

Intertwined spin vestigial orders

Lukas Janssen



Niccolò Francini



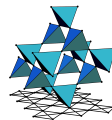
Wilhelm Krüger



ct.qmat

**Complexity and Topology
in Quantum Matter**

Würzburg-Dresden Cluster of Excellence



SFB 1143

OR: "No single continuous transition
in multicomponent system"

Intertwined spin vestigial orders

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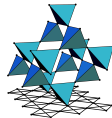
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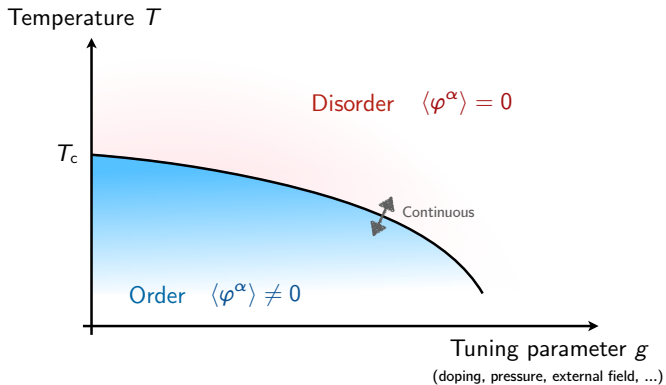
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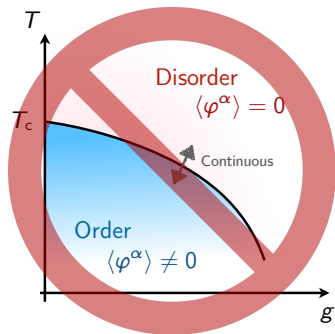
Primary order



Vestigial (“composite”) order

Multicomponent system:

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

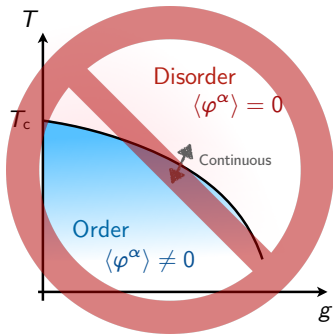


Single continuous **X**

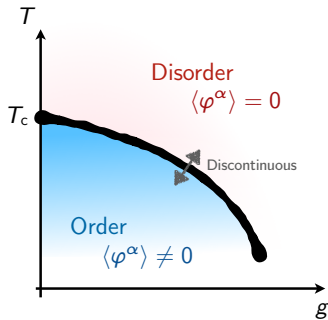
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Single continuous ❌

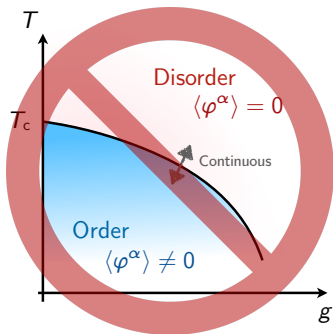


First order ✅

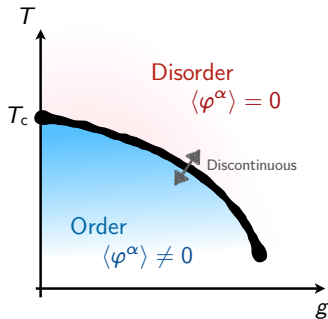
Vestigial ("composite") order

Multicomponent system:

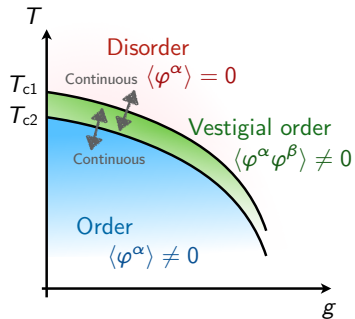
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Single continuous ❌



First order ✅

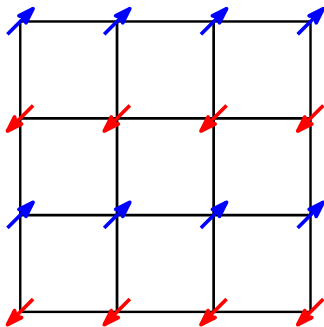


OR:

Two-stage melting ✅

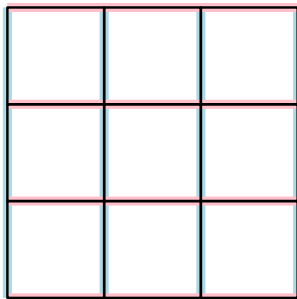
Example #1: Square-lattice spin system

Primary order:



$Q = (0, \pi)$ antiferromagnet

Vestigial order:



Spin nematic

Paramagnet

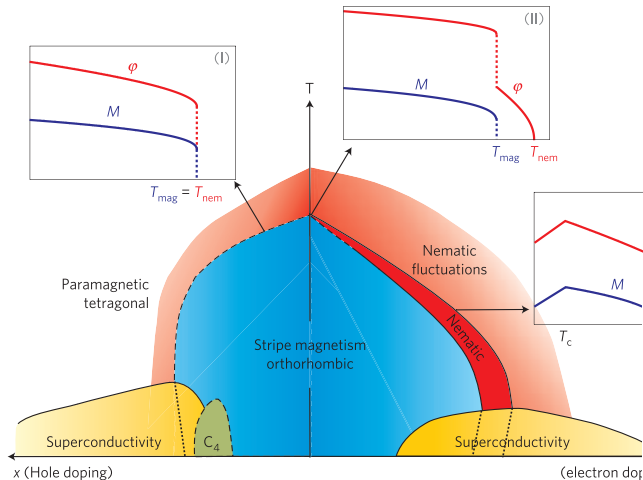
Rotation:



Time reversal:



Example #2: Iron-based superconductors



nature
physics

REVIEW ARTICLE

PUBLISHED ONLINE: 31 JANUARY 2014 | DOI:10.1038/NPHYS2877

What drives nematic order in iron-based superconductors?

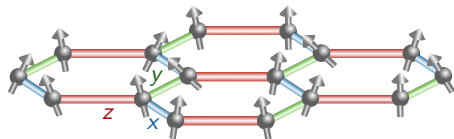
R. M. Fernandes^{1*}, A. V. Chubukov^{2*} and J. Schmalian^{3*}

Although the existence of nematic order in iron-based superconductors is now a well-established experimental fact, its origin remains controversial. Nematic order breaks the discrete lattice rotational symmetry by making the x and y directions in the iron plane non-equivalent. This can happen because of a regular structural transition or as the result of an electronically driven instability — in particular, orbital order or spin-driven Ising-nematic order. The latter is a magnetic state that breaks rotational symmetry but preserves time-reversal symmetry. Symmetry dictates that the development of one of these orders immediately induces the other two, making the origin of nematicity a physics realization of the ‘chicken and egg problem’. In this Review, we argue that the evidence strongly points to an electronic mechanism of nematicity, placing nematic order in the class of correlation-driven electronic instabilities, like superconductivity and density-wave transitions. We discuss different microscopic models for nematicity and link them to the properties of the magnetic and superconducting states, providing a unified perspective on the phase diagram of the iron pnictides.

Example #3: Honeycomb magnet $\text{Na}_2\text{Co}_2\text{TeO}_6$

Kitaev exchange:

$$\mathcal{H} = K \left(\sum_{\langle ij \rangle_x} S_i^x S_j^x + \sum_{\langle ij \rangle_y} S_i^y S_j^y + \sum_{\langle ij \rangle_z} S_i^z S_j^z \right)$$

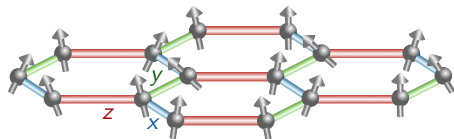


[Kitaev, Ann. Phys. '06]

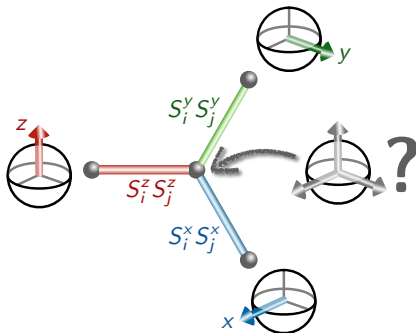
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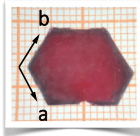


Frustration:



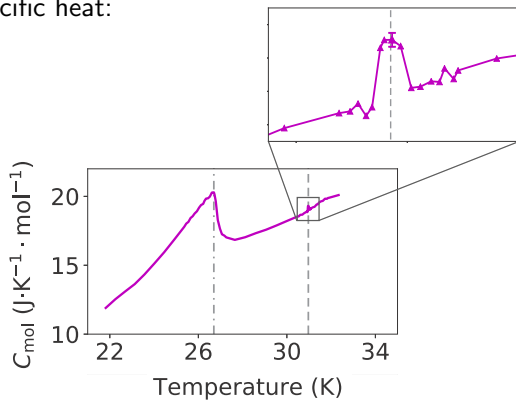
[Kitaev, Ann. Phys. '06]

Experimental phase diagram: $\text{Na}_2\text{Co}_2\text{TeO}_6$



Credit: Yuan Li

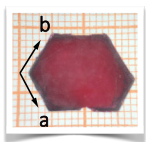
Specific heat:



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

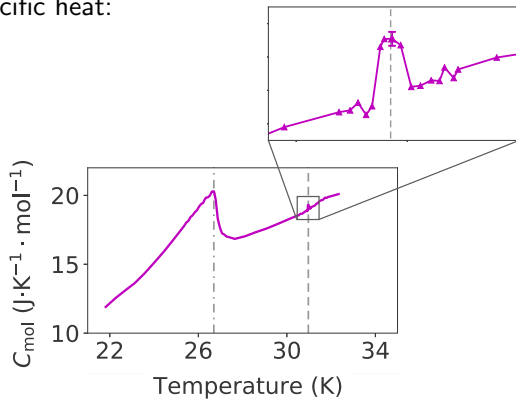
→ Two-stage melting?

Experimental phase diagram: $\text{Na}_2\text{Co}_2\text{TeO}_6$

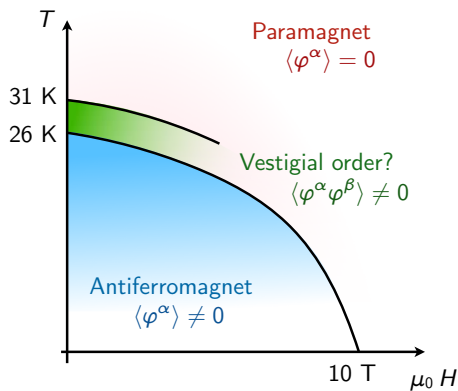


Credit: Yuan Li

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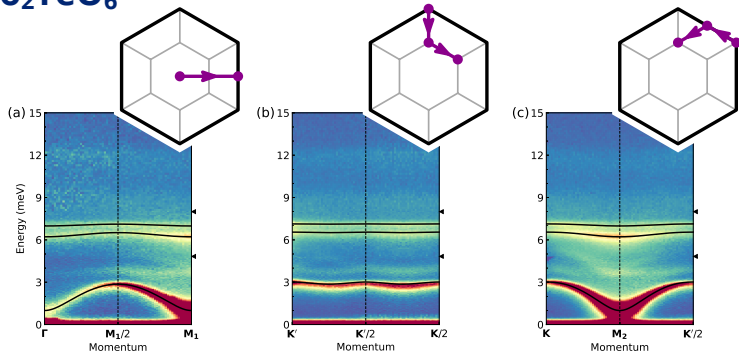


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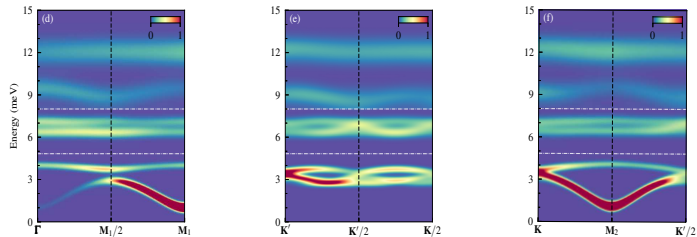
Model building: $\text{Na}_2\text{Co}_2\text{TeO}_6$

Magnetic excitation spectrum

... from neutron scattering:

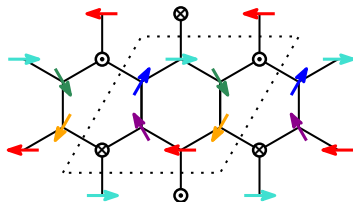


... from spin-wave theory:



Ground state: $\text{Na}_2\text{Co}_2\text{TeO}_6$

High-quality single crystals:

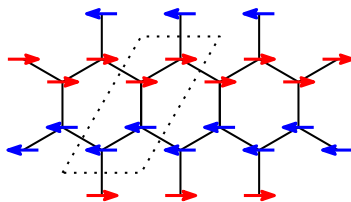


Triple- $\mathbf{q}$ antiferromagnet

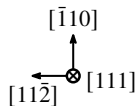
[Krüger, Chen, Jin, Li, LJ, PRL '23]

Other samples:

... sample preparation? disorder?



Zigzag antiferromagnet

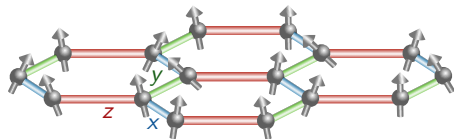


[Sanders *et al.*, PRB '22]

Spin model:

Bilinear exchange:

$$\mathcal{H}_0 = \sum_{\gamma=x,y,z} \sum_{\langle ij \rangle_\gamma} \left[J \mathbf{s}_i \cdot \mathbf{s}_j + K S_i^\gamma S_j^\gamma + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right. \\ \left. + \Gamma' (S_i^\gamma S_j^\alpha + S_i^\alpha S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma) \right]$$



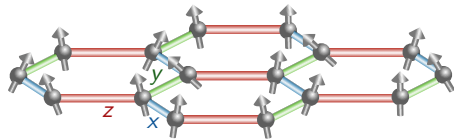
... all symmetry-allowed terms at nearest-neighbor level

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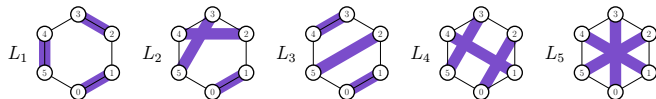
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... all symmetry-allowed terms at nearest-neighbor level



Ring exchange:



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

... 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]

Spin model:

Couplings:

$$(J, K, \Gamma, \Gamma') = (-1/9, -2/3, 8/9, -4/9)A, \quad A > 0$$

... proximate to $\text{Na}_2\text{Co}_2\text{TeO}_6$
[Krüger *et al.*, PRL '23]

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[Krüger *et al.*, PRL '23]

Hidden $\text{SU}(2)$ symmetry for $J_{\square} = 0$:

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


Local rotation

Spin model:

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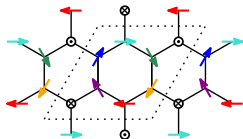
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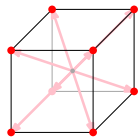
Local rotation

Ground state manifold:

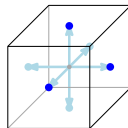
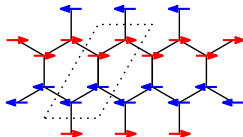
$\mathbf{S}_i$:



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



4 diagonals



3 cubic axes

Spin model:

Couplings:

$$(J, K, \Gamma, \Gamma') = (-1/9, -2/3, 8/9, -4/9)A, \quad A > 0$$

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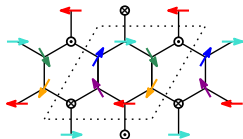
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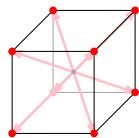
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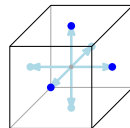
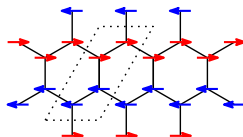


$\tilde{\mathbf{S}}_i$:



4 diagonals

selected for $J_{\square} < 0$



3 cubic axes

selected for $J_{\square} > 0$

Observables

Dual magnetization:

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



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Composite order parameter:

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

... 5 irreducible components of rank-2 tensor

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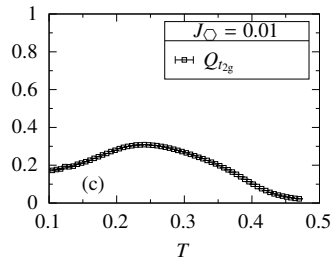
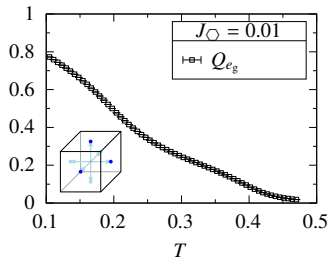
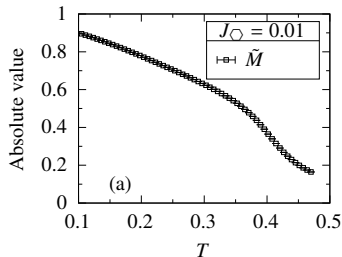
$$= \begin{cases} (0, 1), & \text{for triple-}\mathbf{q} \text{ order} \\ (1, 0), & \text{for z-zigzag order} \end{cases}$$

... 5 irreducible components of rank-2 tensor

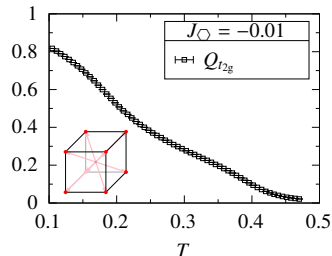
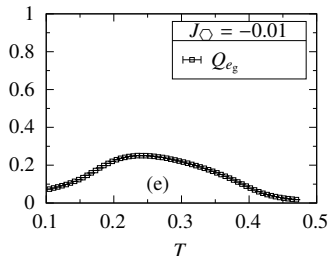
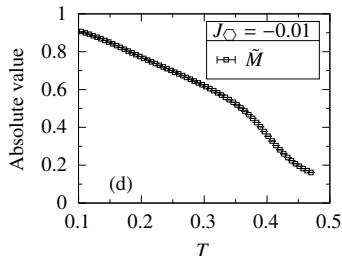
... measurable in finite-size simulations

Classical Monte Carlo simulations ($L = 32$)

$J_{\square} > 0$:

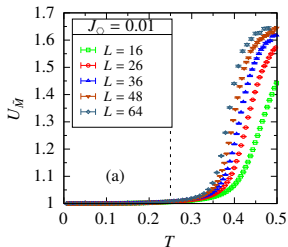


$J_{\square} < 0$:

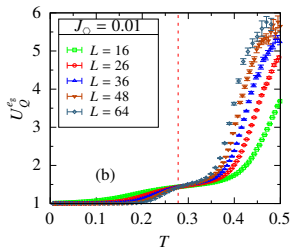


Critical temperatures

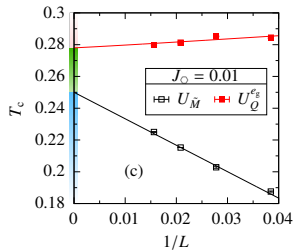
Primary Binder cumulant



Composite Binder cumulant



Crossing points



T

Paramagnet

Vestigial order

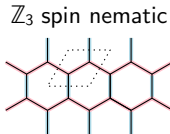
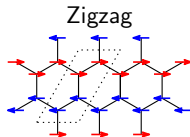
Antiferromagnet

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

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

Two-stage melting

$$J_{\text{hex}} > 0 :$$



Paramagnet

Rotation:

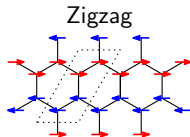


Time reversal:



Two-stage melting

$J_{\square} > 0$:



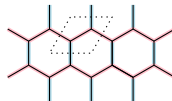
Rotation:



Time reversal:



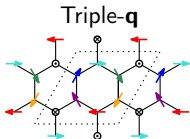
$\mathbb{Z}_3$ spin nematic



Paramagnet



$J_{\square} < 0$:



Rotation:



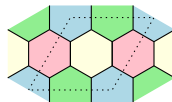
Time reversal:



Translation:



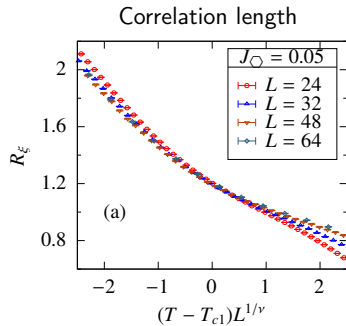
$\mathbb{Z}_4$ spin current density wave



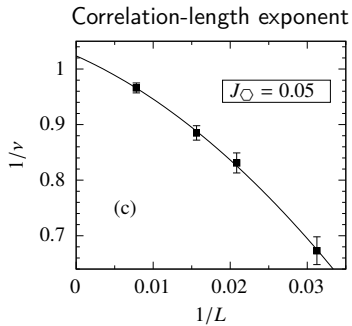
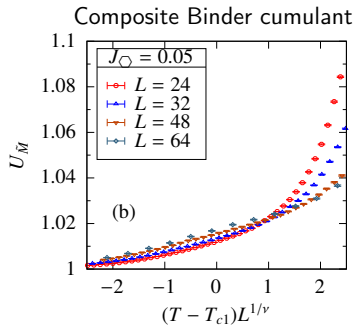
Paramagnet



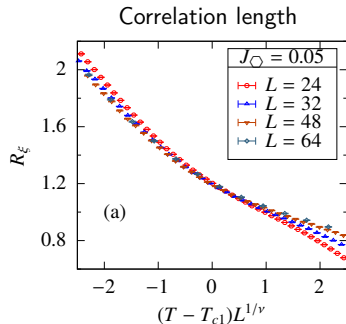
Critical scaling @ T_{c1} (primary-to-vestigial)



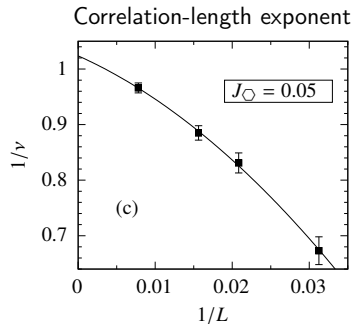
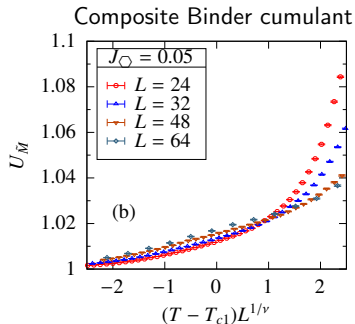
$$R_\xi = \xi/L$$



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



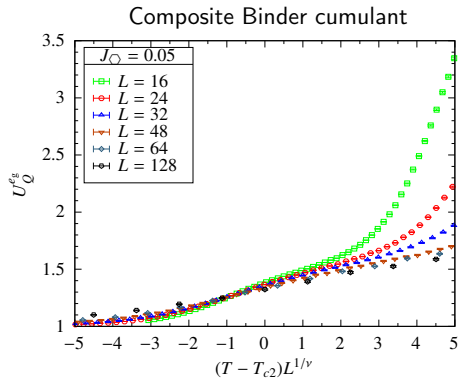
$$R_\xi = \xi/L$$



→ 2D Ising universality

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

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

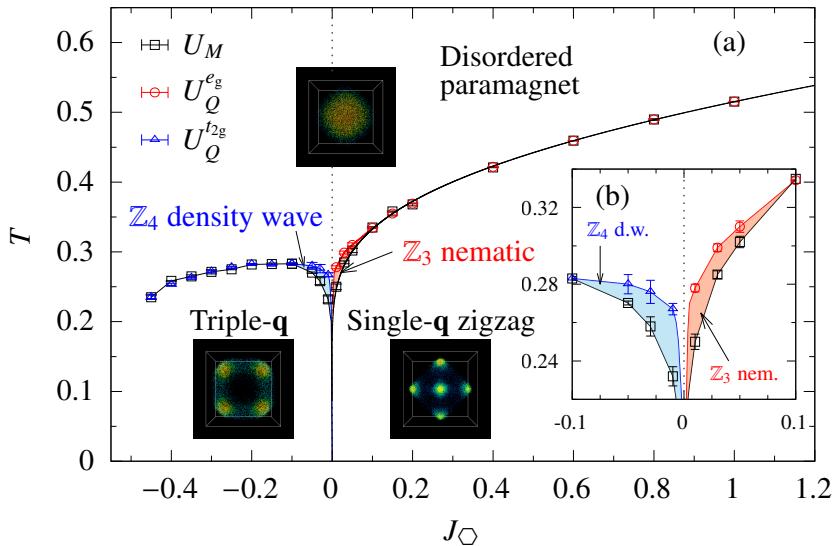


with $1/\nu = 6/5$

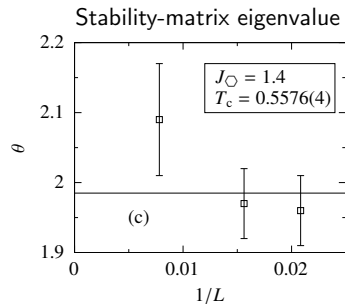
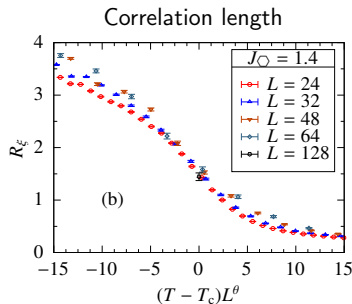
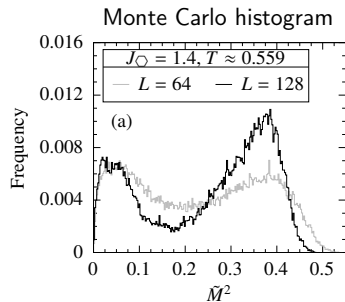
→ 2D three-state Potts universality

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

Phase diagram



Phase coexistence @ primary-to-disorder transition



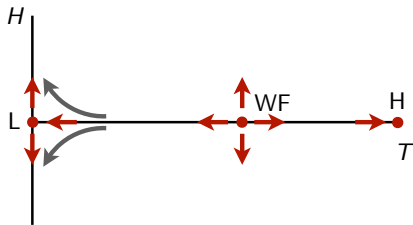
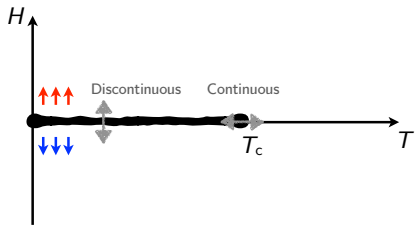
$$\theta = 1.99(3) = d$$

... spatial dimension

→ First-order transition from discontinuity fixed point

Digression: Discontinuity fixed point

Ising model in longitudinal field:



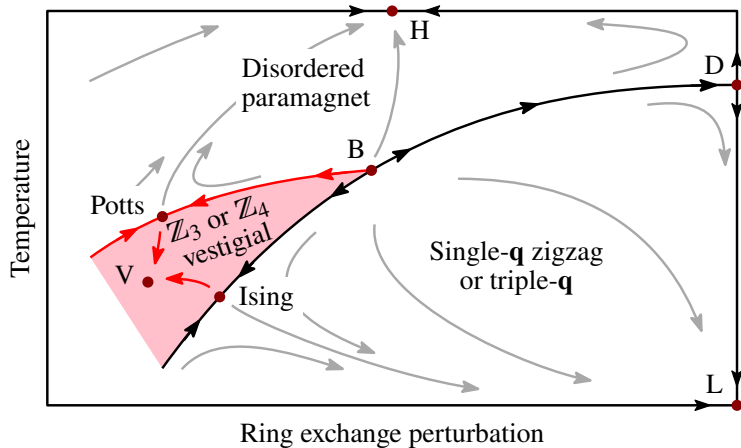
Flow linearization (relevant direction):

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

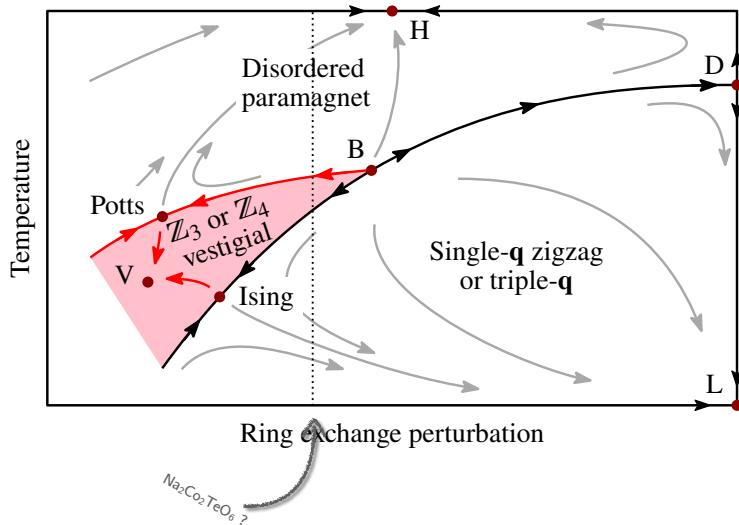
Formal limit of continuous transition:

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

Schematic RG flow

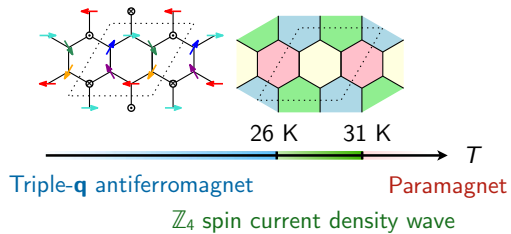


Schematic RG flow



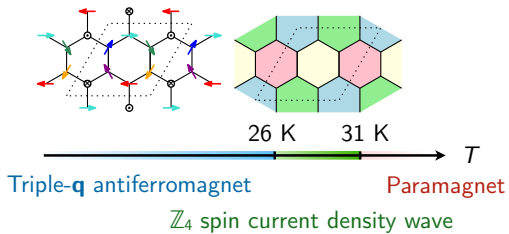
[Francini, LJ, arXiv:2311.08475]

$\text{Na}_2\text{Co}_2\text{TeO}_6$ phase diagram



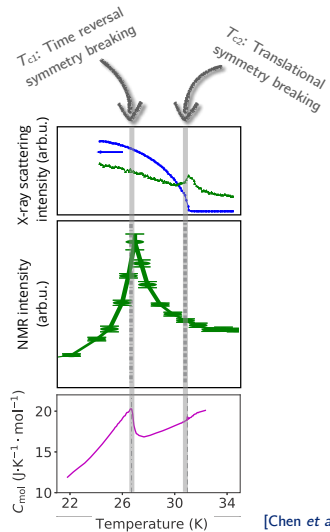
[Francini, LJ, arXiv:2311.08475]

$\text{Na}_2\text{Co}_2\text{TeO}_6$ phase diagram



[Francini, LJ, arXiv:2311.08475]

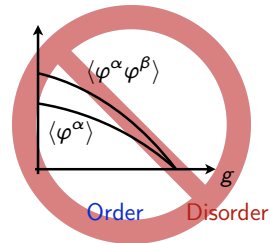
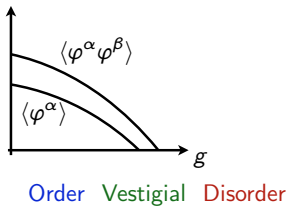
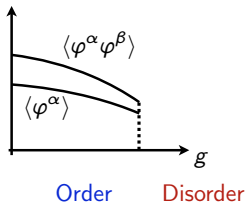
Experiments:



[Chen et al., PRB '21]

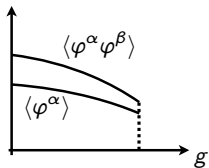
Conclusions

Vestigial-order paradigm: *"No single continuous transition in multicomponent system"*

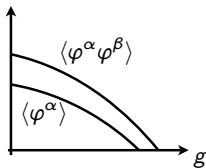


Conclusions

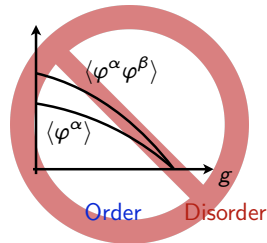
Vestigial-order paradigm: *"No single continuous transition in multicomponent system"*



Order Disorder

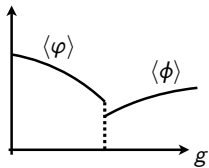


Order Vestigial Disorder

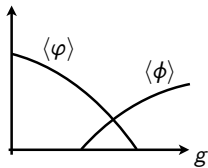


Order Disorder

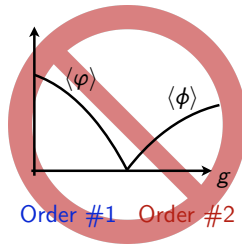
Cf. Landau paradigm: *"No single continuous transition between competing orders"*



Order #1 Order #2



Order #1 Coexistence Order #2



Order #1 Order #2