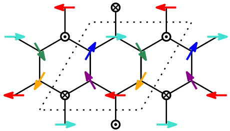
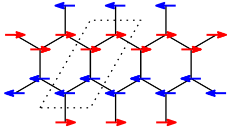
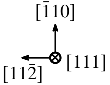
Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM



Single-**q** zigzag AFM





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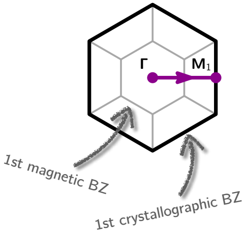

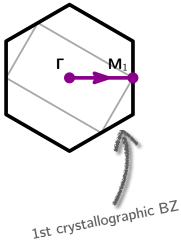

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Multi-q vs single-q order: Magnetic excitation spectrum

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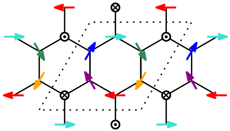

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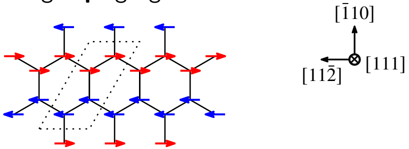

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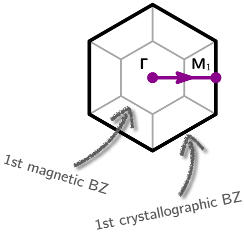
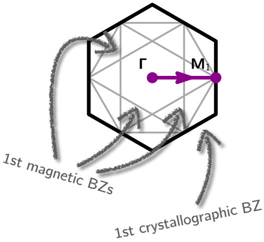




Spectrum necessarily symmetric

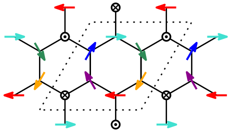
... independent of modeling

Spectrum generically asymmetric

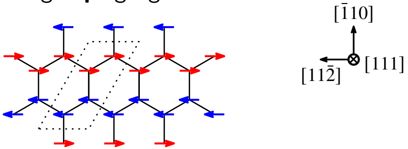
... unless fine-tuned

Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM



Single-**q** zigzag AFM



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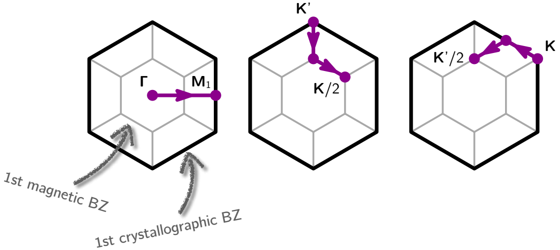
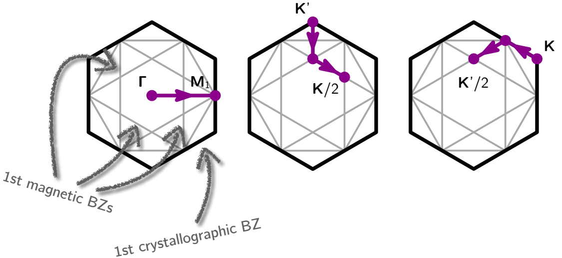




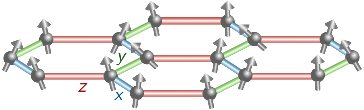
Spectrum necessarily symmetric

... independent of modeling

Spectrum generically asymmetric

... unless fine-tuned

Example: HKΓΓ' model @ hidden SU(2) point



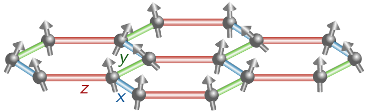
Hamiltonian:

$$\mathcal{H}_0 = \sum_{\langle ij \rangle_\gamma} \Big[J_1 \mathbf{S}_i \cdot \mathbf{S}_j + K_1 S_i^\gamma S_j^\gamma + \Gamma_1 (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma_1' (S_i^\gamma S_j^\alpha + S_i^\alpha S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma) \Big]$$

... with $(J_1, K_1, \Gamma_1, \Gamma'_1) = (-1/9, -2/3, 8/9, -4/9)\ A$

[Chaloupka, Khaliullin, PRB '15]

Example: HKΓΓ’ model @ hidden SU(2) point



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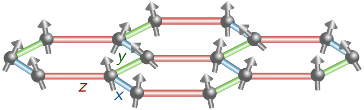
... with $(J_1, K_1, \Gamma_1, \Gamma'_1)$ = (-1/9, -2/3, 8/9, -4/9) A

[Chaloupka, Khaliullin, PRB '15]

Hidden SU(2) symmetry: $\mathbf{S}_i \mapsto \tilde{\mathbf{S}}_i = T_{14} \mathbf{S}_i$: $\quad \mathcal{H}_0 \mapsto \tilde{\mathcal{H}}_0 = A \sum_{\langle ij \rangle} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j$

Local rotation

Example: HKΓΓ' model @ hidden SU(2) point



Hamiltonian:

$$\mathcal{H}_0 = \sum_{\langle ij \rangle_\gamma} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_j + K_1 S_i^\gamma S_j^\gamma + \Gamma_1 (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma_1' (S_i^\gamma S_j^\alpha + S_i^\alpha S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma) \right]$$

... with (J_1, K_1, Γ_1, Γ'_1) = (-1/9, -2/3, 8/9, -4/9) A

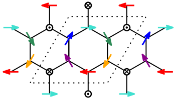
[Chaloupka, Khaliullin, PRB '15]

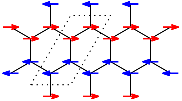
Hidden SU(2) symmetry: $\mathbf{S}_i \mapsto \tilde{\mathbf{S}}_i = T_{14} \mathbf{S}_i$: $\mathcal{H}_0 \mapsto \tilde{\mathcal{H}}_0 = A \sum_{\langle ij \rangle} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j$

Local rotation

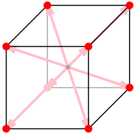
Ground state manifold:

$\mathbf{S}_i$:

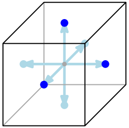




$\tilde{\mathbf{S}}_i$:

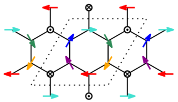


4 diagonals

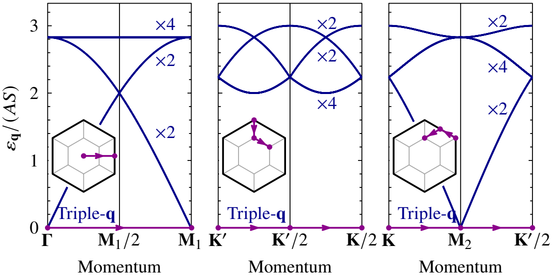


3 cubic axes

Magnon spectrum @ hidden SU(2) point

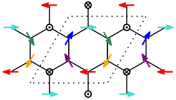


Triple-**q** AFM

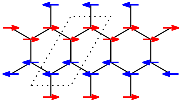


… fully symmetric

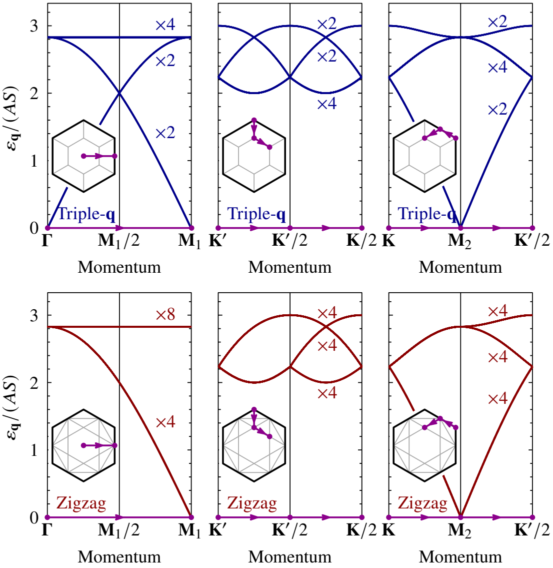
Magnon spectrum @ hidden SU(2) point



Triple-**q** AFM



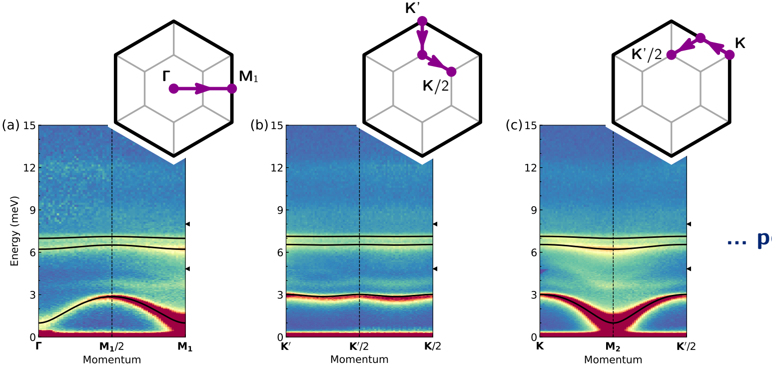
Zigzag AFM



... fully symmetric

... at least some bands asymmetric

$Na_2Co_2TeO_6$: Inelastic neutron scattering

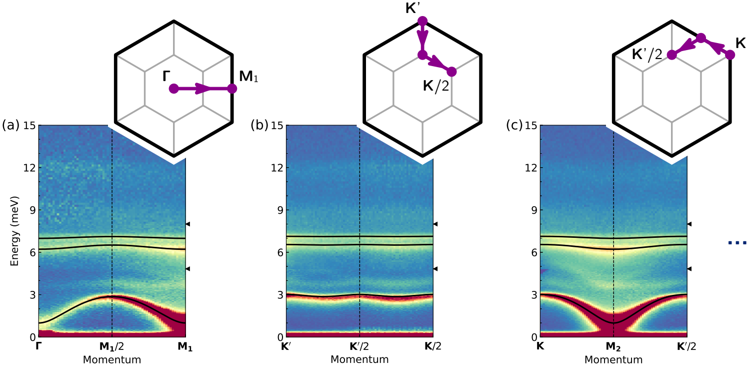


... perfectly symmetric magnon bands

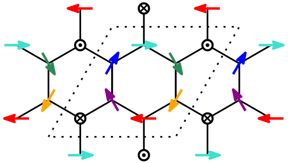
[Krüger, Chen, Jin, Li, LJ, PRL '23]

→ Poster by W. Krüger

$Na_2Co_2TeO_6$: Inelastic neutron scattering



… perfectly symmetric magnon bands



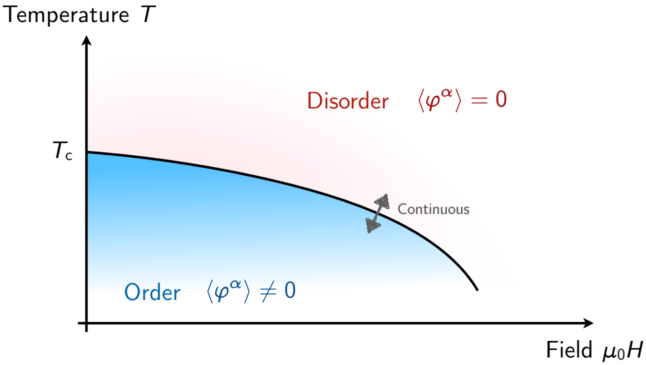
Message #1: $Na_2Co_2TeO_6$ features triple-**q** AFM order at low temperatures

[Krüger, Chen, Jin, Li, LJ, PRL '23]

→ Poster by W. Krüger

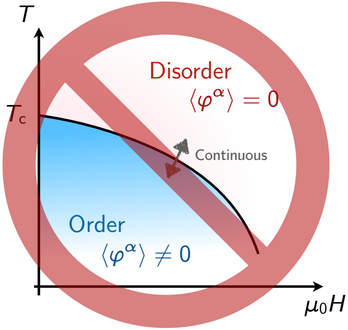
Finite-temperature phase diagram: Simple system

... order parameter has only 1 component
or breaks only 1 symmetry



Finite-temperature phase diagram: Multicomponent system

... order parameter has > 1 component
and breaks > 1 symmetry



Single continuous ✘

[Fernandes, Orth, Schmalian, ARCMP '19]

Finite-temperature phase diagram: Multicomponent system

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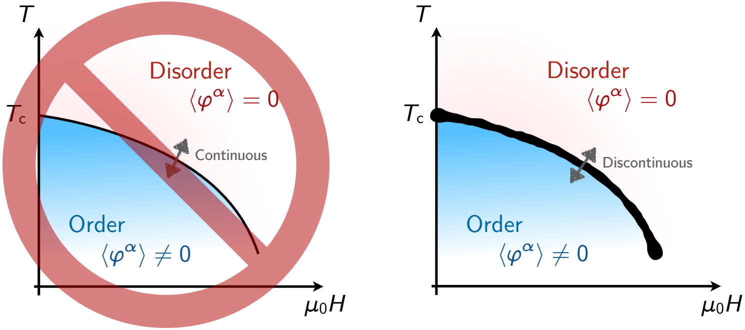


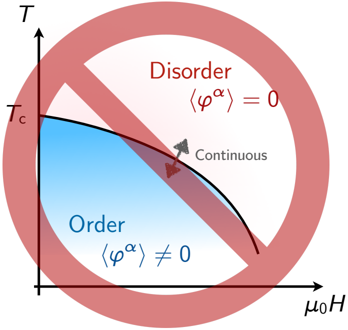
Single continuous ✗

First order ✓

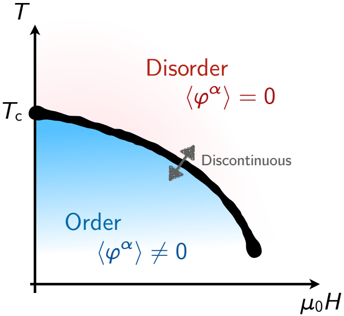
[Fernandes, Orth, Schmalian, ARCMP '19]

Finite-temperature phase diagram: Multicomponent system

... order parameter has $>$ 1 component
and breaks $>$ 1 symmetry

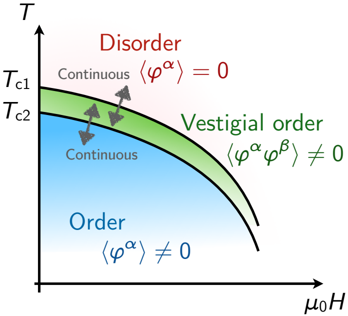


Single continuous ✗



First order ✓

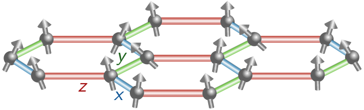
OR



Two-stage melting ✓

[Fernandes, Orth, Schmalian, ARCMP ’19]

HKΓΓ' model with ring perturbation



Hamiltonian:

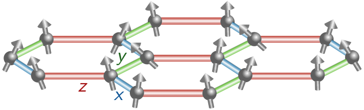
$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\hexagon}$$

Bilinear exchange:

$$\mathcal{H}_0 = \sum_{\langle ij \rangle_\gamma} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_j + K_1 S_i^\gamma S_j^\gamma + \Gamma_1 (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma_1' (S_i^\gamma S_j^\alpha + S_i^\alpha S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma) \right]$$

... with (J_1, K_1, Γ_1, Γ'_1) = (-1/9, -2/3, 8/9, -4/9) A

HKΓΓ' model with ring perturbation



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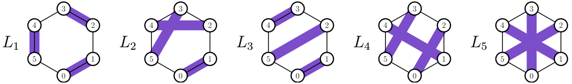
Ring exchange:



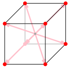
$$\mathcal{H}_{\hexagon} = J_{\hexagon} \sum_{\langle ijklmn \rangle} L_{ijklmn} (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l)(\mathbf{S}_m \cdot \mathbf{S}_n)$$

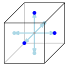
... with $L_1 = 1/3$, $L_2 = -1$, $L_3 = 1/2$, $L_4 = 1/2$, $L_5 = -1/6$
from strong-coupling expansion of honeycomb-lattice Hubbard model
[Yang, Albuquerque, Capponi, Läuchli, Schmidt, NJP '12]

Observables

Dual magnetization:

$$\tilde{M} = \langle |\tilde{\mathbf{M}}| \rangle \qquad \text{with} \qquad \tilde{\mathbf{M}} := \frac{1}{N} \sum_i (-1)^i T_{14}^{\top} \mathbf{S}_i = \begin{cases} \frac{1}{\sqrt{3}}(1,1,1), & \text{for triple-}\mathbf{q}\text{ order} \\ (0,0,1), & \text{for } z\text{-zigzag order} \end{cases}$$





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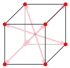

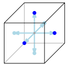

Composite order parameter:

$$(Q_{e_g}, Q_{t_{2g}}) = (\langle|\mathbf{Q}_{e_g}|\rangle, \langle|\mathbf{Q}_{t_{2g}}|\rangle) \qquad \text{with} \qquad \begin{aligned} \mathbf{Q}_{e_g} &:= \tfrac{1}{2}\left(2\tilde{M}_z^2 - \tilde{M}_x^2 - \tilde{M}_y^2, \sqrt{3}[\tilde{M}_x^2 - \tilde{M}_y^2]\right) \\ \mathbf{Q}_{t_{2g}} &:= \sqrt{3}\left(\tilde{M}_y\tilde{M}_z, \tilde{M}_z\tilde{M}_y, \tilde{M}_x\tilde{M}_y\right) \end{aligned}$$

... 5 irreducible components of rank-2 tensor

Observables

Dual magnetization:

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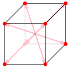

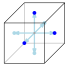

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... 5 irreducible components of rank-2 tensor

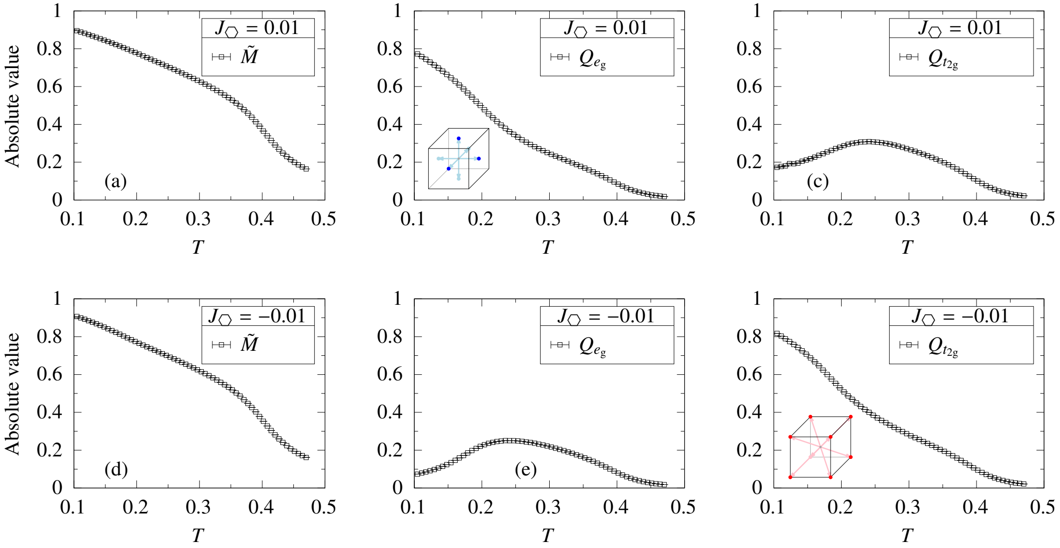
$$= \begin{cases} (0,1), & \text{for triple-}\mathbf{q}\text{ order} \\ (1,0), & \text{for } z\text{-zigzag order} \end{cases}$$

... measurable in finite-size simulations

Classical Monte Carlo simulations ($L = 32$)

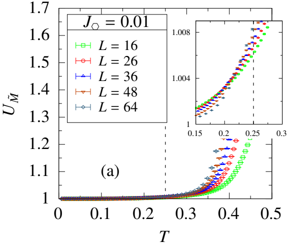
$J_{\hexagon} > 0$:

$J_{\hexagon} < 0$:

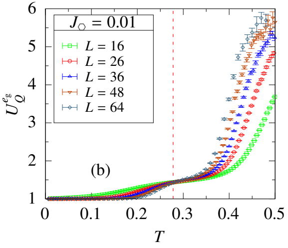


Critical temperatures

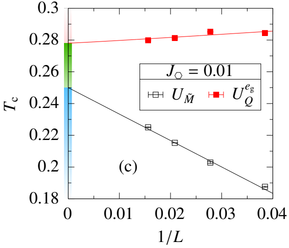
Primary Binder cumulant

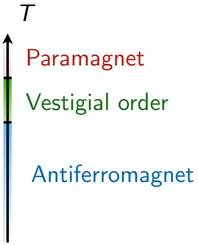


Composite Binder cumulant



Crossing points

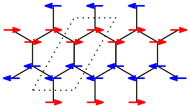
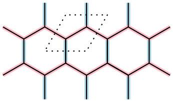




$$U_{\tilde{M}} = \frac{\langle \tilde{\mathbf{M}}^4 \rangle}{\langle \tilde{\mathbf{M}}^2 \rangle^2}$$

$$U_Q^{e_g} = \frac{\langle \mathbf{Q}_{e_g}^4 \rangle}{\langle \mathbf{Q}_{e_g}^2 \rangle^2}$$

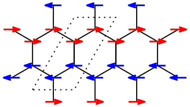
Two-stage melting

$J_{\hexagon} > 0$:	Zigzag	$\mathbb{Z}_3$ spin nematic	Paramagnet
			
Rotation:	✗	✗	✓
Time reversal:	✗	✓	✓

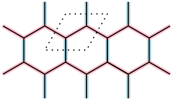
Two-stage melting

$J_{\hexagon} > 0$:

Zigzag



$\mathbb{Z}_3$ spin nematic

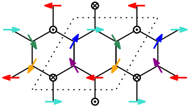


Paramagnet

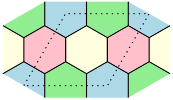
	Zigzag	$\mathbb{Z}_3$ spin nematic	Paramagnet
Rotation:	✘	✘	✔
Time reversal:	✘	✔	✔

$J_{\hexagon} < 0$:

Triple-**q**



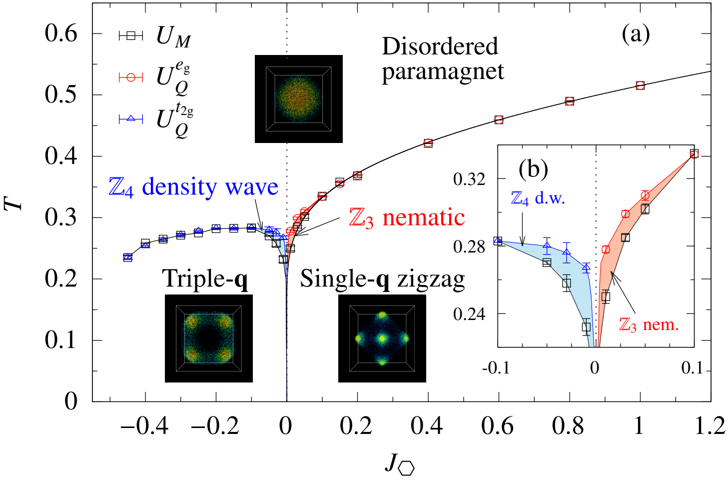
$\mathbb{Z}_4$ spin current density wave



Paramagnet

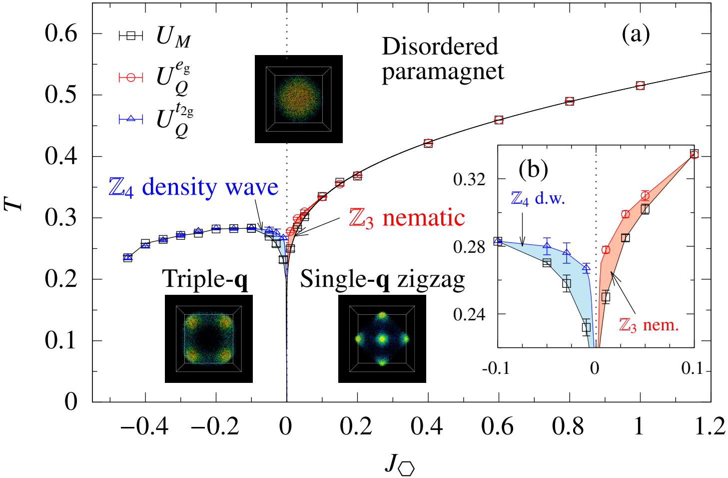
	Triple-**q**	$\mathbb{Z}_4$ spin current density wave	Paramagnet
Rotation:	✔	✔	✔
Time reversal:	✘	✔	✔
Translation:	✘	✘	✔

Phase diagram: HKΓΓ′ model



[Francini, LJ, arXiv:2311.08475]

Phase diagram: HKΓΓ' model



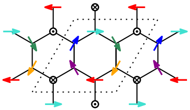
Message #2: Triple-**q** order can melt in two stages

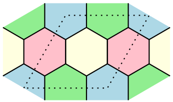
... same is true for zigzag order

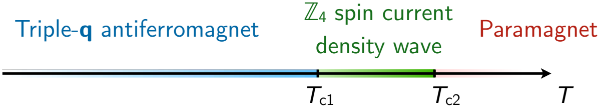
[Francini, LJ, arXiv:2311.08475]

Phase diagram: $Na_2Co_2TeO_6$

Theory:







[Francini, LJ, arXiv:2311.08475]

Phase diagram: $Na_2Co_2TeO_6$

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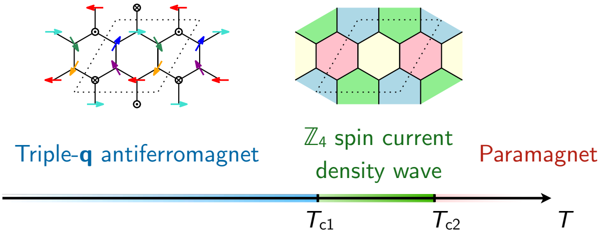
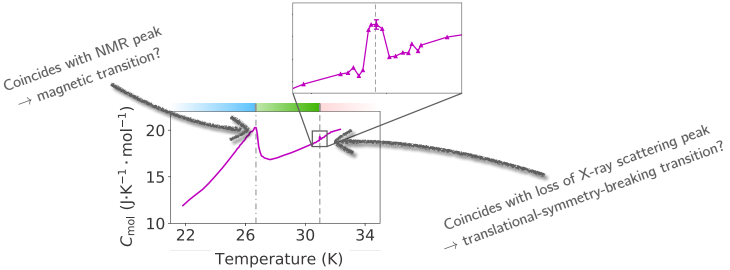


[Francini, LJ, arXiv:2311.08475]

Experiment:



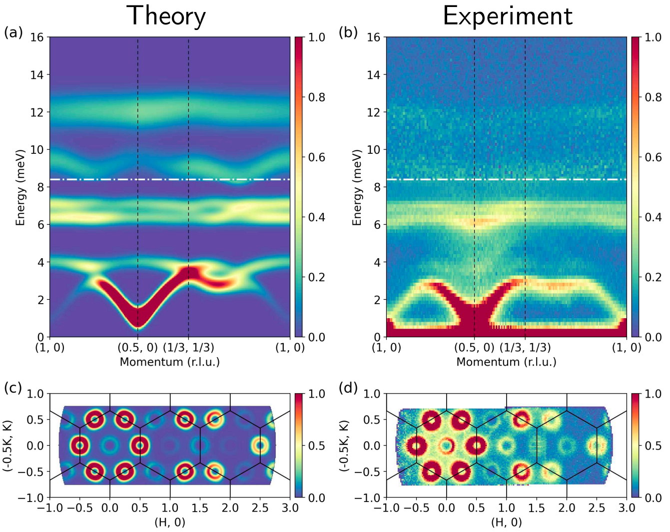
[Chen *et al.*, PRB '21]

$Na_2Co_2TeO_6$: Magnon excitation spectrum

$$(J, K, \Gamma, \Gamma') = (1.2, -8.3, 1.9, -2.3, 0.5)\,\mathrm{meV}$$

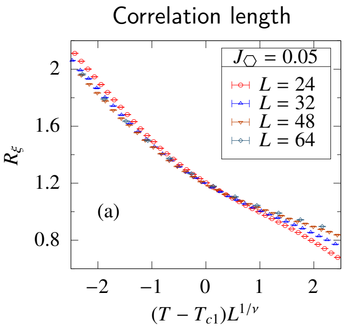
$$(J_3, J_2^A, J_2^B) = (1.5, 0.32, -0.24)\,\mathrm{eV}$$

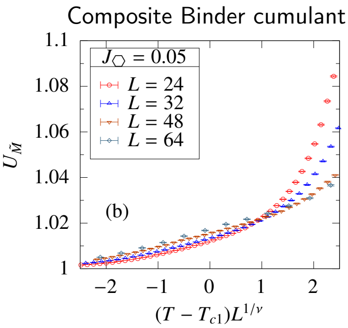
$$+\ \text{nonbilinear exchange}$$

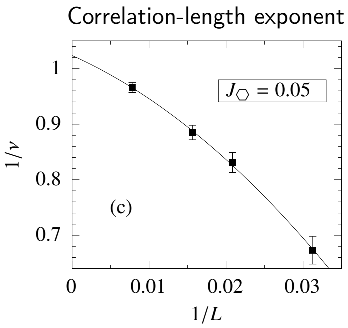


[Krüger, Chen, Jin, Li, LJ, PRL '23]

Critical scaling @ T_{c1} (primary-to-vestigial)

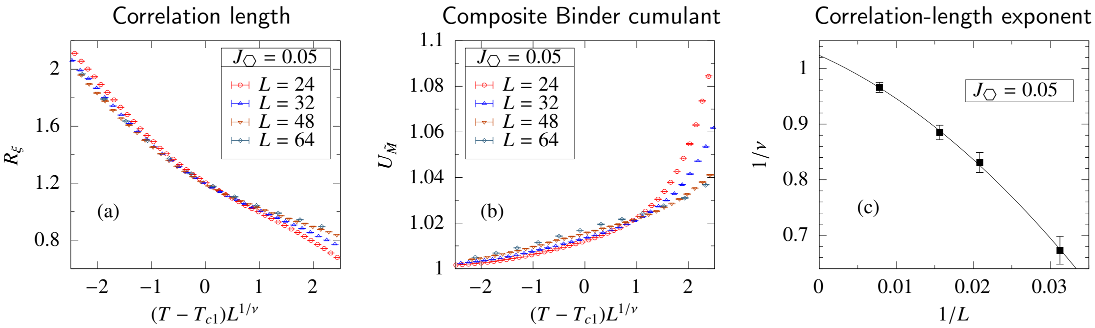






$$R_\xi = \xi / L$$

Critical scaling @ T_{c1} (primary-to-vestigial)

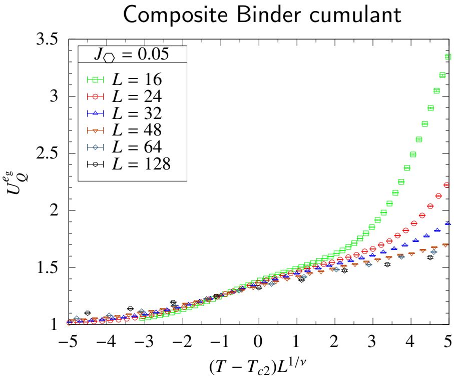


$$R_\xi = \xi / L$$

→ 2D Ising universality

… consistent with $\mathbb{Z}_2$ time reversal symmetry breaking

Critical scaling @ T_{c2} (vestigial-to-paramagnet)



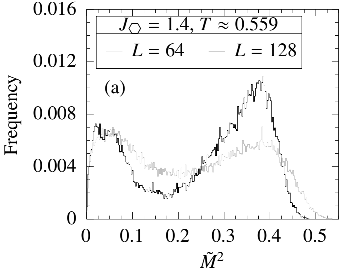
with $1/\nu = 6/5$

$\rightarrow$ 2D three-state Potts universality

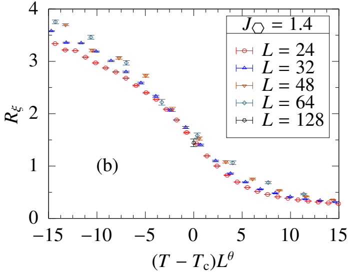
... consistent with $\mathbb{Z}_3$ symmetry breaking

Phase coexistence @ primary-to-disorder transition

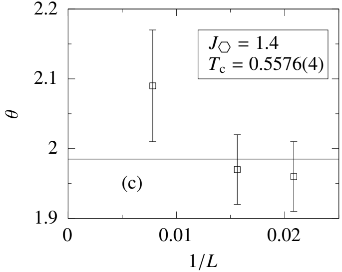
Monte Carlo histogram



Correlation length



Stability-matrix eigenvalue

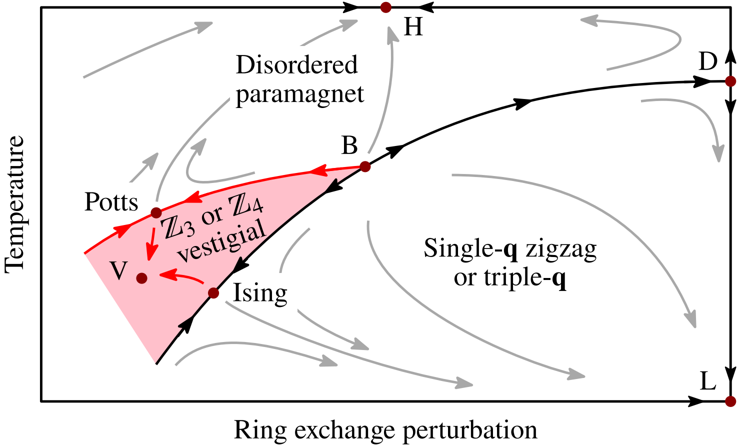


$\theta = 1.99(3) = d$

... spatial dimension

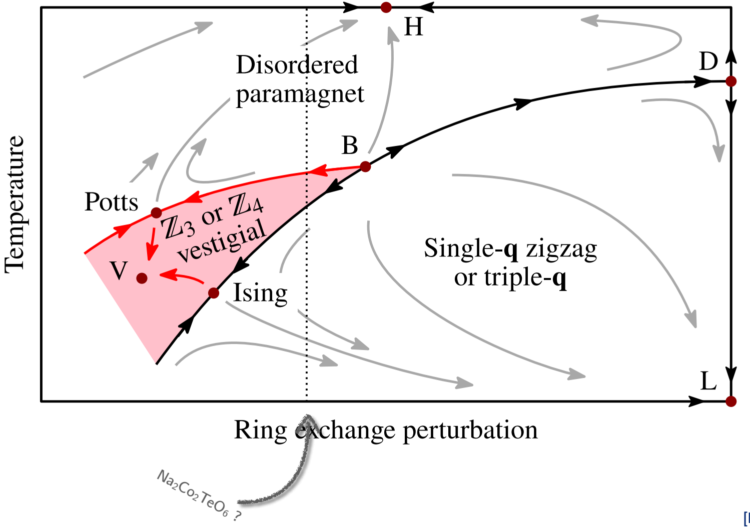
→ First-order transition from discontinuity fixed point

Schematic RG flow



[Francini, LJ, arXiv:2311.08475]

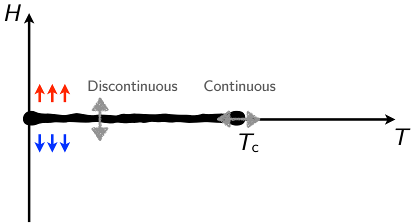
Schematic RG flow

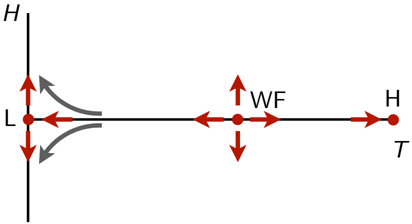


[Francini, LJ, arXiv:2311.08475]

Digression: Discontinuity fixed point

Ising model in longitudinal field:





Flow linearization (relevant direction):

$$\beta_H = -\theta H + \mathcal{O}(H^2) \qquad \text{with} \qquad \theta = d = 2$$

Formal limit of continuous transition:

$$\begin{aligned} U &\propto |t|^{1-\alpha} \\ M &\propto (-t)^{\beta} \quad (t < 0) \end{aligned} \qquad \text{with} \qquad \begin{aligned} \alpha &\to 1 \\ \beta &\to 0 \end{aligned} \qquad \Rightarrow \qquad 1/\nu \to d = 2$$

[Nienhuis, Nauenberg, PRL '75]

High-spin d^7 Mott insulators

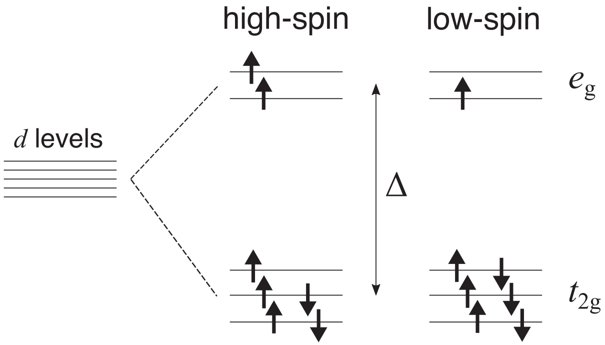


FIG. 1. Atomic d levels splitting into two groups under the octahedral CEF Δ: e_g levels at a higher energy and t_{2g} levels at a lower energy. The d^7 electron configuration can take either high-spin (middle) or low-spin state (right), depending on the strength of Coulomb interactions and Δ.

[Sano, Kato, Motome, PRB '18]