

Fractionalized fermionic quantum criticality in spin-orbital Mott insulators

Lukas Janssen
(TU Dresden)



Urban Seifert



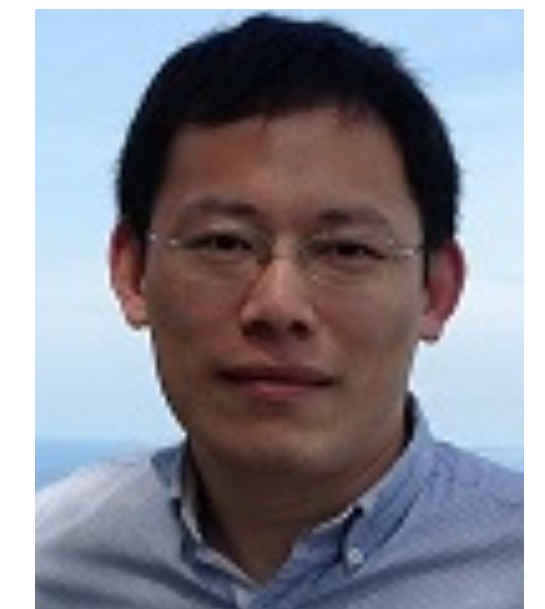
Xiao-Yu Dong



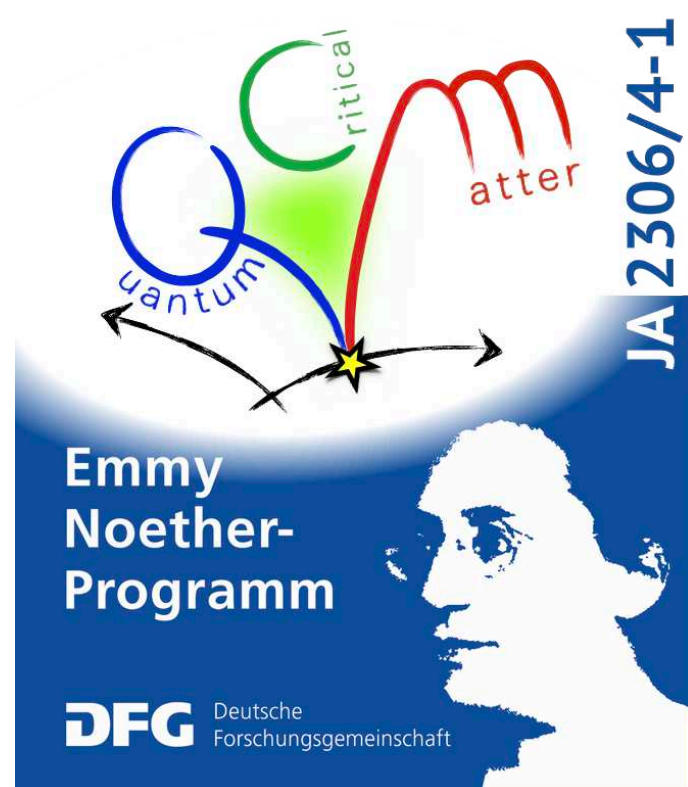
Sreejith Chulliparambil



Matthias Vojtá



Hong-Hao Tu



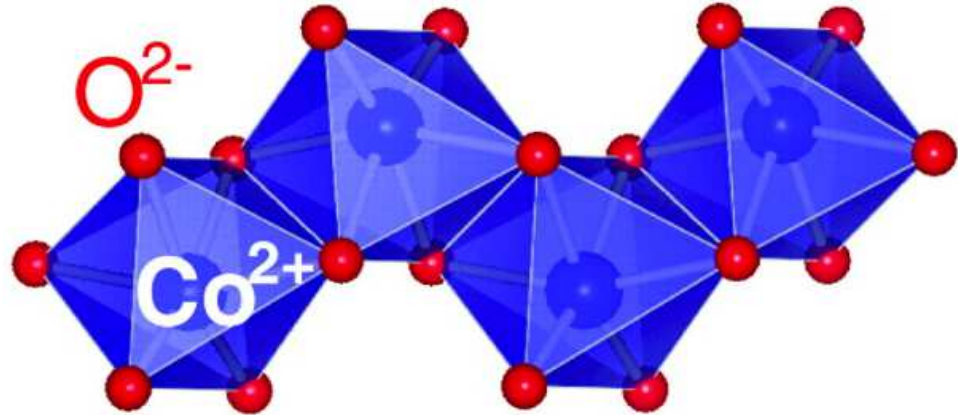
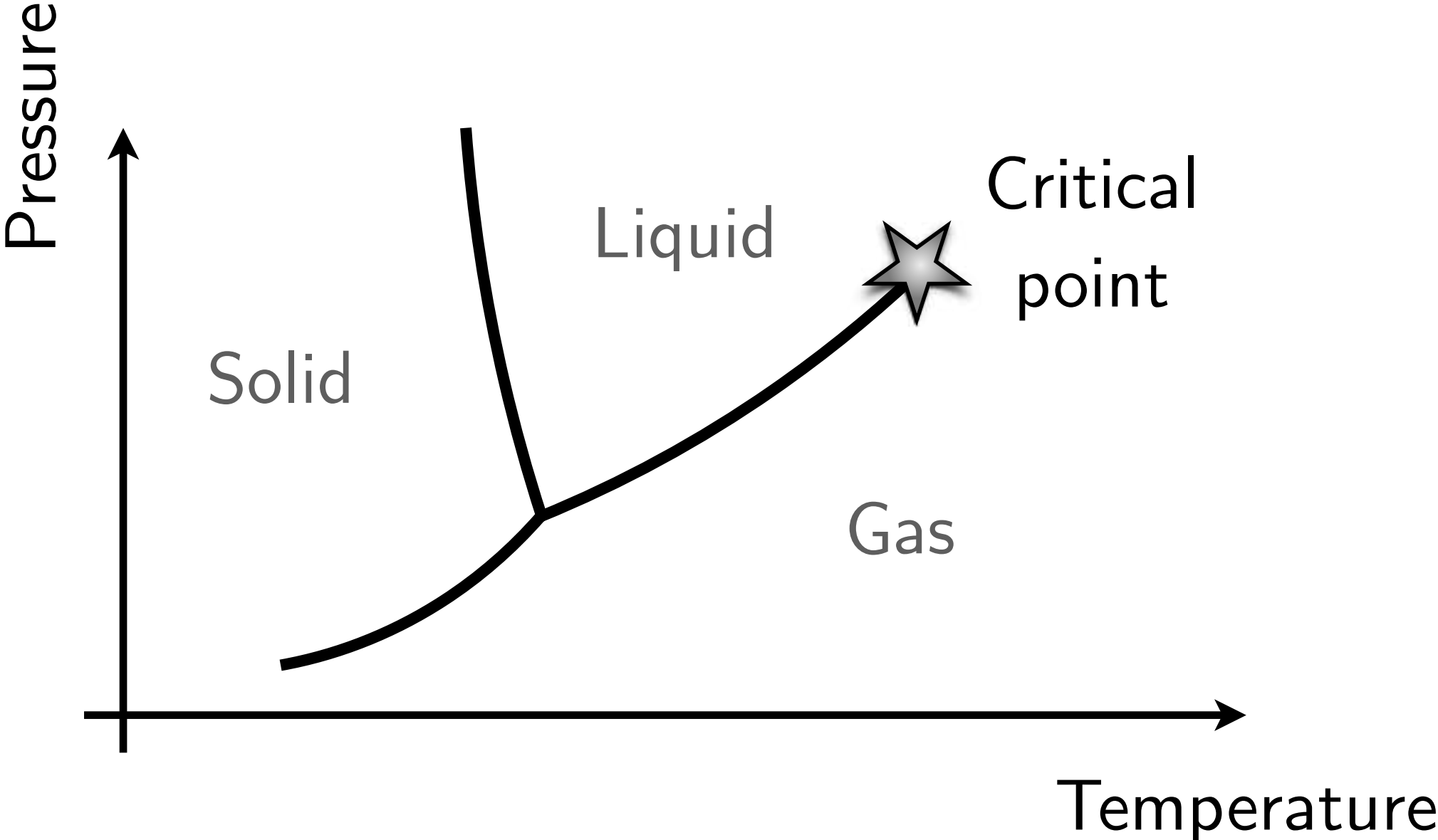
Outline

- (1) Introduction: *“Beyond-Landau” quantum criticality*
- (2) Spin-1/2: *Field-induced criticality in Kitaev materials*
- (3) Spin-3/2: *Fractionalized fermionic criticality in spin-orbital models*
- (4) Conclusions

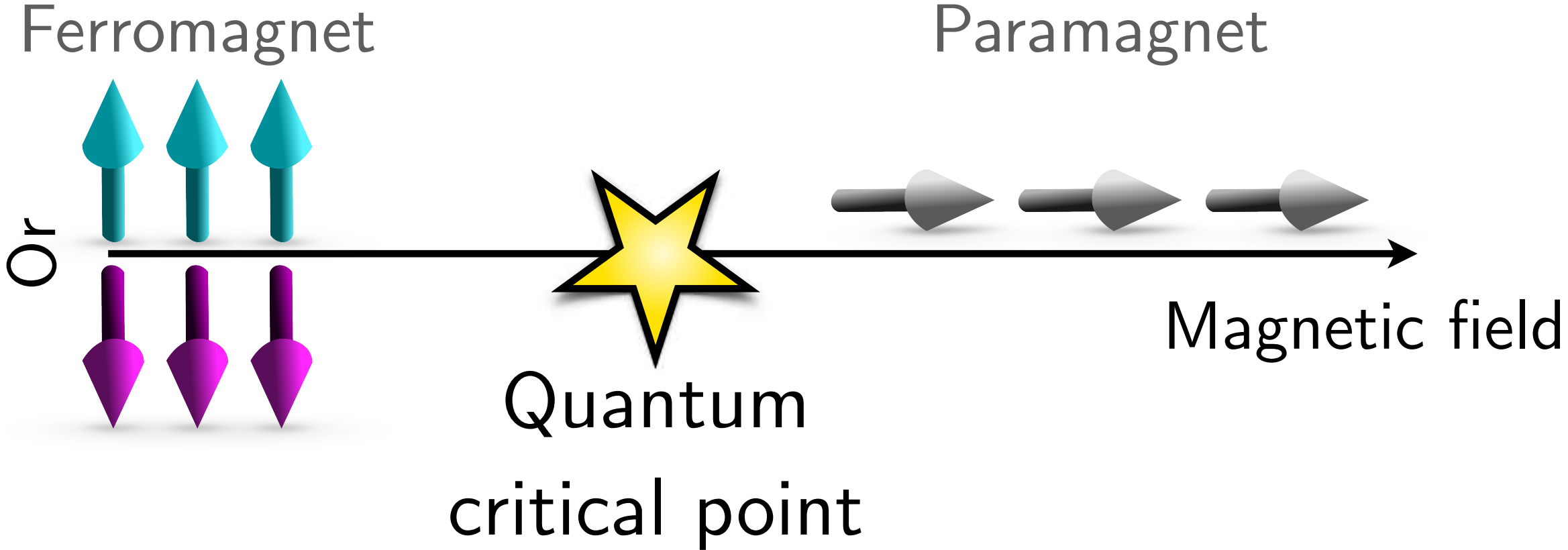
Classical vs quantum criticality



H_2O $T > 0$



CoNb_2O_6 $T \rightarrow 0$

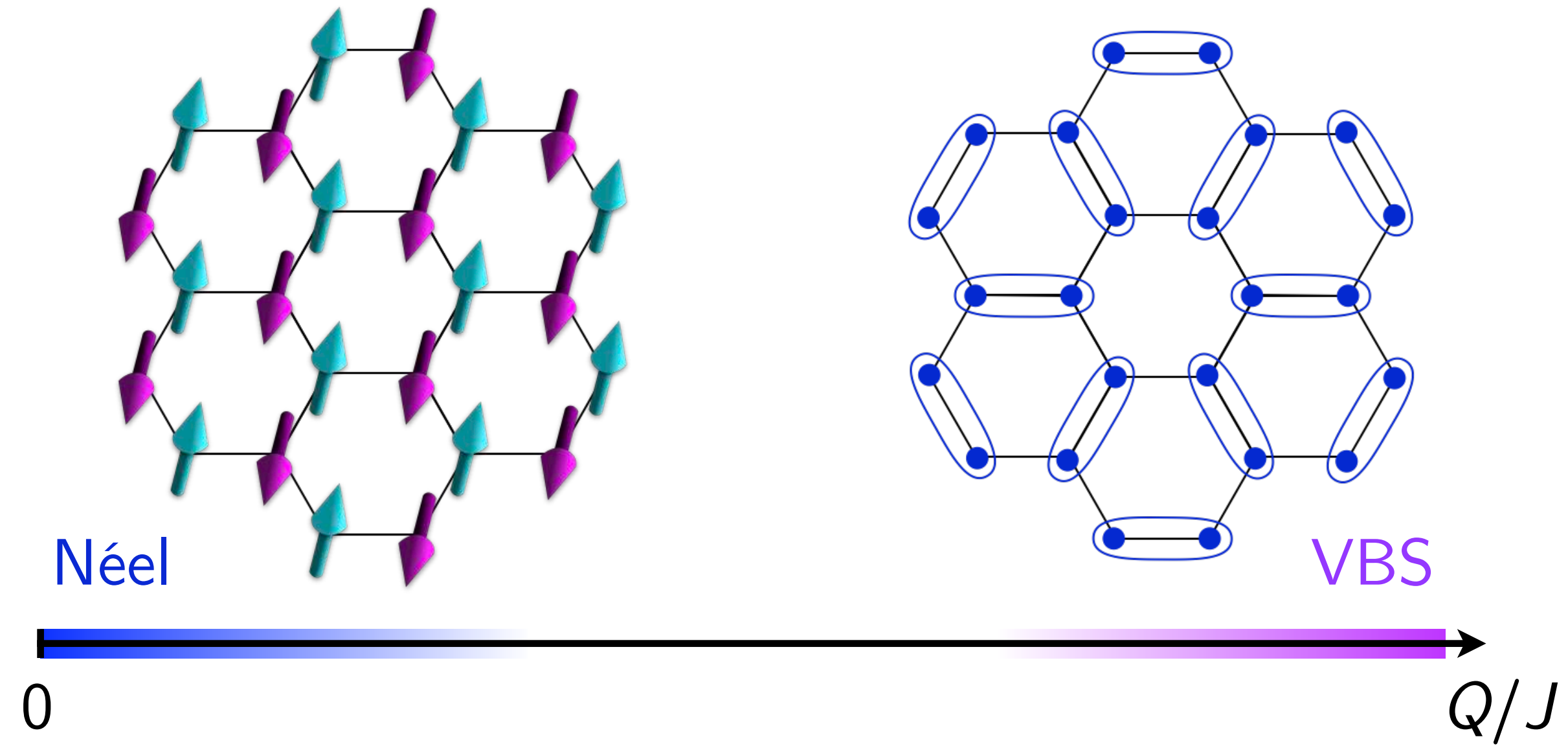


[Coldea *et al.*, Science '10]
 [Kinross *et al.*, PRX '14]

...

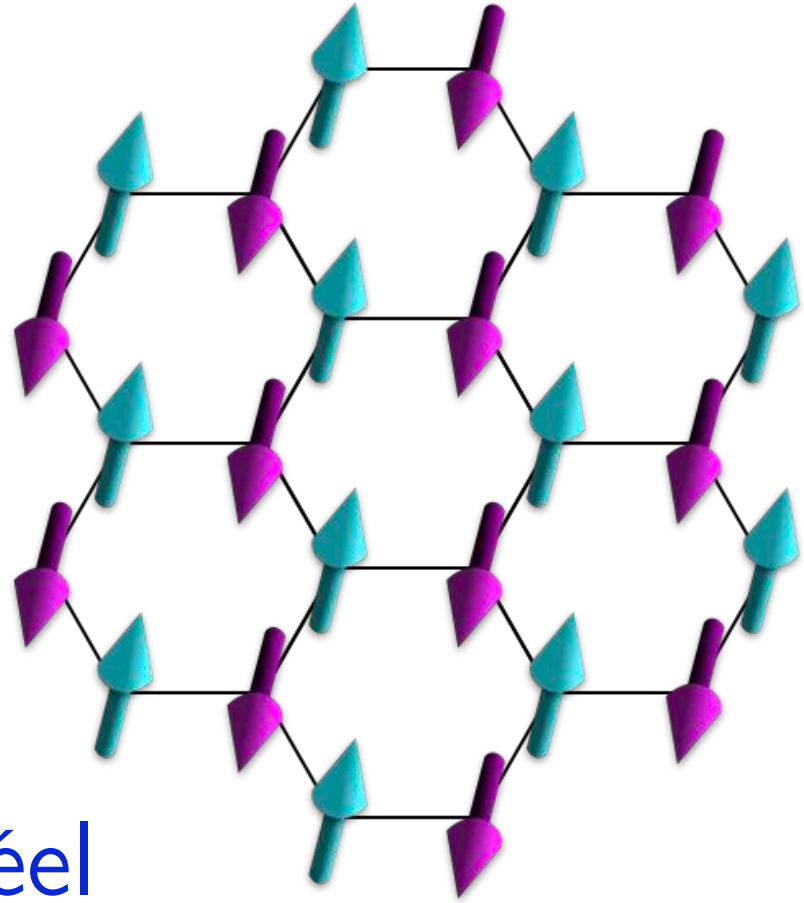
Deconfined quantum criticality

$$\text{---} = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$$

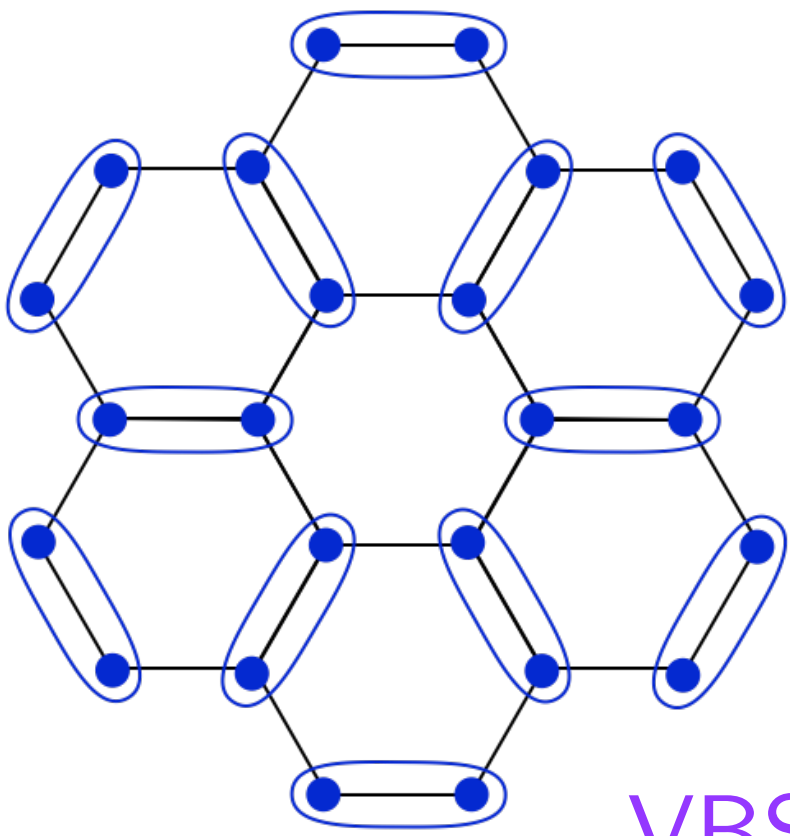


Deconfined quantum criticality

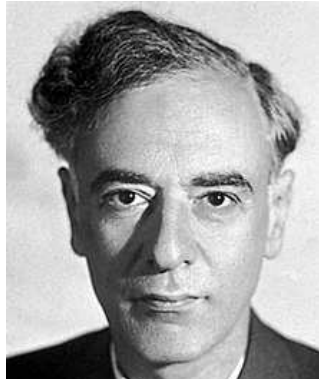
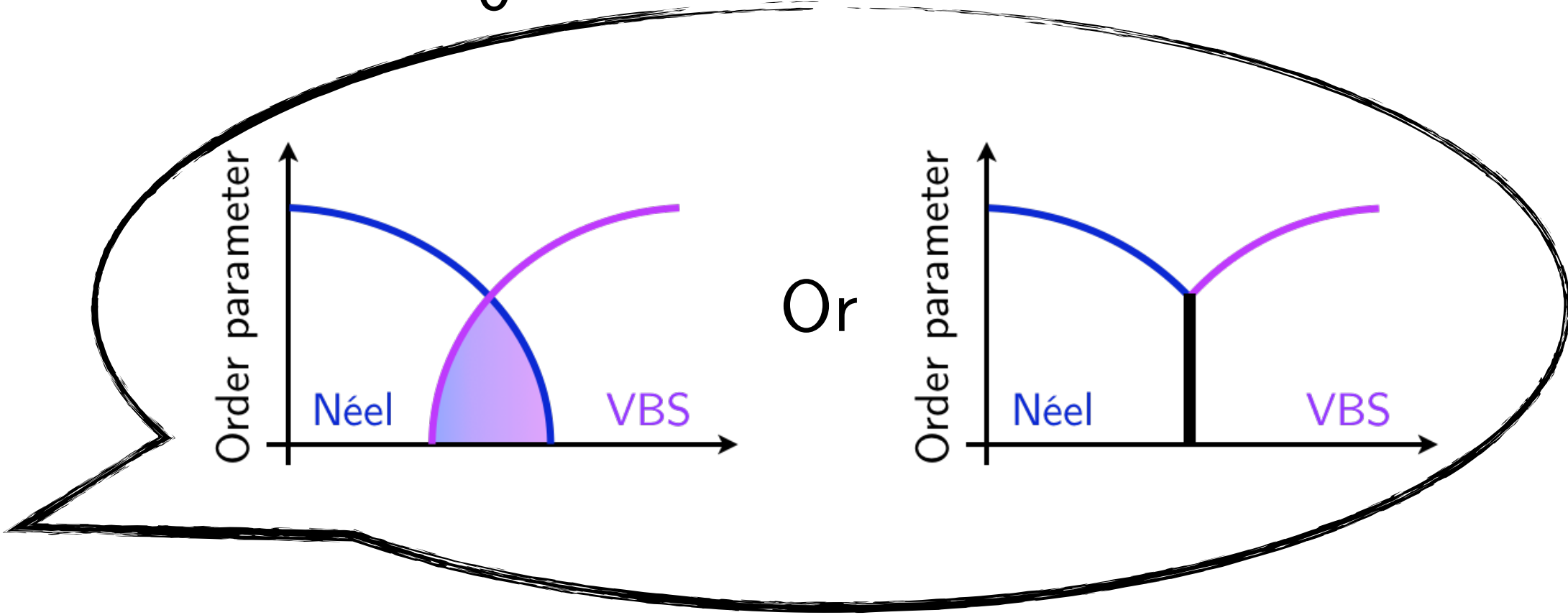
$$\text{---} = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$$



Néel



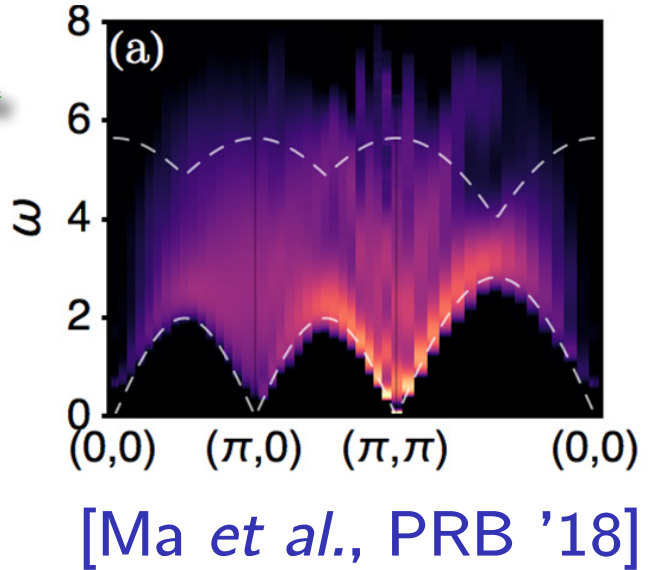
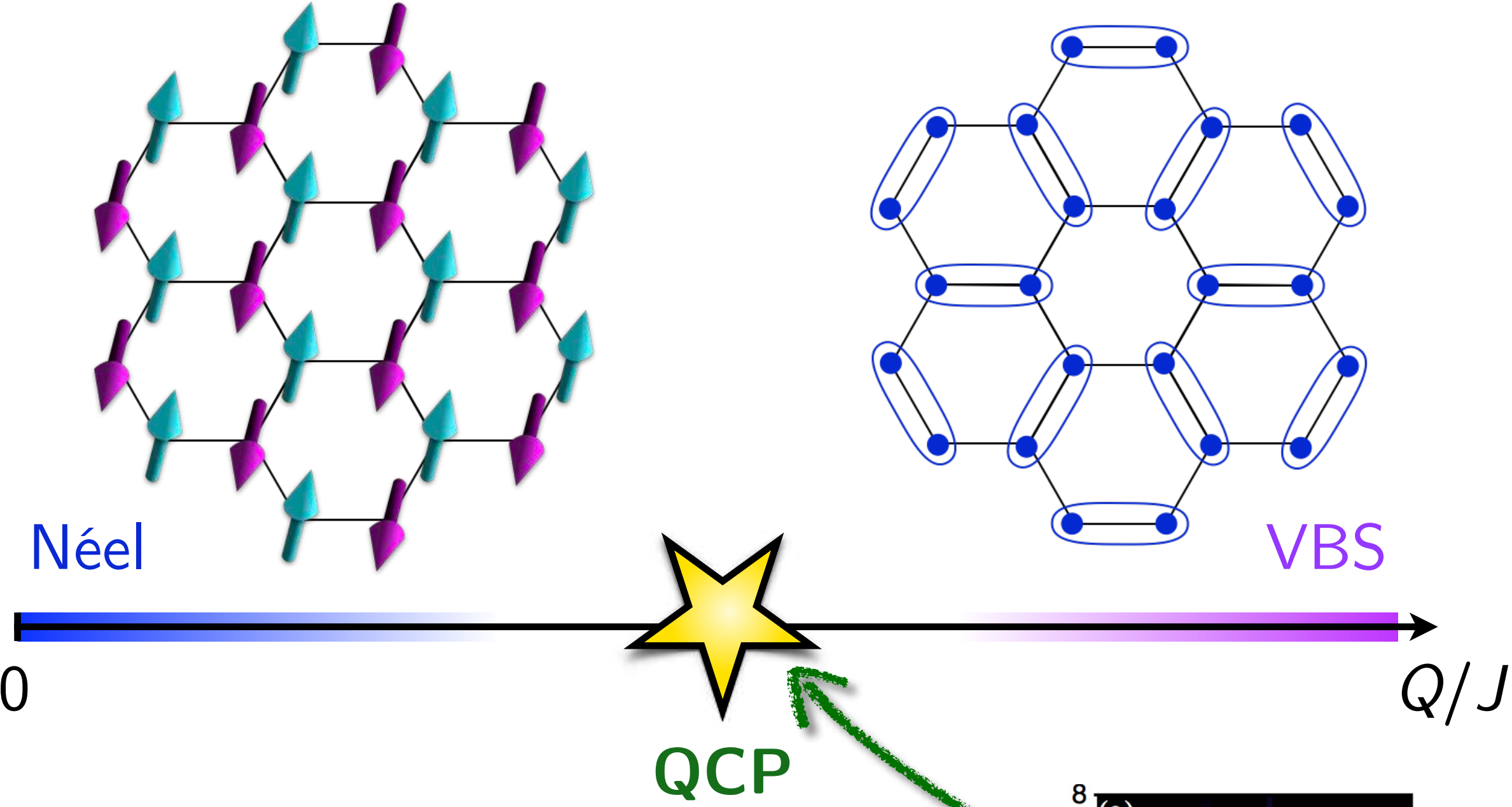
VBS



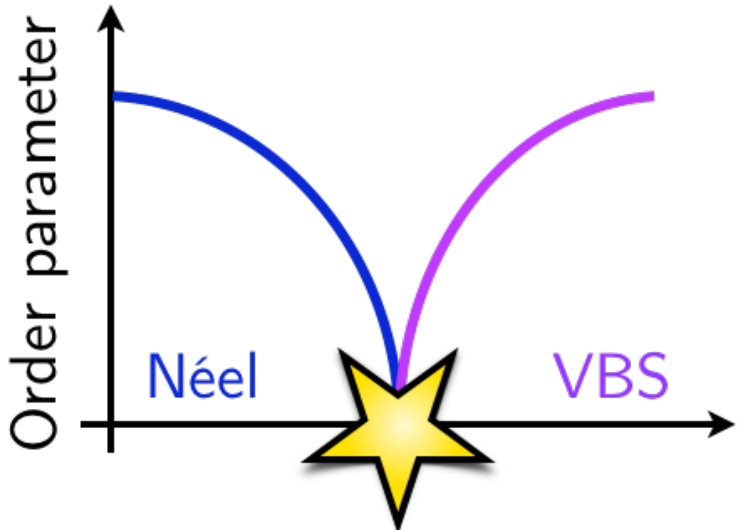
Landau

Deconfined quantum criticality

$$\text{---} = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$$

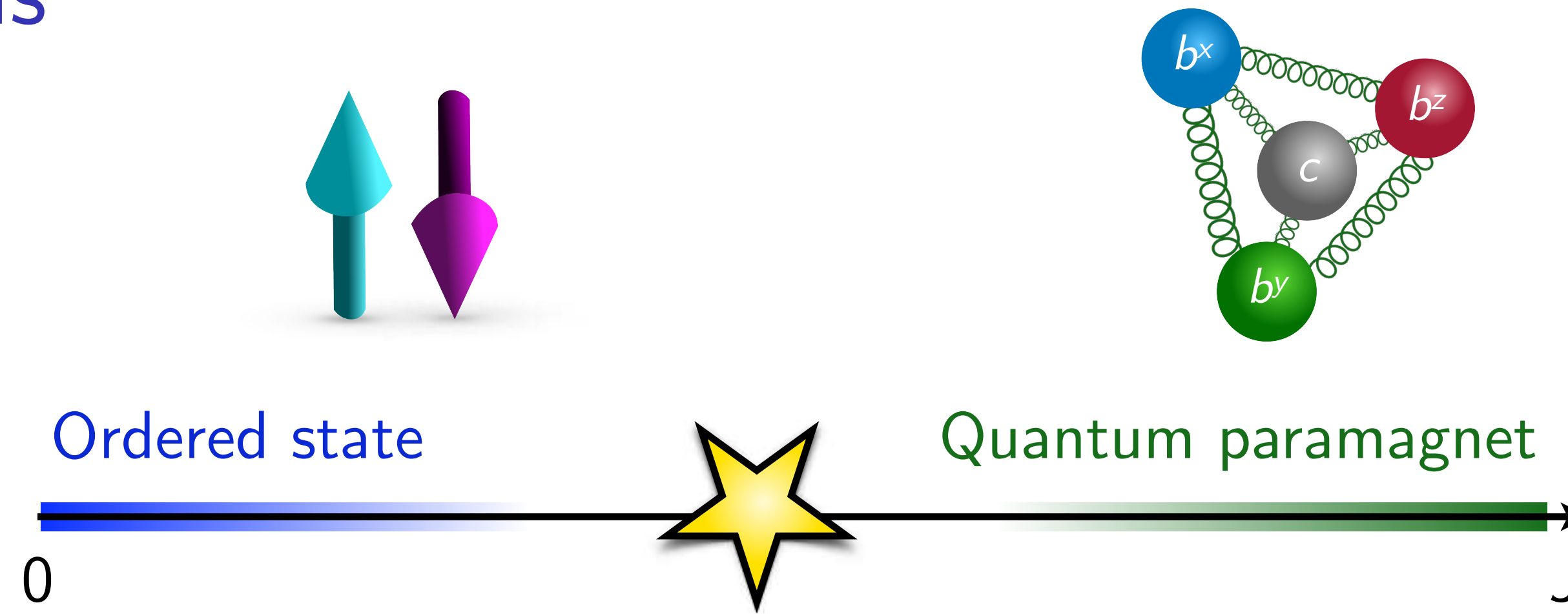


“Deconfined” quasiparticles B and \bar{B}



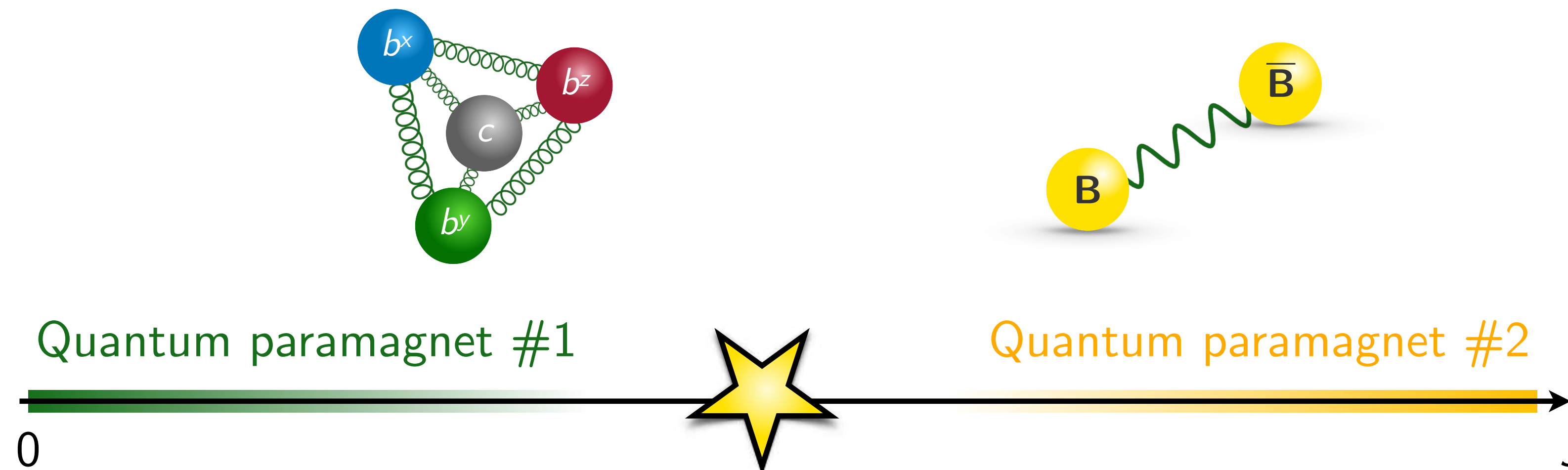
[Senthil *et al.*, Science '04]
 [Pujari, Damle, Alet, PRL '13]
 [Block, Melko, Kaul, PRL '13]
 [Shao, Guo, Sandvik, Science '16]
 ...

Spin-liquid transitions



[Assaad & Grover, PRX '16]
[LJ, Wang, Scherer, Meng, Xu, PRB '20]

...



[Metlitski, Mross, Sachdev, Senthil, PRB '15]
[LJ & He, PRB '17]
[Boyack, Lin, Zerf, Rayyan, Maciejko, PRB '18]

...

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Frustrated magnets

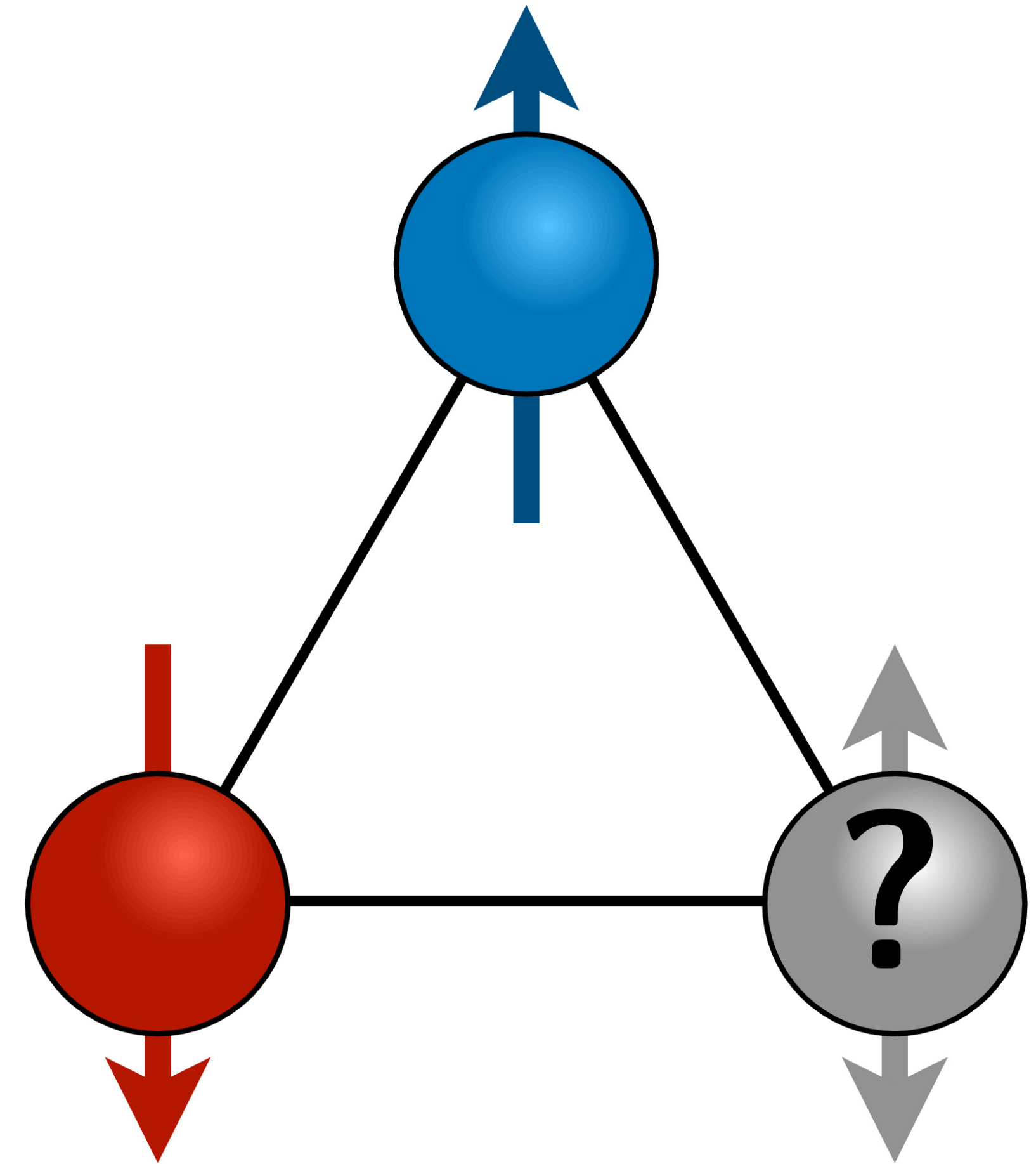
Frustration:

Not all local constraints can be simultaneously **satisfied**

Consequences:

Classical: Exponentially large ground-state manifold

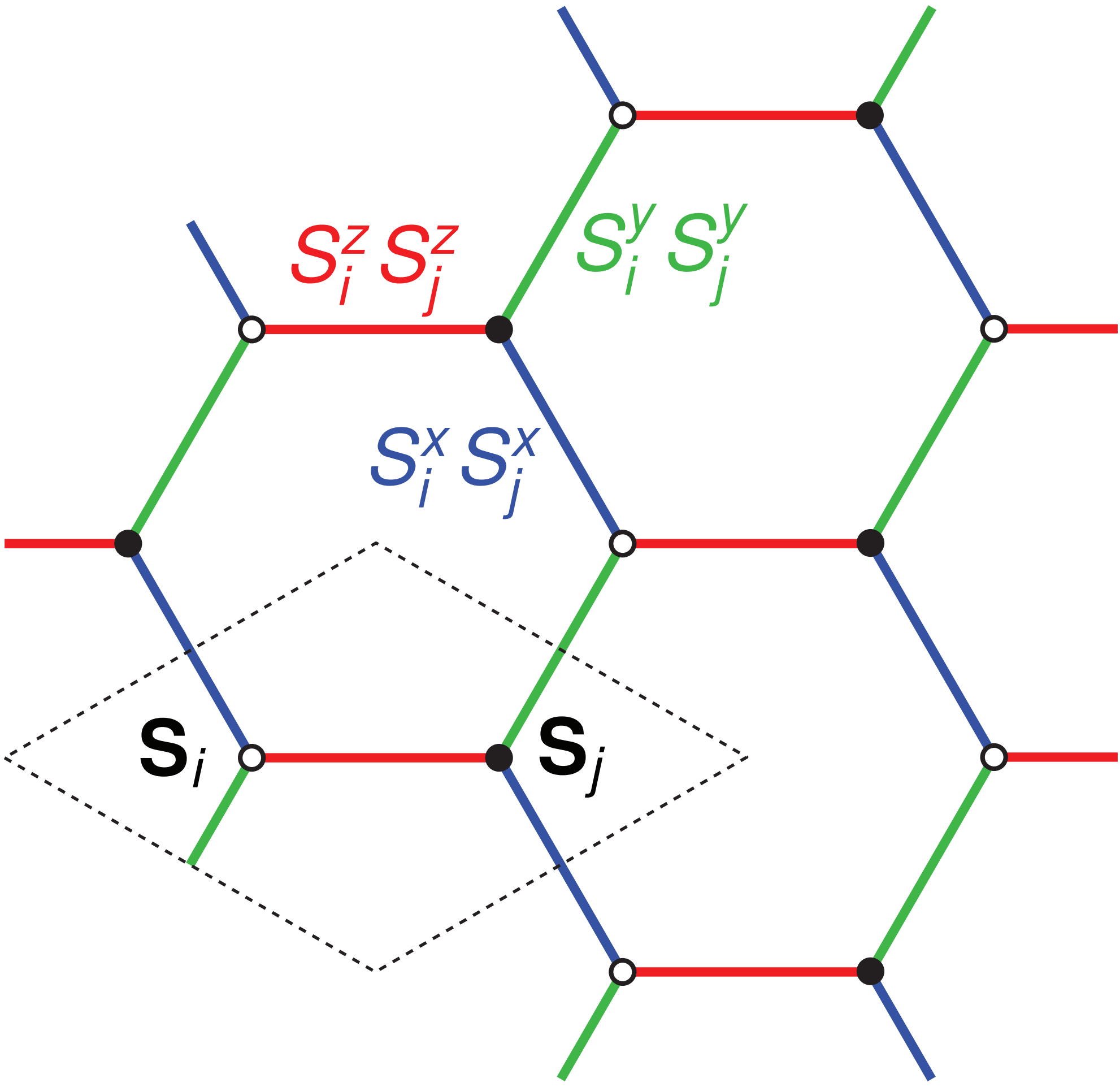
Quantum: New phases of matter?



Antiferromagnetic coupling of **3** Ising spins

Kitaev honeycomb model

Spin-1/2 on honeycomb lattice:



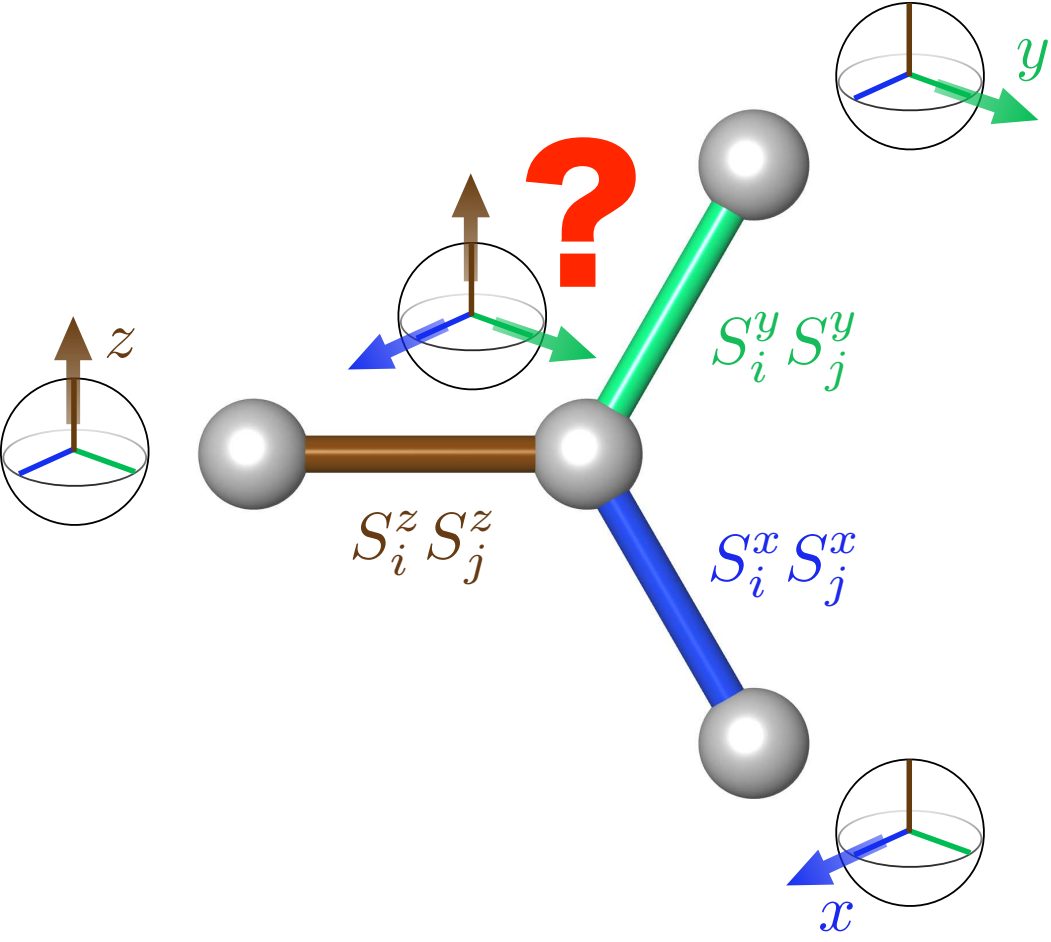
Hamiltonian:

$$H = -K_x \sum_{\text{blue links}} \sigma_i^x \sigma_j^x - K_y \sum_{\text{green links}} \sigma_i^y \sigma_j^y - K_z \sum_{\text{red links}} \sigma_i^z \sigma_j^z$$

[Kitaev, Ann. Phys. '06]



Alexei Kitaev



Exchange frustration

Review: [Trebst, arXiv:1701.07056]

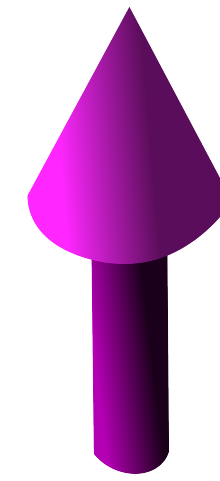
Parton construction

Majorana representation:

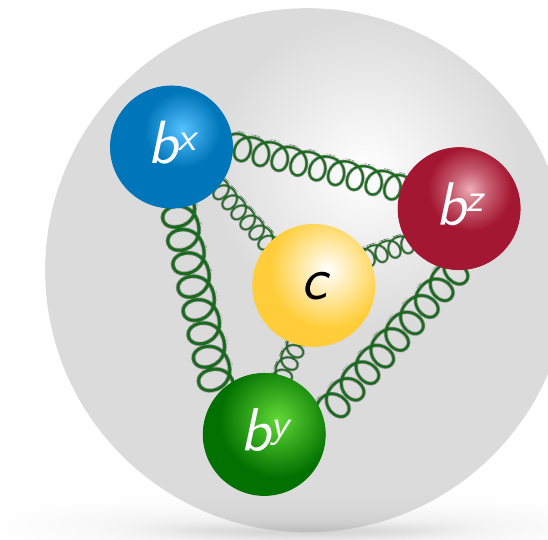
$$\sigma^x \mapsto \tilde{\sigma}^x = ib^x c$$

$$\sigma^y \mapsto \tilde{\sigma}^y = ib^y c$$

$$\sigma^z \mapsto \tilde{\sigma}^z = ib^z c$$



1 spin



4 Majoranas
with gauge constraint

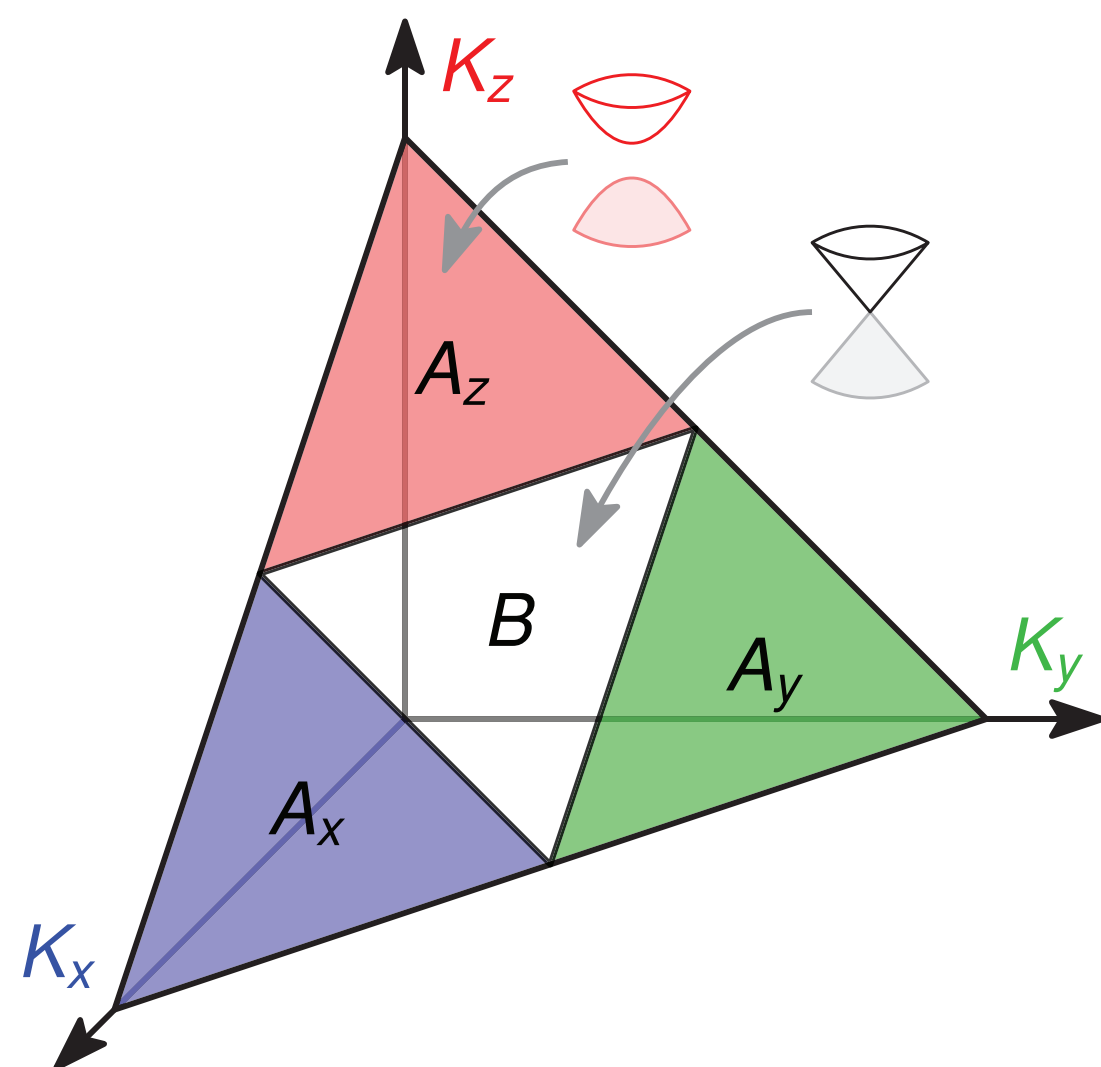
Fractionalization:

$$H \mapsto \tilde{H} = -i \sum_{\langle ij \rangle_\gamma} K_\gamma \underbrace{(ib_i^\gamma b_j^\gamma)}_{\equiv \hat{u}_{ij} = \hat{u}_{ij}^\dagger} c_i c_j$$

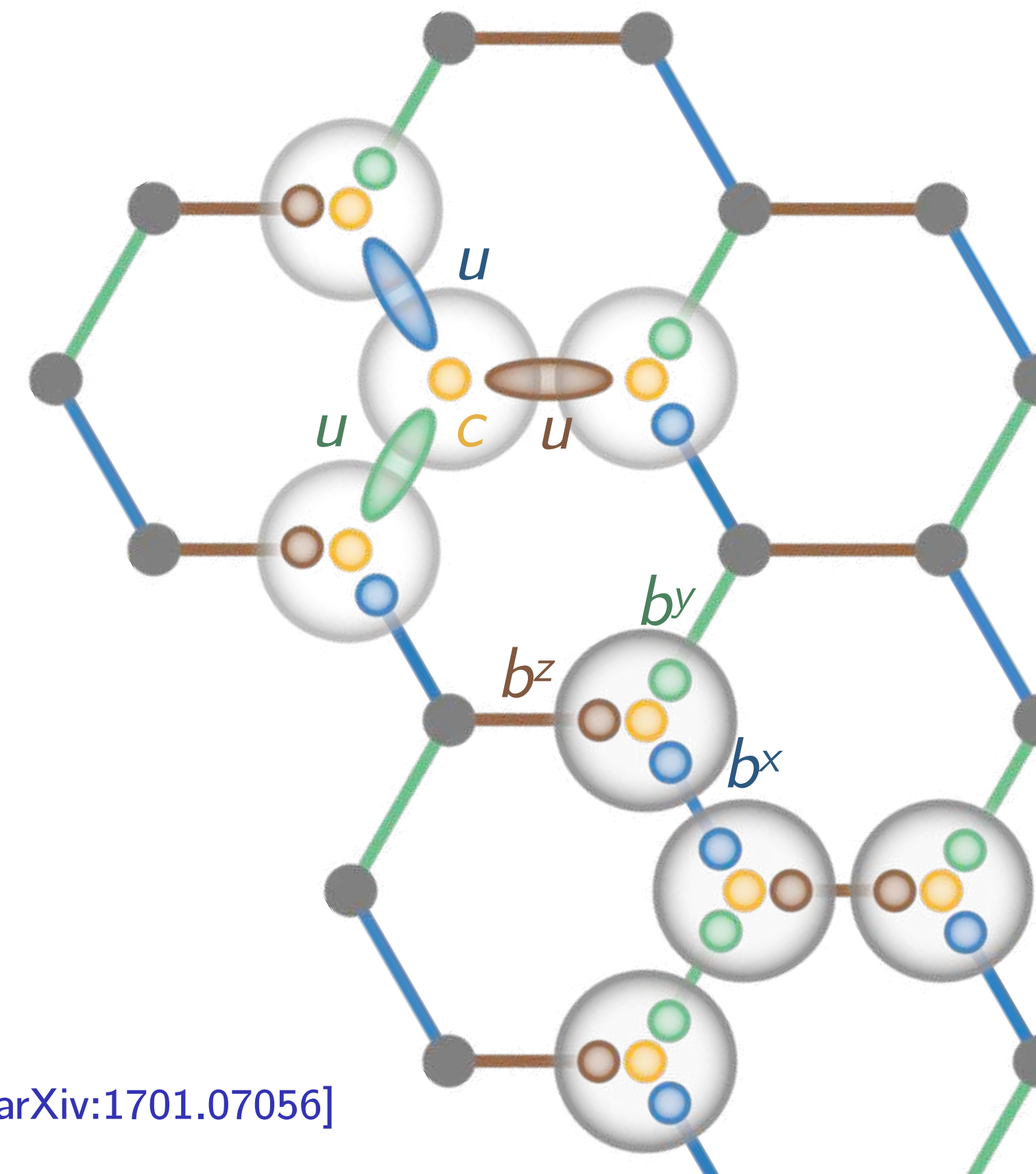
static!

Ground-state flux pattern: $u \equiv 1$
[Lieb, PRL '94]

Fermion spectrum:

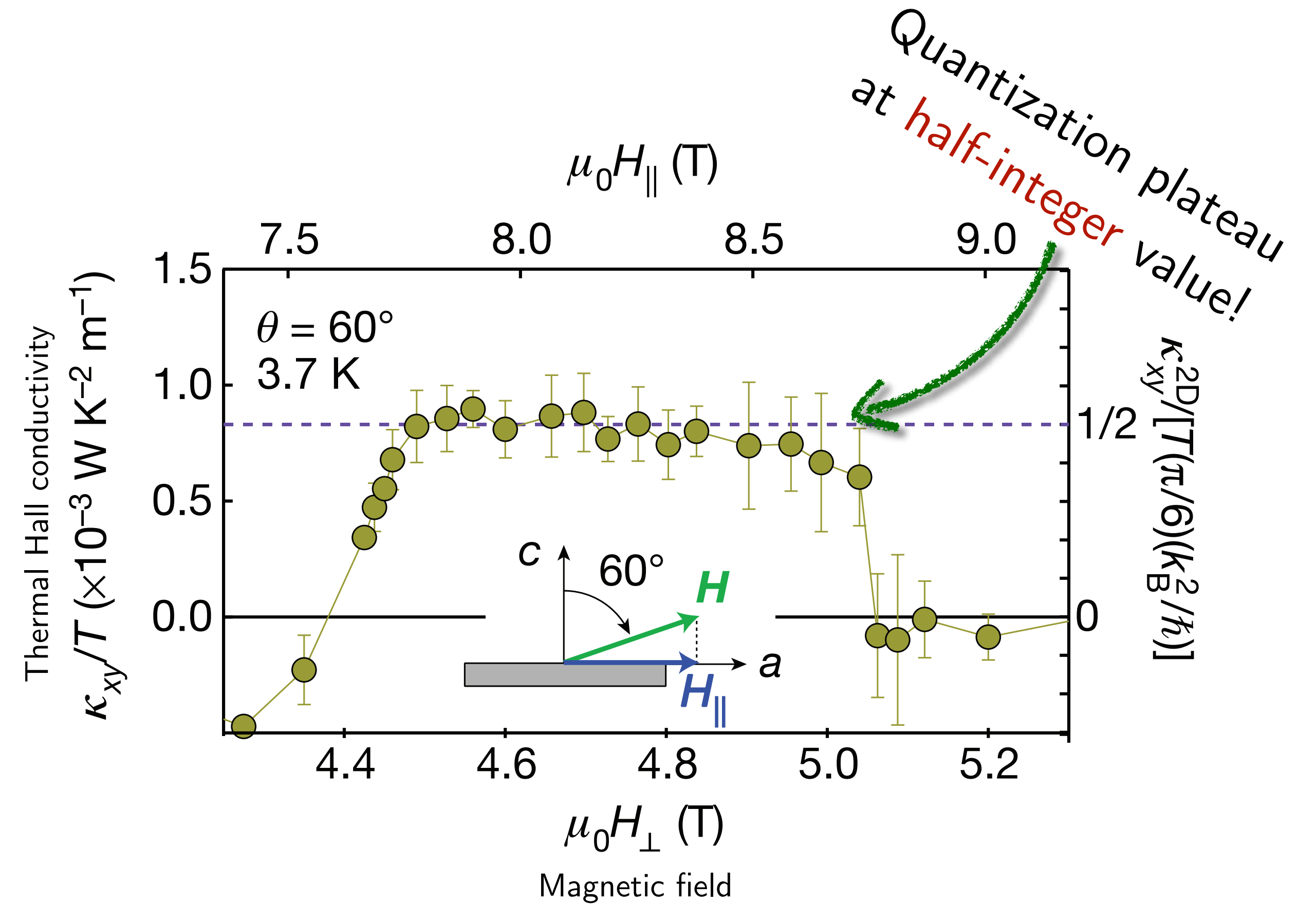
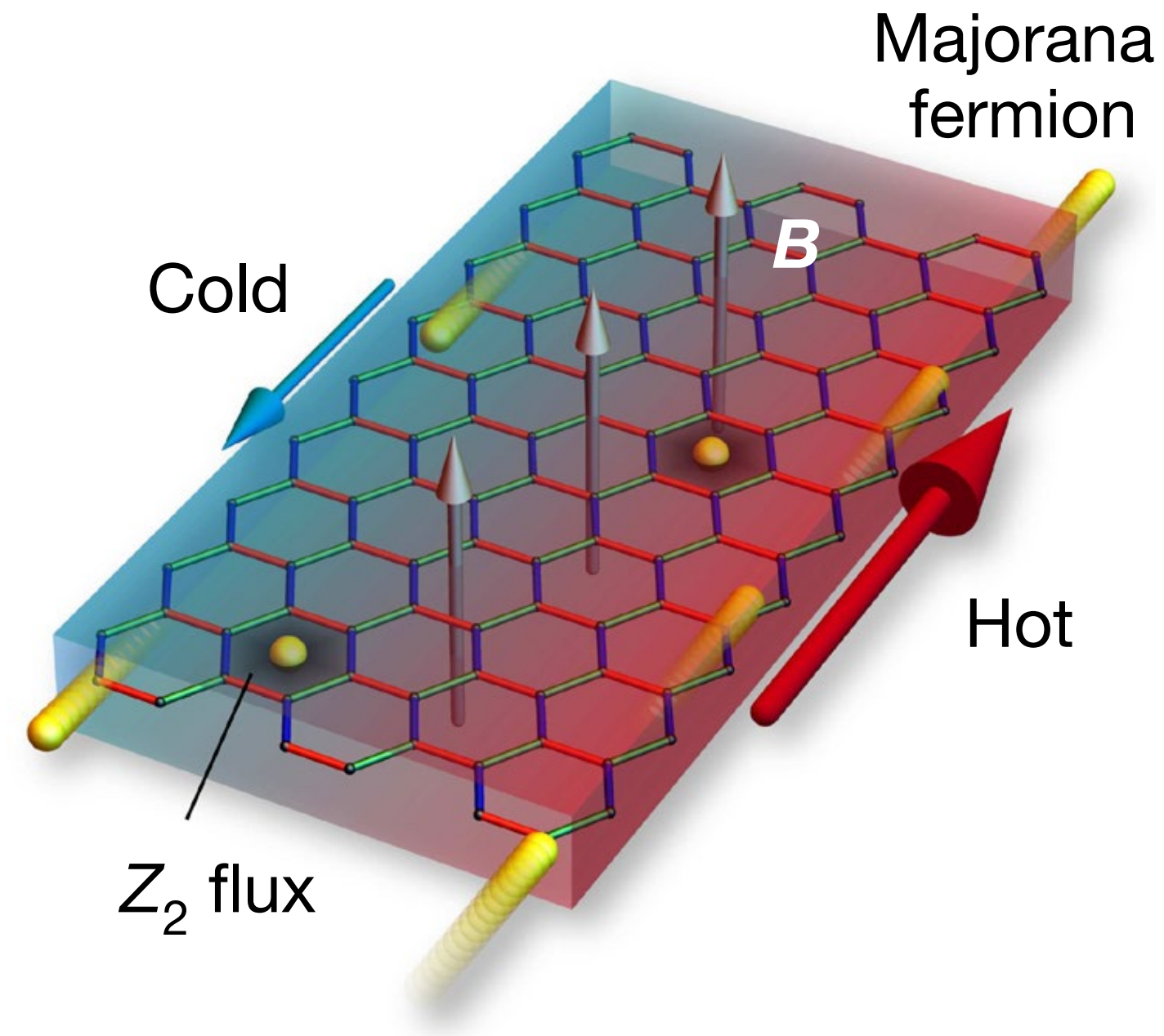


Review: [Trebst, arXiv:1701.07056]



Experimental search: α -RuCl₃ in field

Half-integer thermal Quantum Hall effect:



[Kasahara *et al.*, Nature '18]

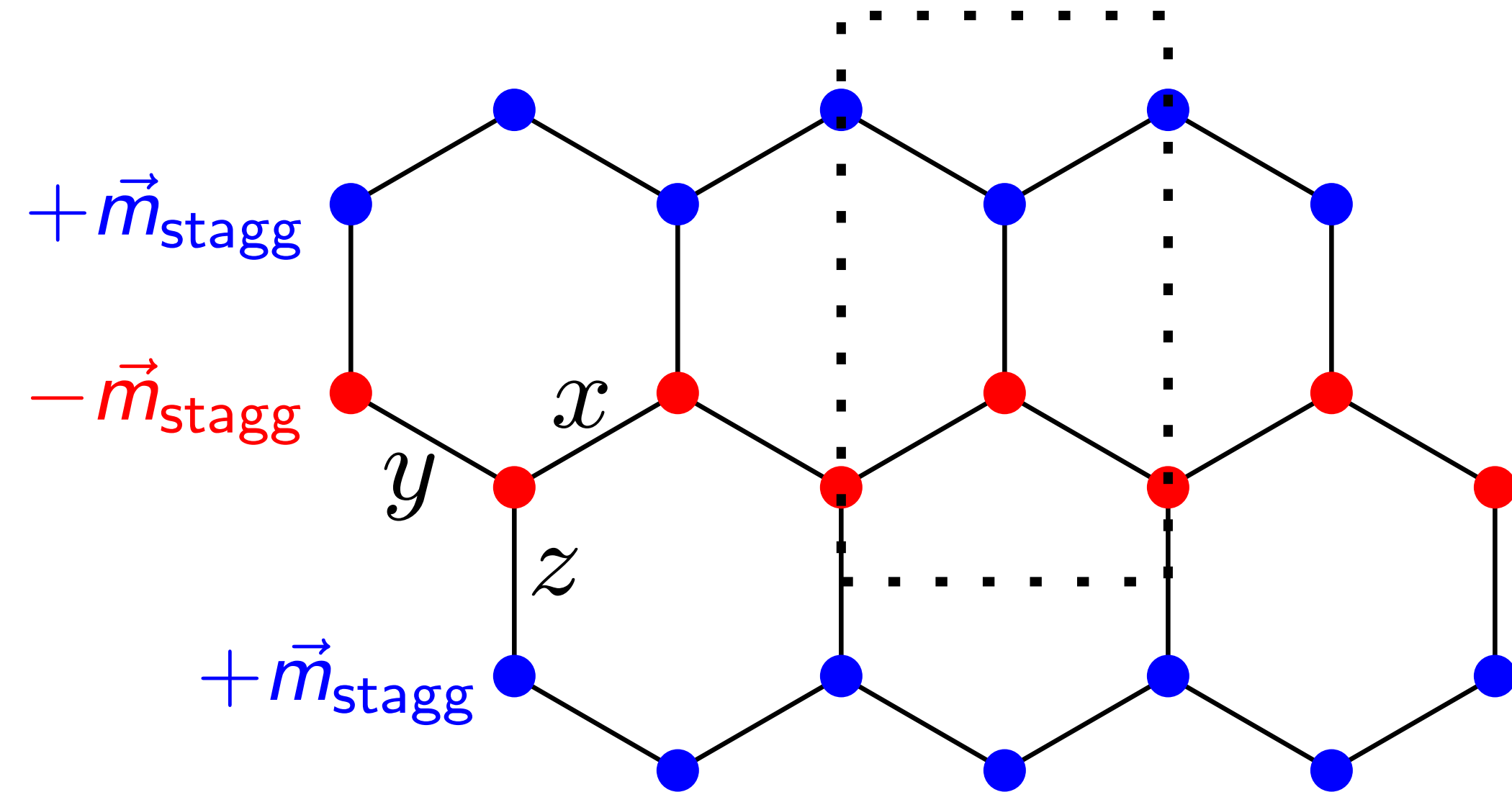
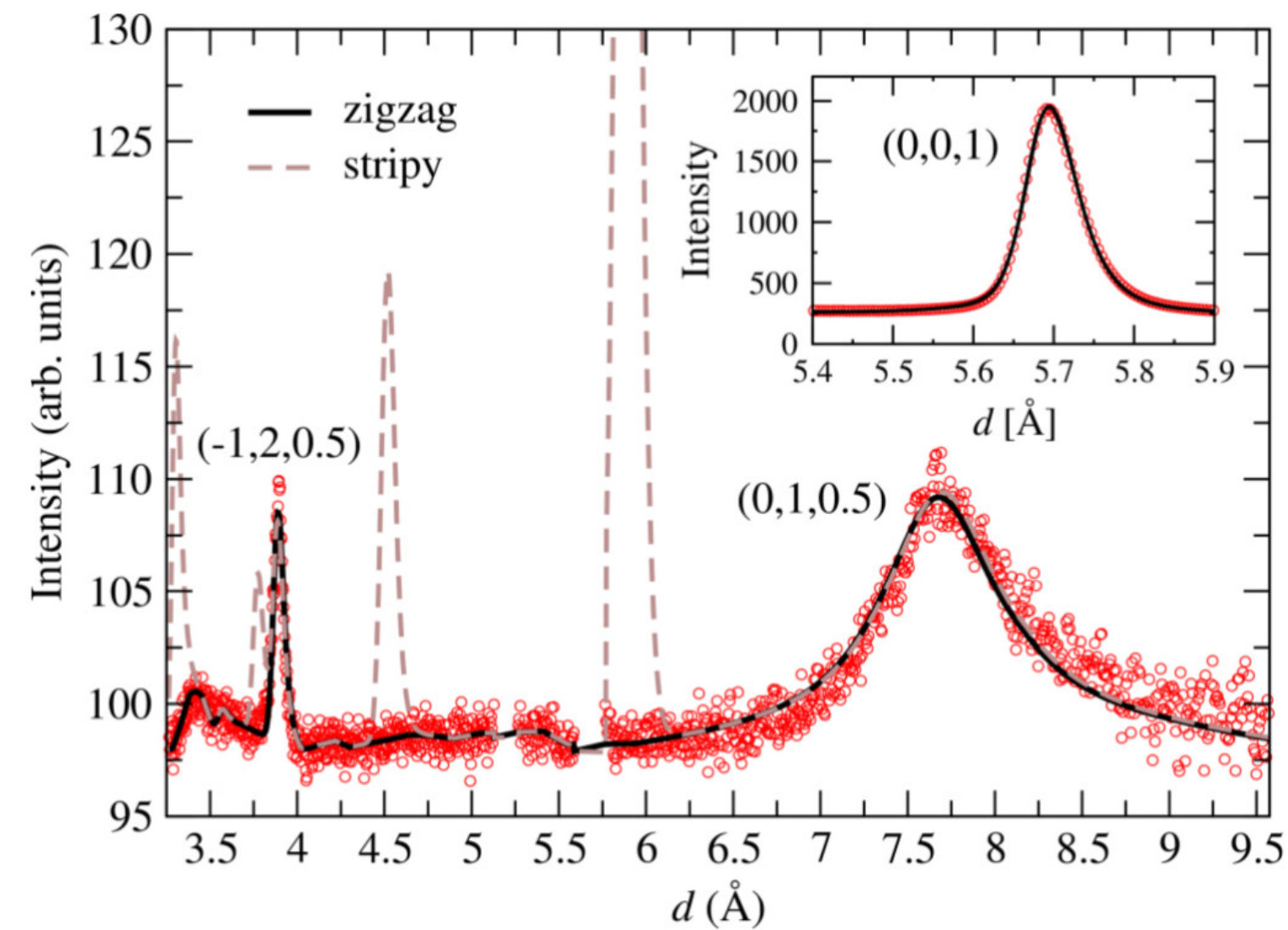
Topical Review: [LJ & Vojta, JPCM '19]

Smoking-gun signature of Majorana edge states?

α -RuCl₃ in zero field: Zigzag antiferromagnet

Neutron diffraction:

[Johnson *et al.*, PRB '15]



Extended Heisenberg-Kitaev models:

$$\mathcal{H} = \sum_{\langle ij \rangle} \left[J_1 \vec{S}_i \cdot \vec{S}_j + K_1 S_i^\gamma S_j^\gamma + \Gamma_1 (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right] + \sum_{\langle\langle\langle ij \rangle\rangle\rangle} J_3 \vec{S}_i \cdot \vec{S}_j + \dots$$

[Winter *et al.*, PRB '16]

[LJ, Andrade, Vojta, PRB '17]

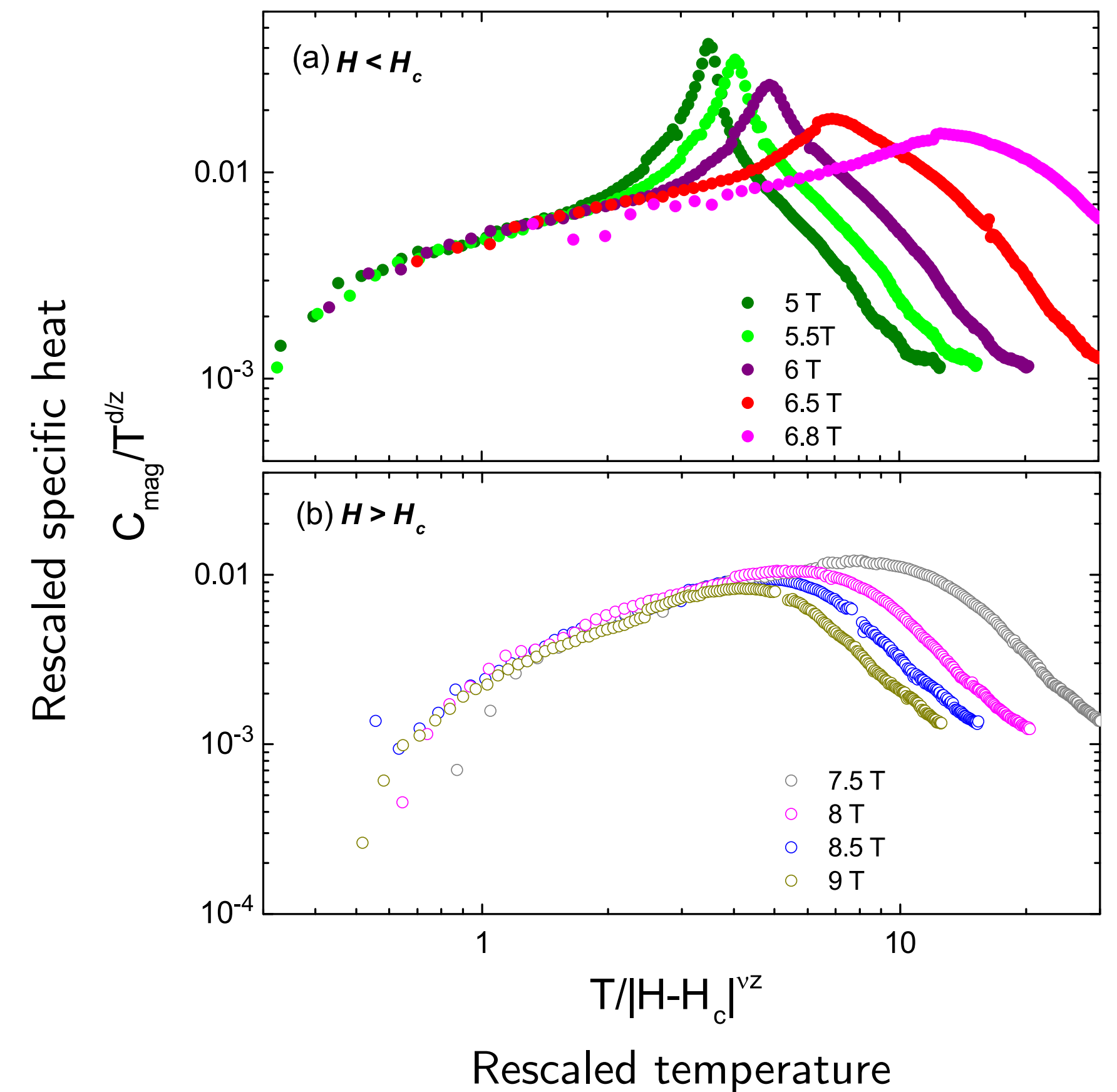
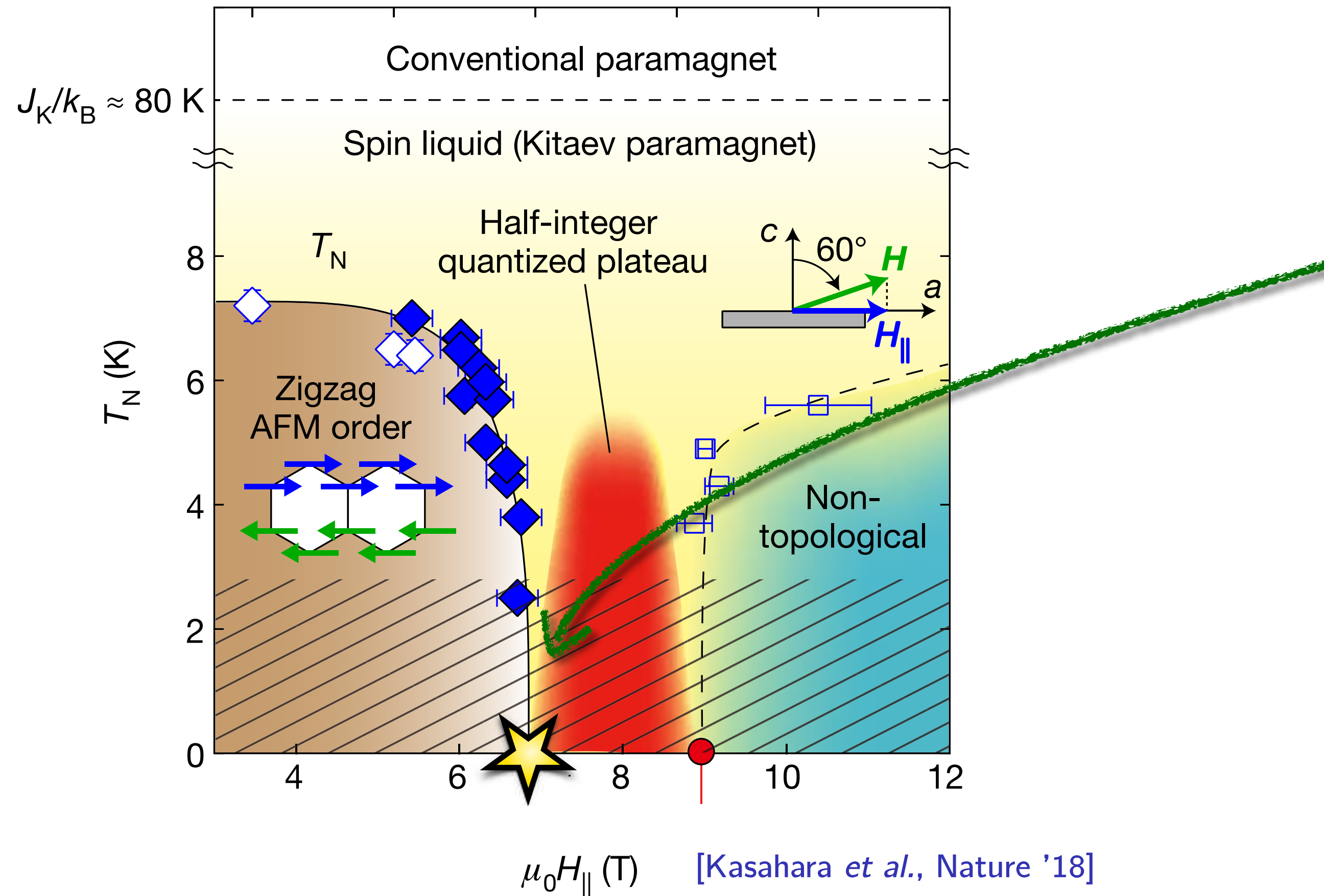
[Kaib, Winter, Valentí, PRB '19]

[LJ, Koch, Vojta, PRB '20]

[Maksimov & Chernyshev, PRR '20]

...

α -RuCl₃: Field-induced quantum criticality



... with $z \approx 1$ and $\nu \approx 0.7$

[Wolter, Corredor, LJ, *et al.*, PRB '17]

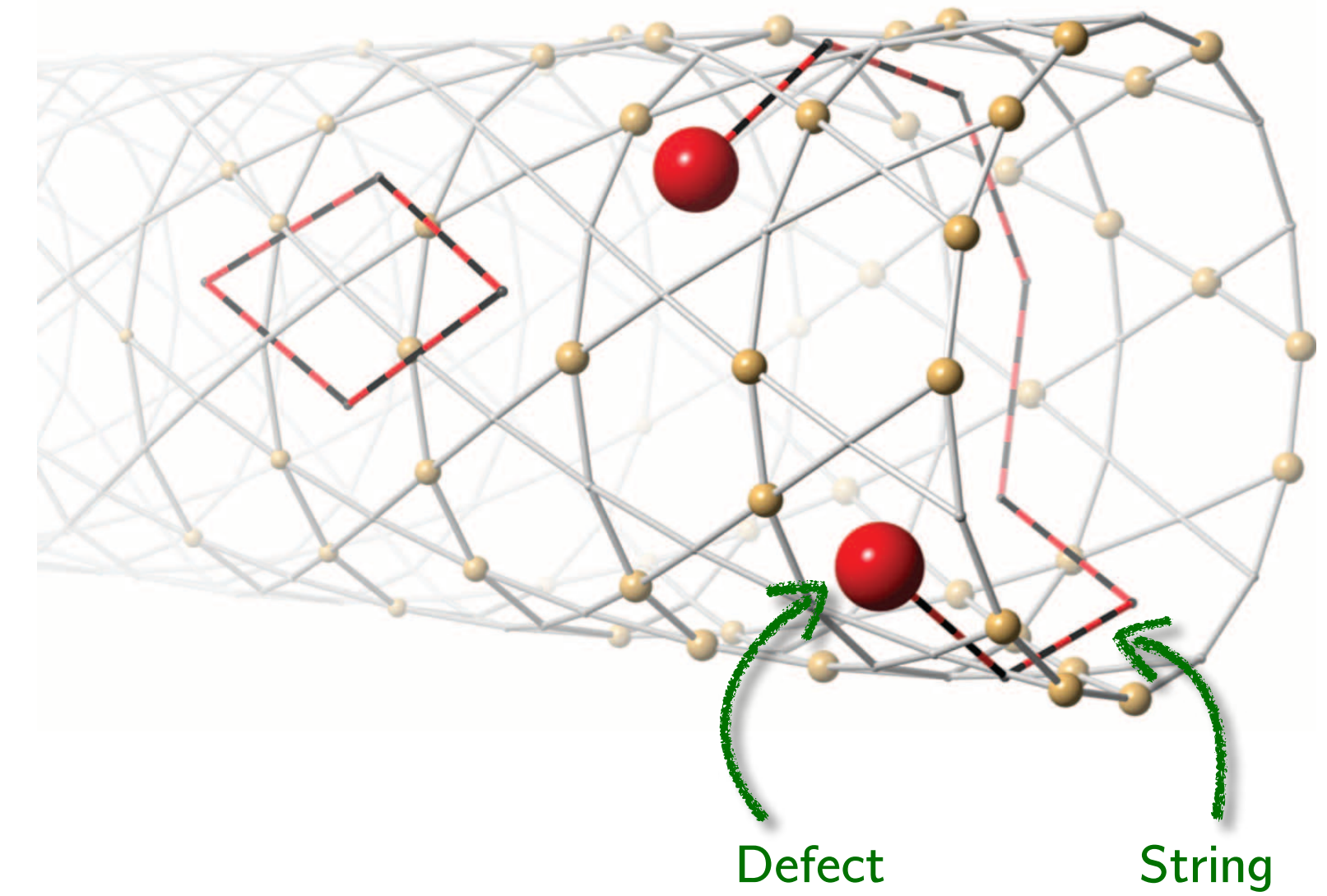
Fractionalized transition?

Fractionalized quantum criticality: XY*

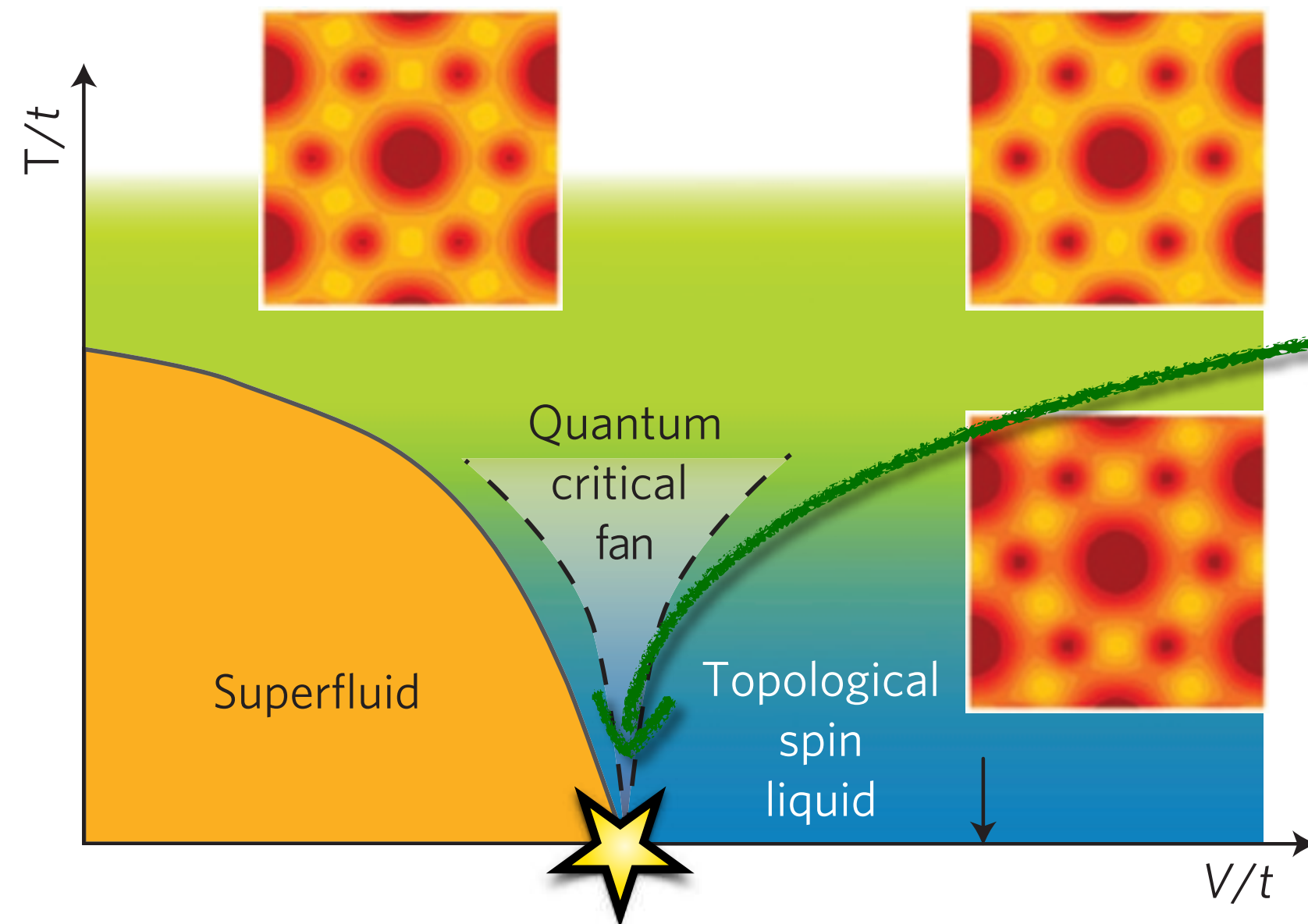
Bose-Hubbard-like model (kagome lattice):

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \left[b_i^\dagger b_j + b_i b_j^\dagger \right] + V \sum_{\text{hex}} (n_{\text{hex}})^2$$

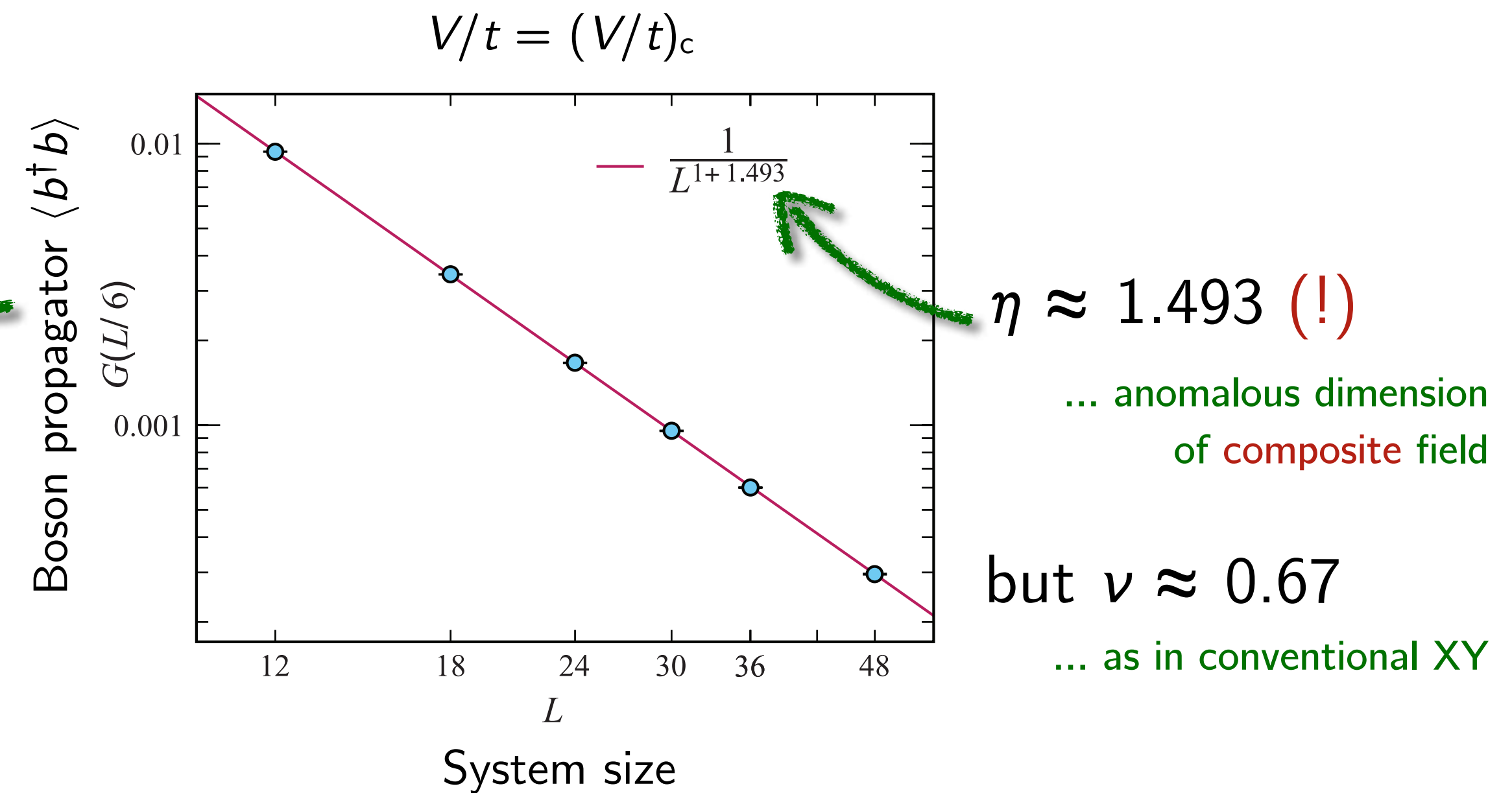
↑ Hopping bosons
↑ Boson density in plaquette



Phase diagram:

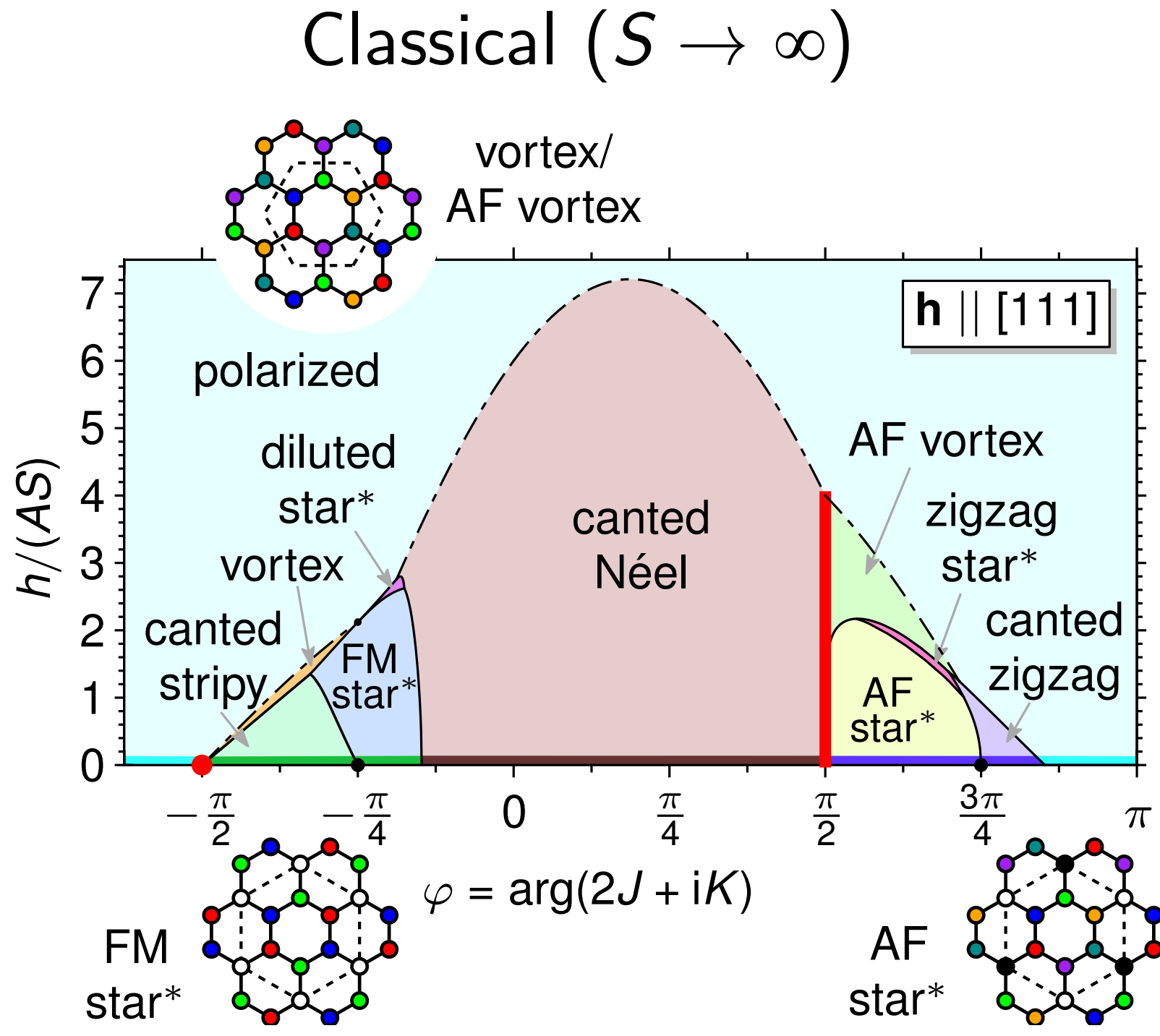


[Isakov, Hastings, Melko, Nat. Phys. '11]

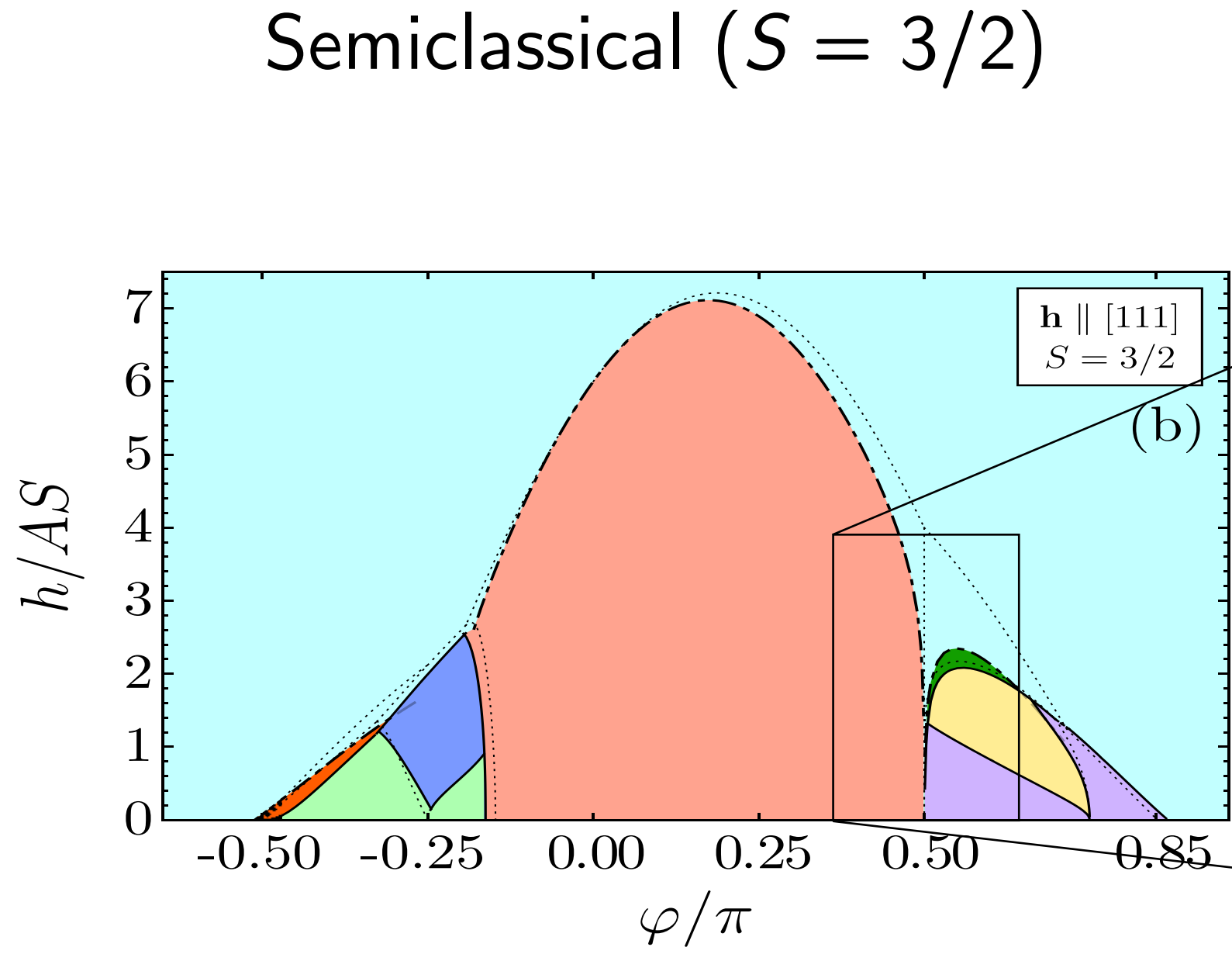


[Isakov, Melko, Hastings, Science '12]
 [Chubukov, Senthil, Sachdev, PRL '94]

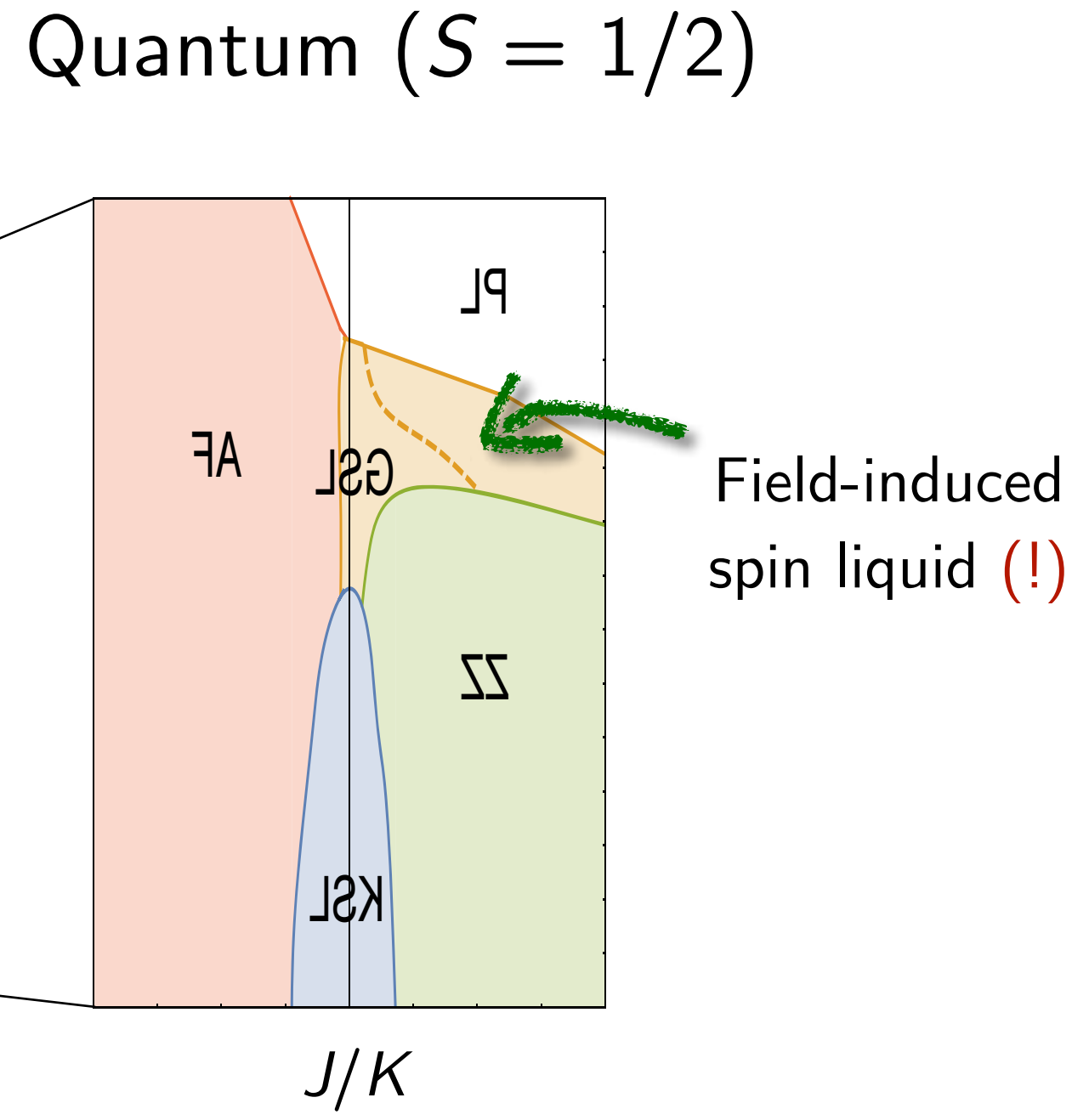
Heisenberg-Kitaev models in field



[LJ, Andrade, Vojta, PRL '16]
... linear spin-wave theory
& classical Monte Carlo



[Consoli, LJ, Vojta, Andrade, PRB '20]
... nonlinear spin-wave theory



[Hickey & Trebst, Nat. Commun. '19]
... 24-site ED

Technical challenge: Dynamical \mathbb{Z}_2 gauge field!

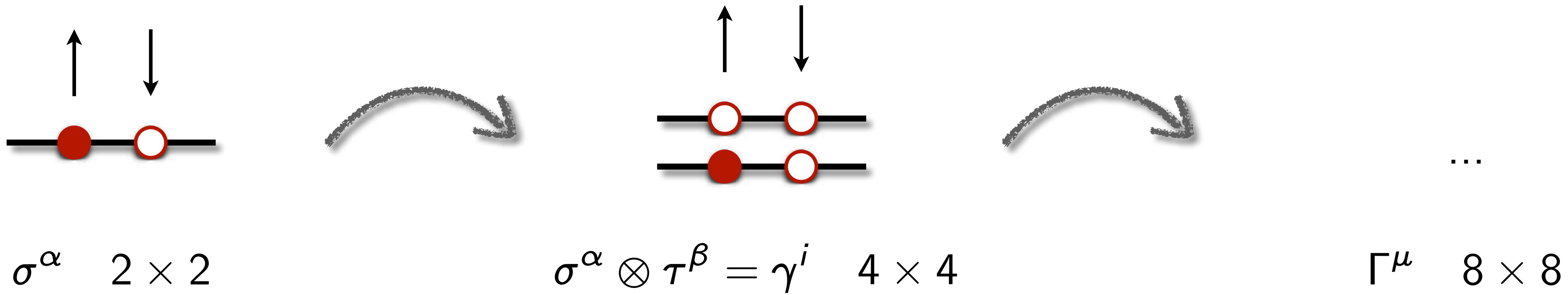
... no sign-problem-free QMC available

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Generalizations of Kitaev model: Spin-orbital liquids

Spin + orbital + ... degrees of freedom:



... can realize all 16 \mathbb{Z}_2 topological superconductors
 [Chulliparambil, ..., LJ, Tu, arXiv:2005.13683]

Example #1 (square lattice):

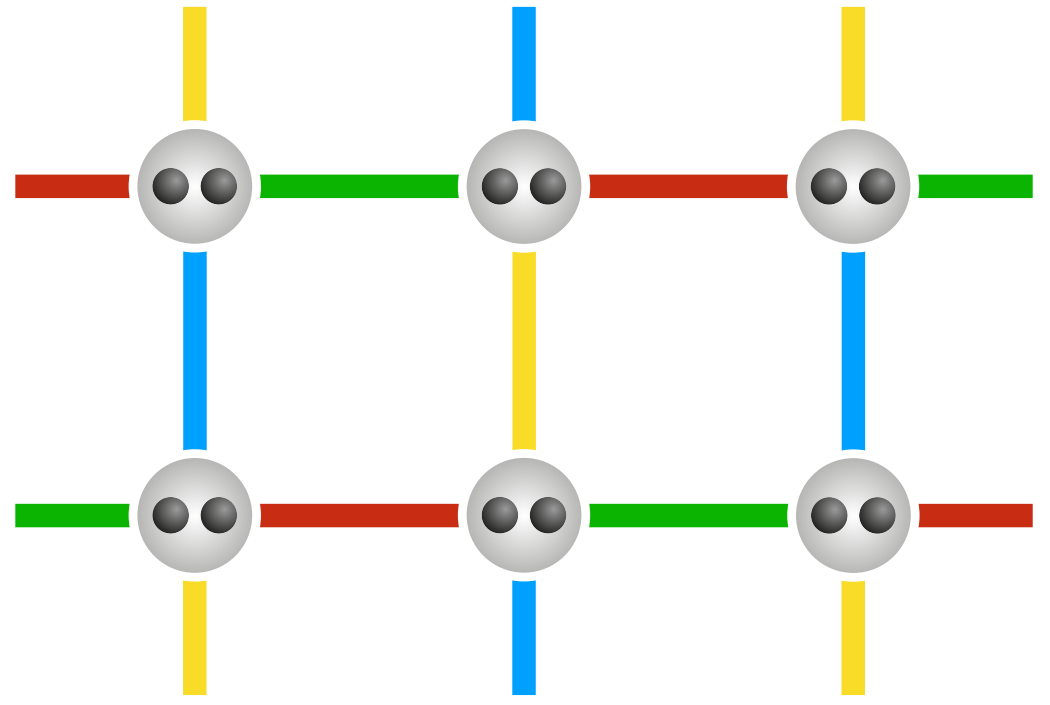
$$H_K = -K \sum_{\langle ij \rangle_\gamma} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \otimes \tau_i^\gamma \tau_j^\gamma$$

XY spin Kitaev orbital

Majorana representation:

- $\sigma^y \otimes \tau^x = ib^1 c^x$
- $\sigma^y \otimes \tau^y = ib^2 c^x$
- $\sigma^y \otimes \tau^z = ib^3 c^x$
- $\sigma^x \otimes \mathbb{1} = ib^4 c^x$
- $\sigma^z \otimes \mathbb{1} = ic^y c^x$

... recover known model for $j = 3/2$ spin liquid:
 [Yao, Zhang, Kivelson, PRL '09]
 [Nakai, Ryu, Furusaki, PRB '12]

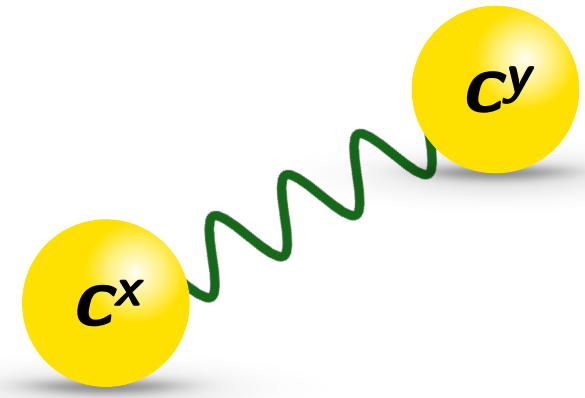


2 itinerant fermions

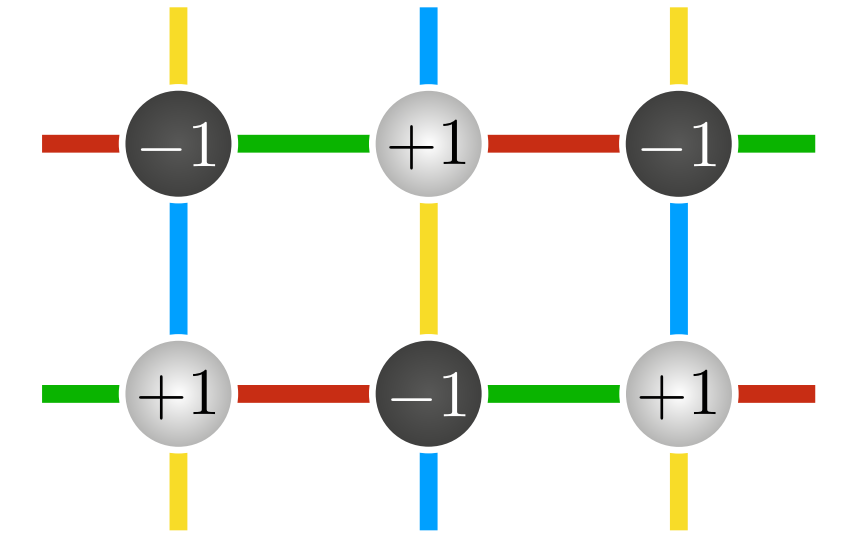
Static perturbations

“Heisenberg-Kitaev” spin-orbital model:

$$H = H_K + J^z \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \otimes \mathbb{1}_i \mathbb{1}_j$$



“Kitaev” spin-orbital liquid



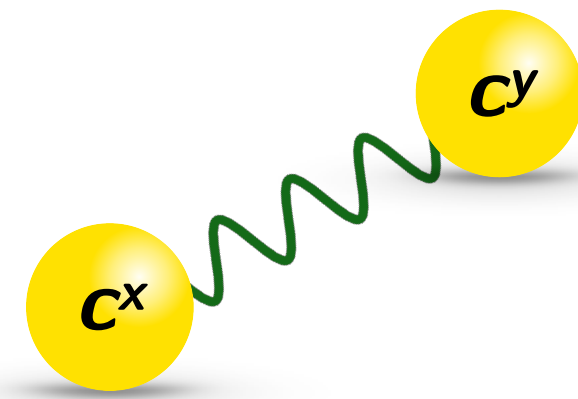
Ising spin order



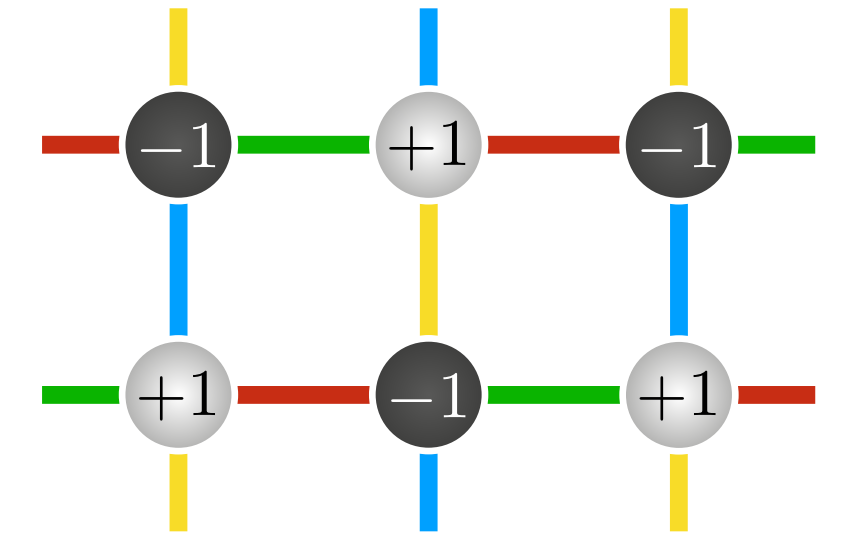
Static perturbations

“Heisenberg-Kitaev” spin-orbital model:

$$H = H_K + J^z \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \otimes \mathbb{1}_i \mathbb{1}_j$$



“Kitaev” spin-orbital liquid



Ising spin order



Parton representation:

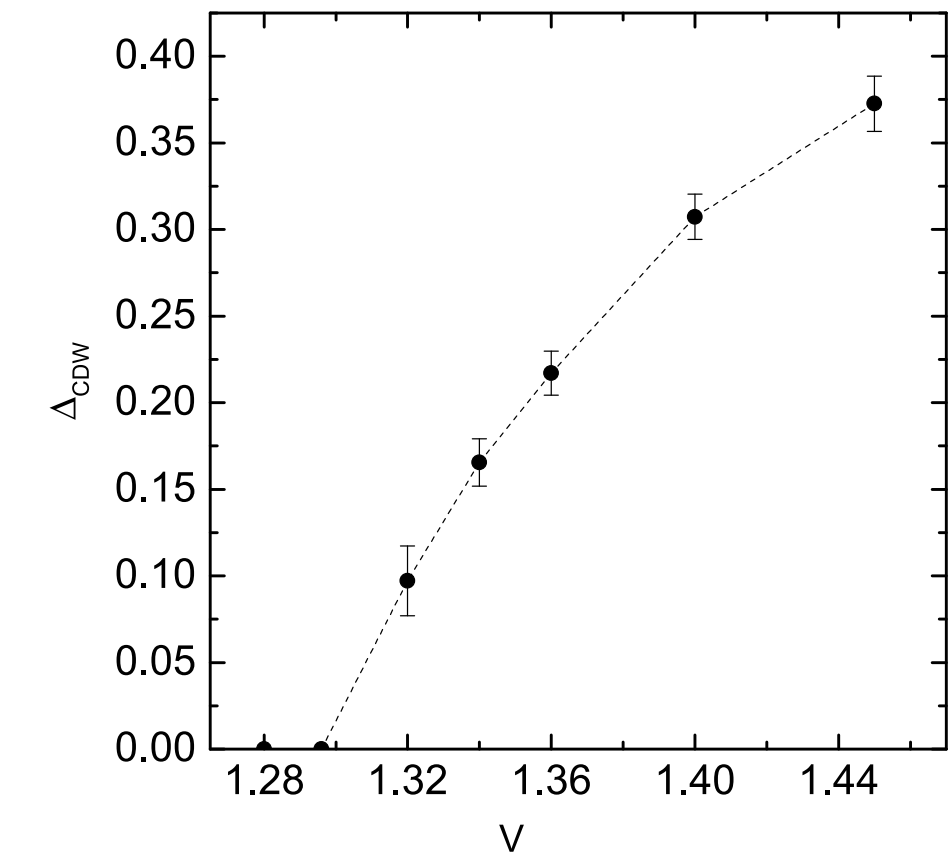
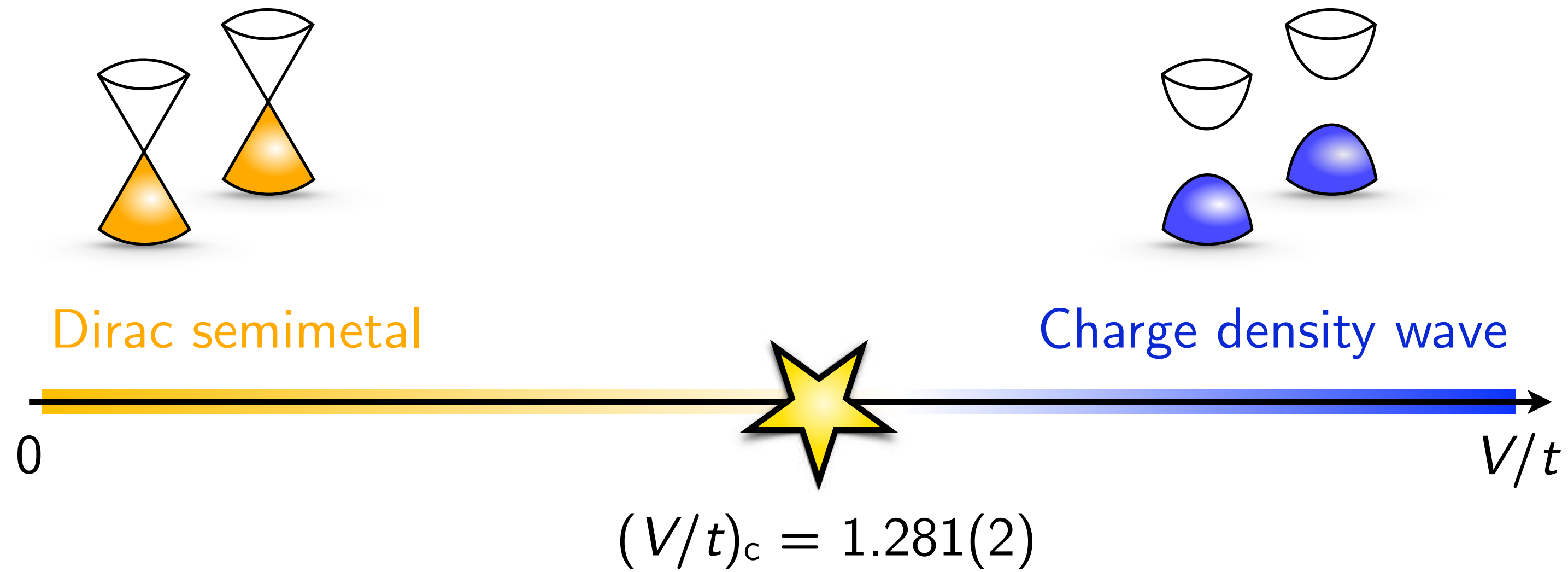
$$H \mapsto \sum_{\langle ij \rangle} \left[2K u_{ij} (f_i^\dagger f_j + f_j^\dagger f_i) + 4J^z (n_i - \frac{1}{2})(n_j - \frac{1}{2}) \right]$$

hopping parameter $t = 2K$
 π flux
nearest-neighbor repulsion $V = 4J^z$
 $f = \frac{1}{2}(c^x + ic^y)$
electron density $f^\dagger f$

Ground-state flux pattern:
[Lieb, PRL '94]

Spin-orbital model \mapsto interacting fermions on π -flux lattice

Spinless fermions on π -flux lattice: QMC



[Wang, Corboz, Troyer, NJP '14]

[Li, Jiang, Yao, NJP '15]

[Huffman & Chandrasekharan, PRD '17; PRD '20]

Gross-Neveu- \mathbb{Z}_2 universality:

$$1/\nu = 1.12(1), \quad \eta_\phi = 0.51(3), \quad \eta_\psi \approx 0.1$$

[Gracey, IJMP '94]

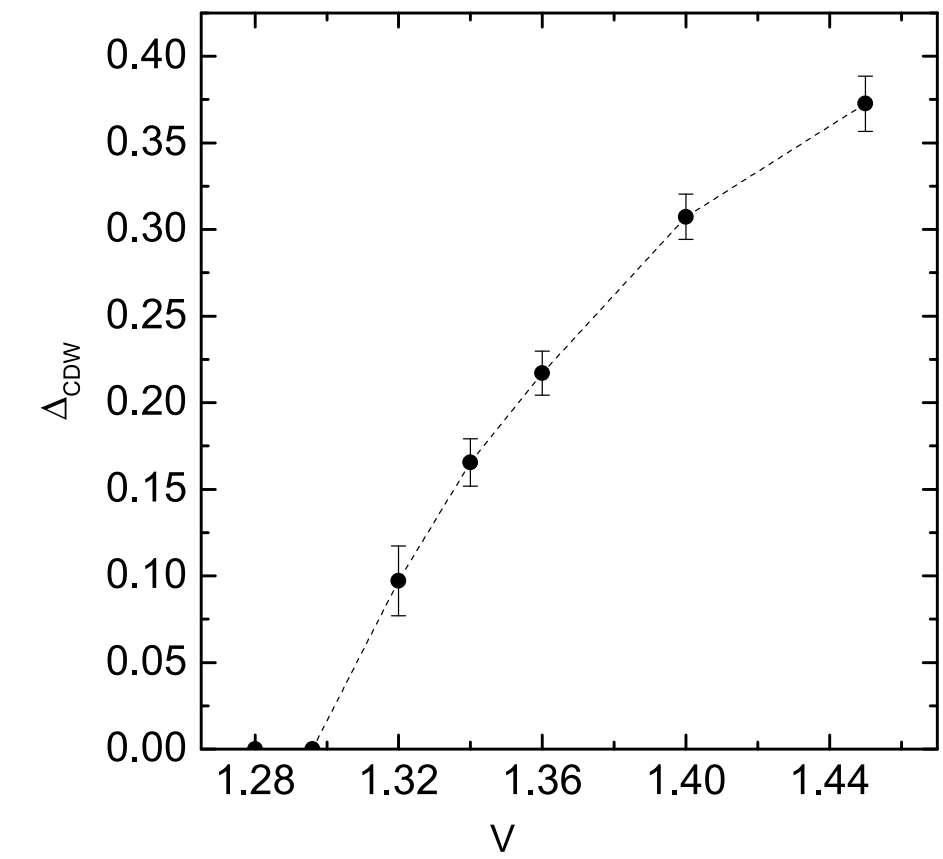
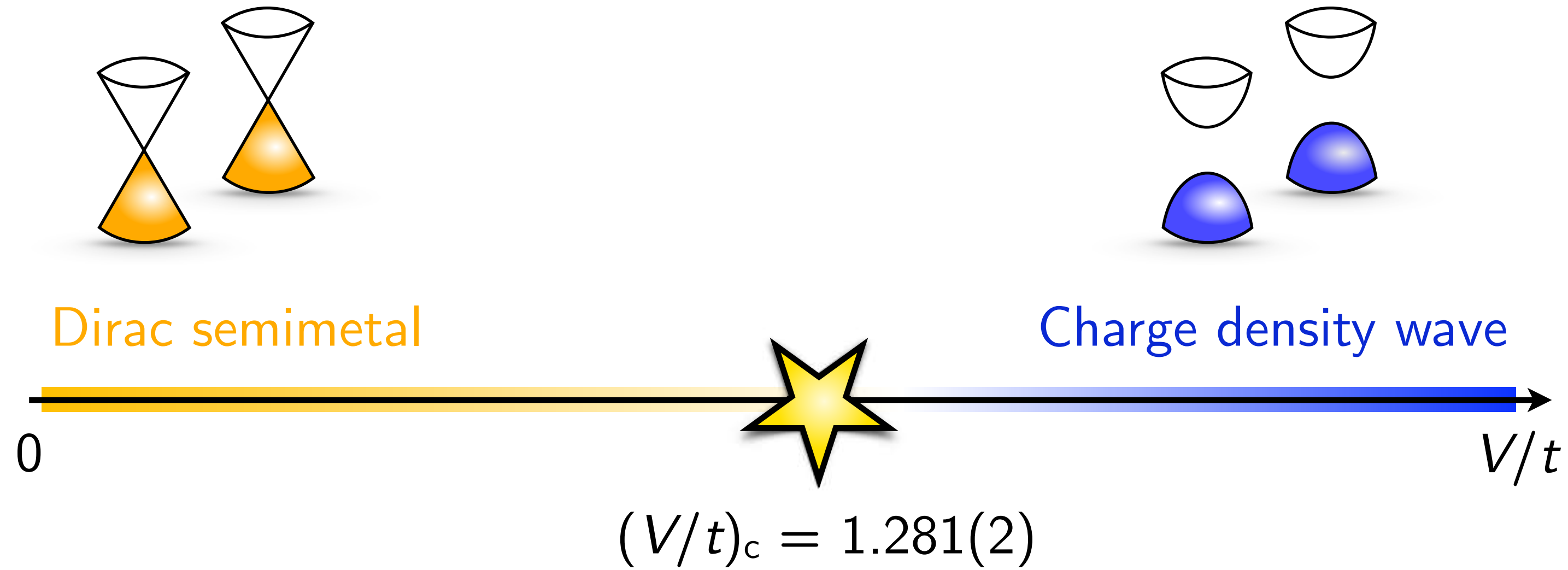
[LJ & Herbut, PRB '14]

[Iliesiu *et al.*, JHEP '18]

[Ihrig, Mihaila, Scherer, PRB '18]

...

Spinless fermions on π -flux lattice: QMC



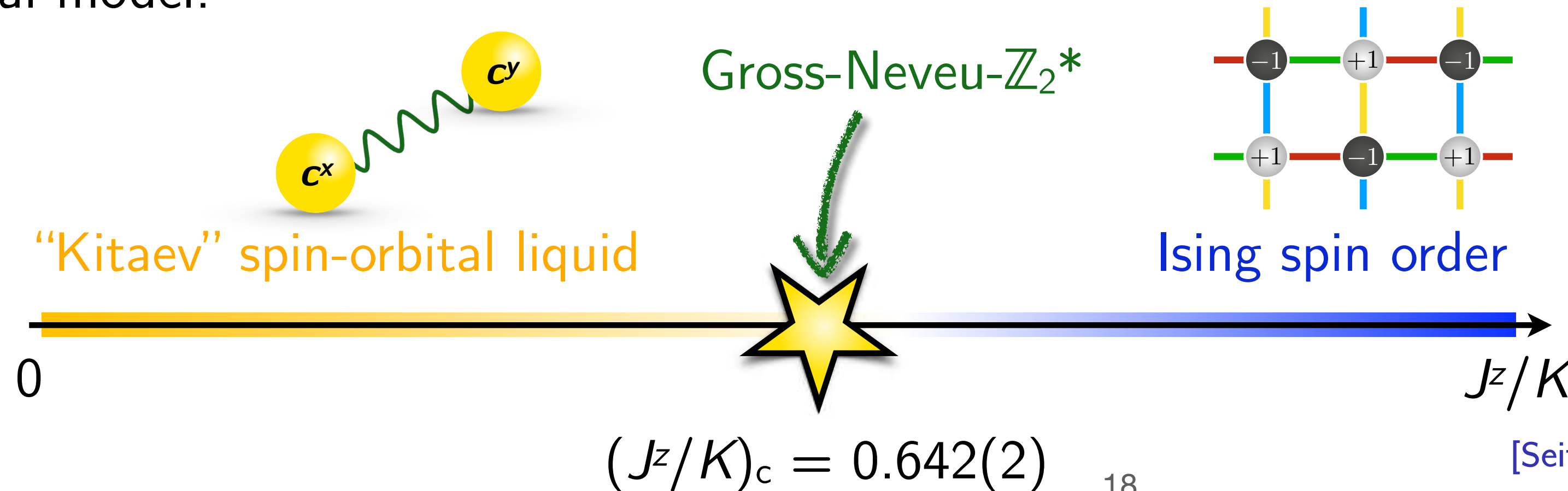
[Wang, Corboz, Troyer, NJP '14]
 [Li, Jiang, Yao, NJP '15]
 [Huffman & Chandrasekharan, PRD '17; PRD '20]

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 [LJ & Herbut, PRB '14]
 [Iliesiu *et al.*, JHEP '18]
 [Ihrig, Mihaila, Scherer, PRB '18]

Spin-orbital model:

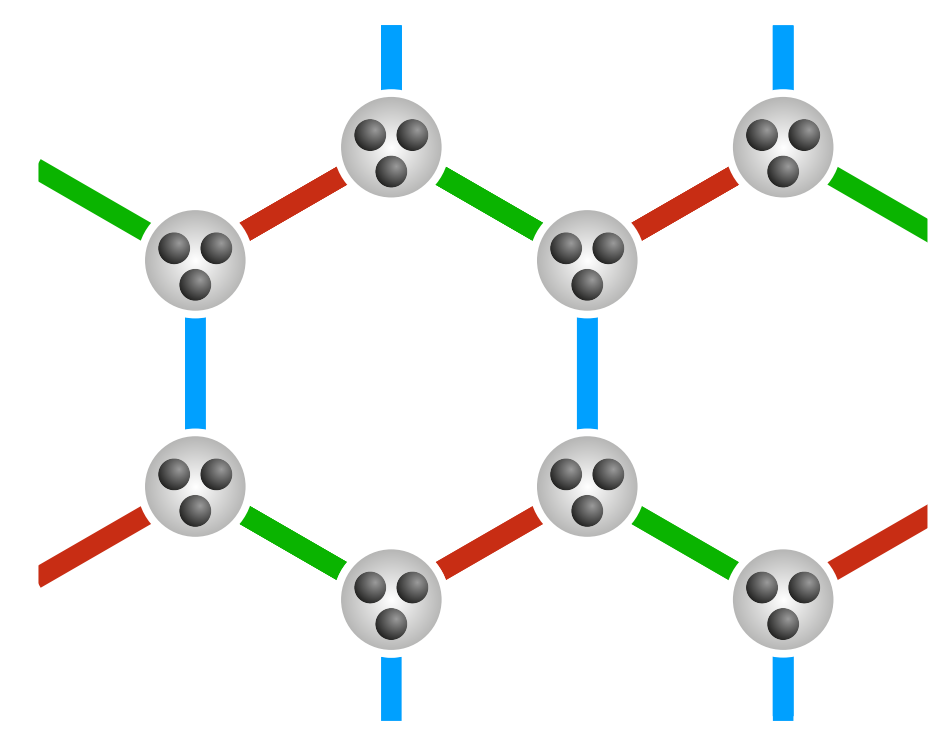


[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, arXiv:2009.05051]

Fractionalized fermionic universality classes

Example #2 (honeycomb lattice):

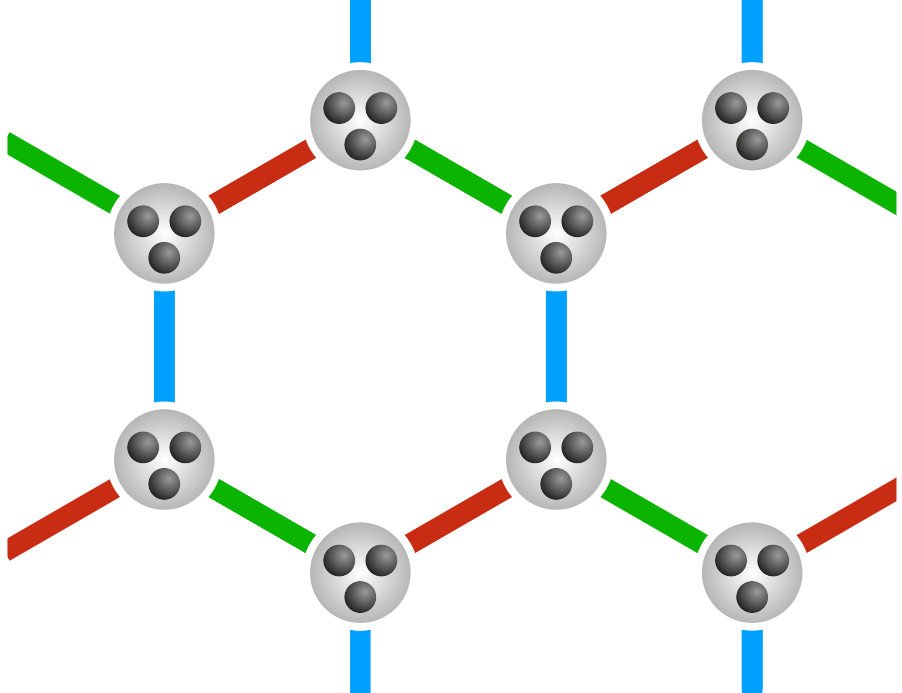
$$H = -K \sum_{\langle ij \rangle_\gamma} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma + J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j$$



Fractionalized fermionic universality classes

Example #2 (honeycomb lattice):

$$H = -K \sum_{\langle ij \rangle_\gamma} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma + J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j$$



3 itinerant fermions

Majorana representation:

$$H \mapsto \sum_{\langle ij \rangle} \left[K u_{ij} c_i^\top c_j + \frac{J}{4} (c_i^\top \vec{L} c_i) \cdot (c_j^\top \vec{L} c_j) \right]$$

$c \equiv \begin{pmatrix} c^x \\ c^y \\ c^z \end{pmatrix}$ spin-1 matrices

0 flux

Ordered state:

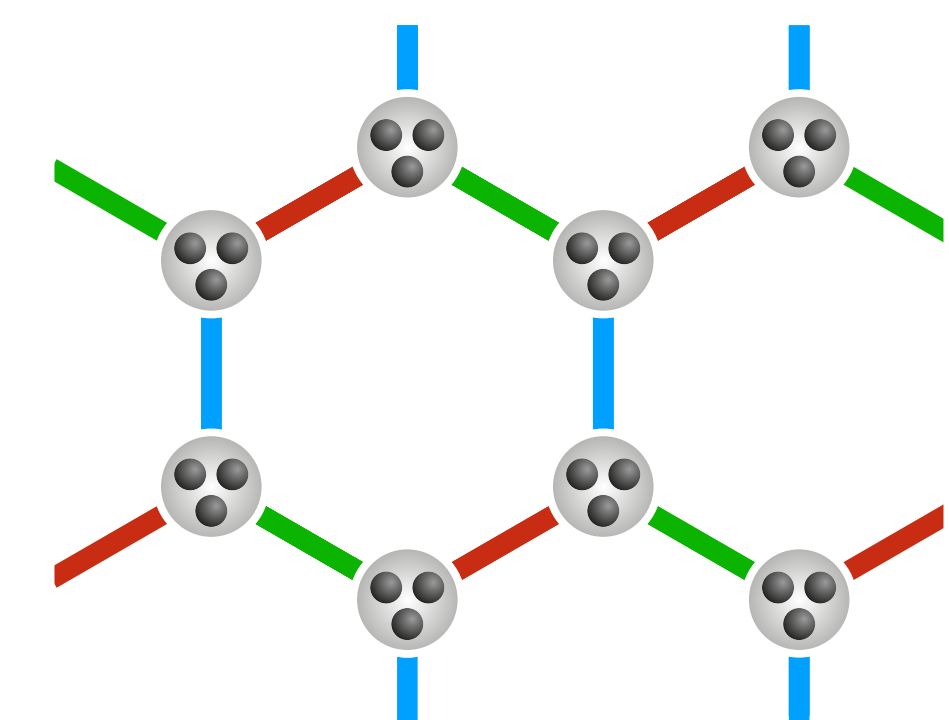
$$\langle c_{iA}^\top \vec{L} c_{iA} \rangle \neq \langle c_{jB}^\top \vec{L} c_{jB} \rangle \quad \text{spin density wave}$$



Fractionalized fermionic universality classes

Example #2 (honeycomb lattice):

$$H = -K \sum_{\langle ij \rangle_\gamma} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma + J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j$$



3 itinerant fermions

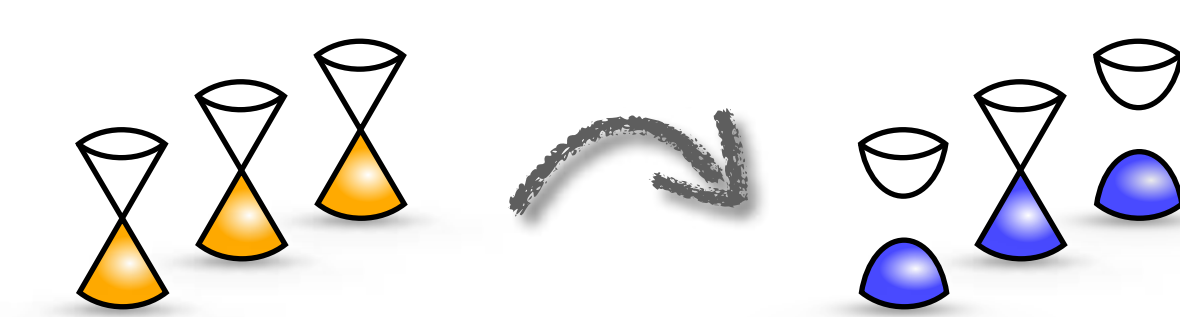
Majorana representation:

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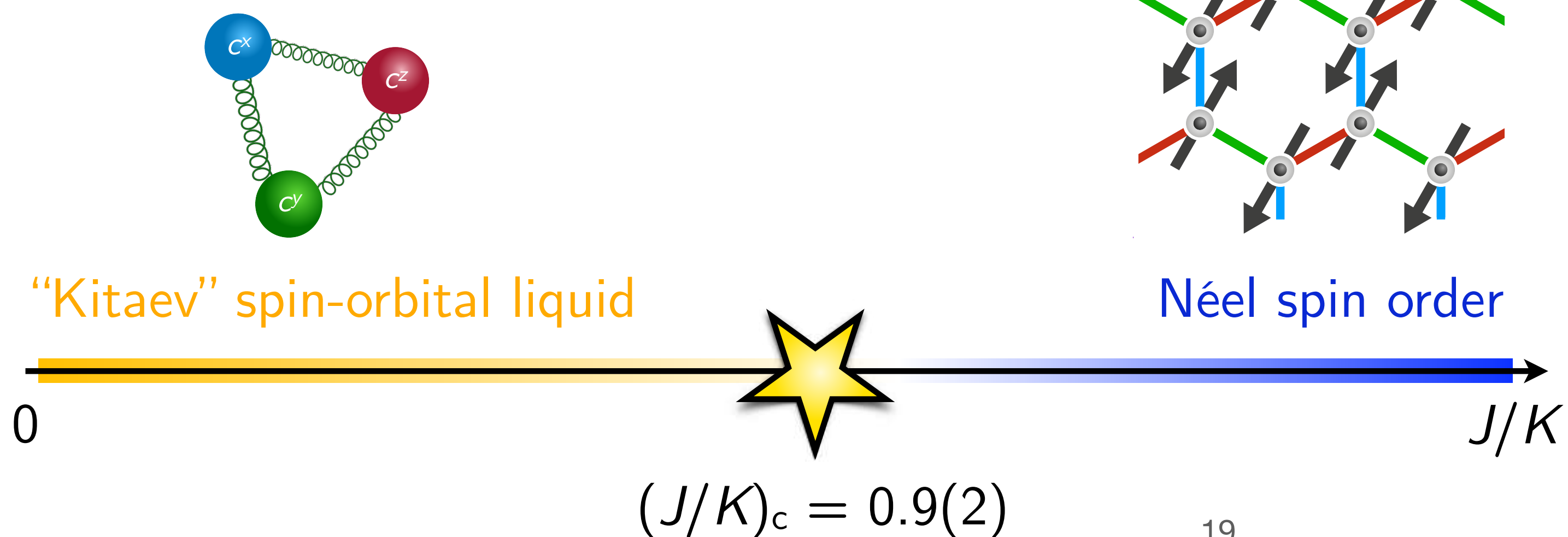
$c \equiv \begin{pmatrix} c^x \\ c^y \\ c^z \end{pmatrix}$ (spin-1 matrices)
 0 flux

Ordered state:

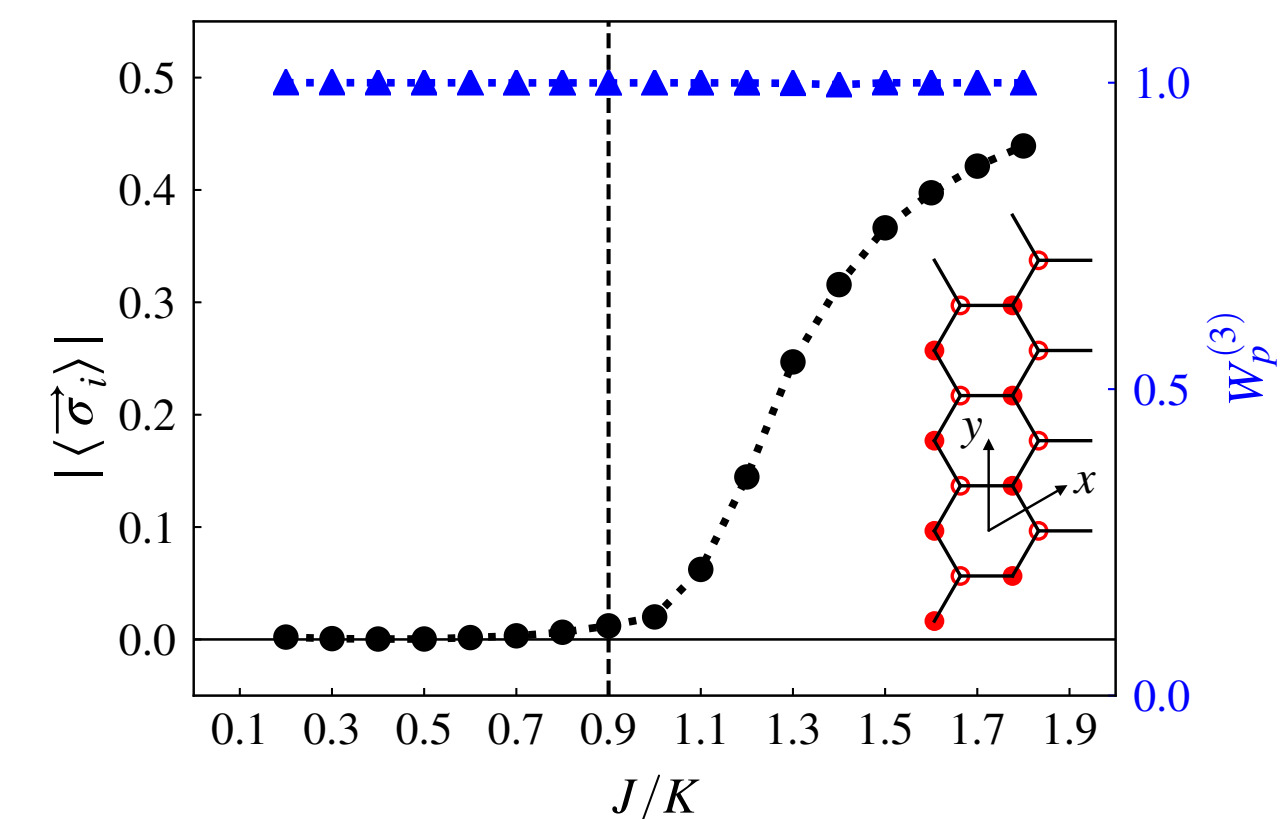
$$\langle c_{iA}^\top \vec{L} c_{iA} \rangle \neq \langle c_{jB}^\top \vec{L} c_{jB} \rangle \quad \text{spin density wave}$$



Phase diagram:



DMRG:



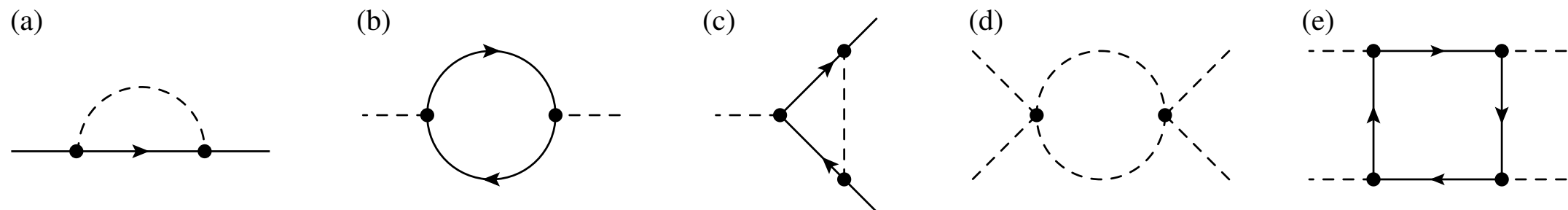
[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, arXiv:2009.05051]

Effective field theory: Gross-Neveu-SO(3)

Action:

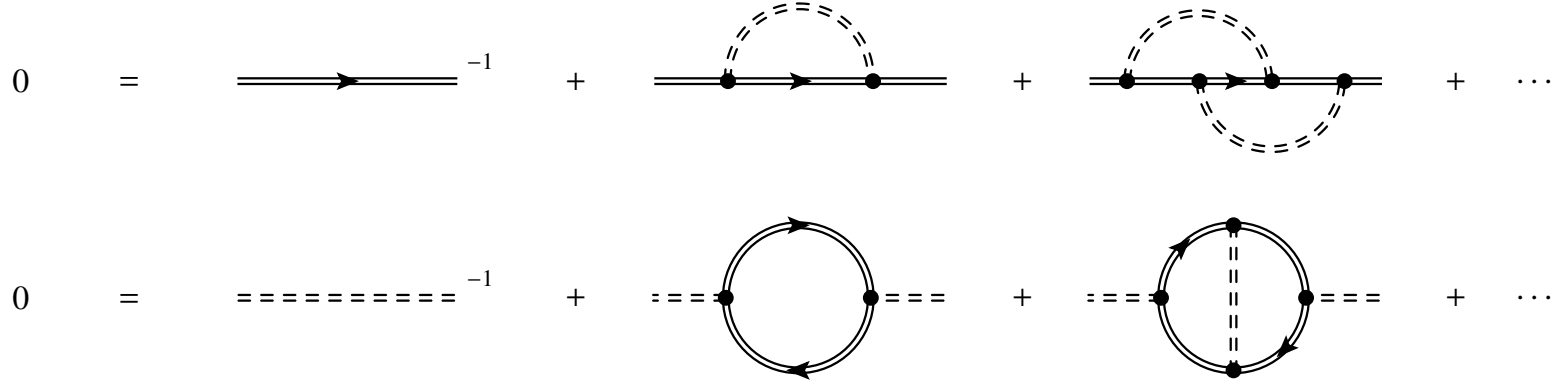
$$\mathcal{S} = \int d^2\vec{x}d\tau \left[\bar{\psi}\gamma^\mu\partial_\mu\psi + g\vec{\varphi} \cdot \bar{\psi}(\mathbb{1}_2 \otimes \vec{L})\psi + \frac{1}{2}\vec{\varphi} \cdot (-\partial_\mu^2 + m^2)\vec{\varphi} + \lambda(\vec{\varphi} \cdot \vec{\varphi})^2 \right]$$

4 - ϵ expansion:



$$1/\nu \approx 1.1, \quad \eta_\phi \approx 0.33, \quad \eta_\psi \approx 0.17$$

1/N expansion:



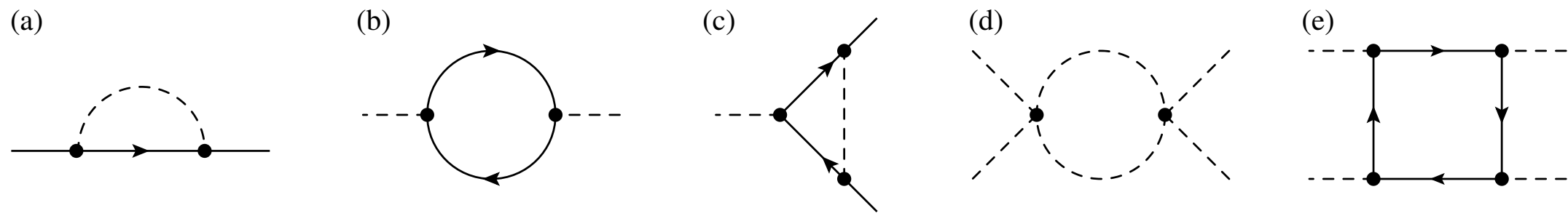
$$1/\nu \approx 0.5, \quad \eta_\phi \approx 0.32, \quad \eta_\psi \approx 0.14$$

Effective field theory: Gross-Neveu-SO(3)

Action:

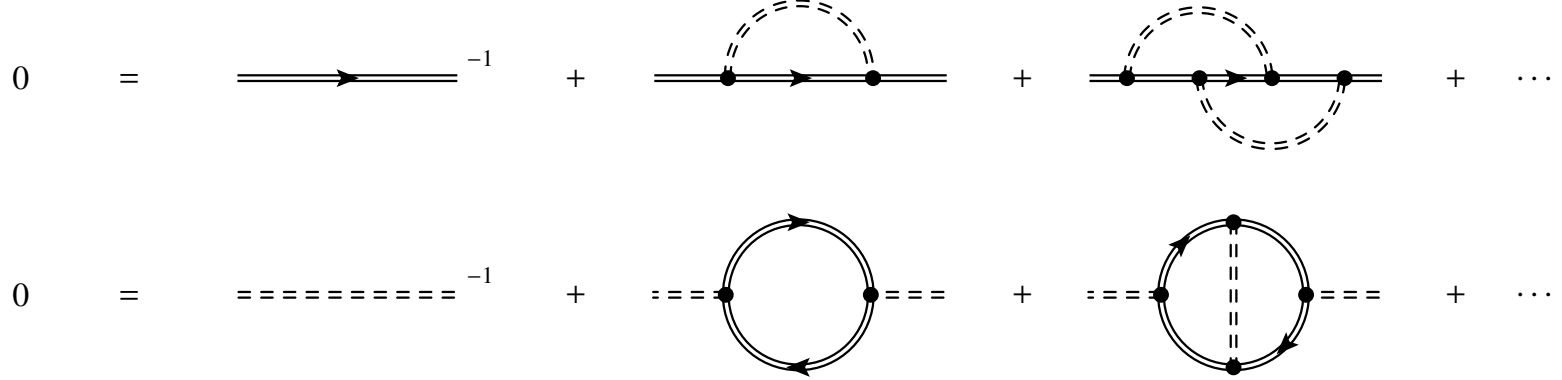
$$\mathcal{S} = \int d^2\vec{x}d\tau \left[\bar{\psi}\gamma^\mu\partial_\mu\psi + g\vec{\varphi} \cdot \bar{\psi}(\mathbb{1}_2 \otimes \vec{L})\psi + \frac{1}{2}\vec{\varphi} \cdot (-\partial_\mu^2 + m^2)\vec{\varphi} + \lambda(\vec{\varphi} \cdot \vec{\varphi})^2 \right]$$

4 - ϵ expansion:

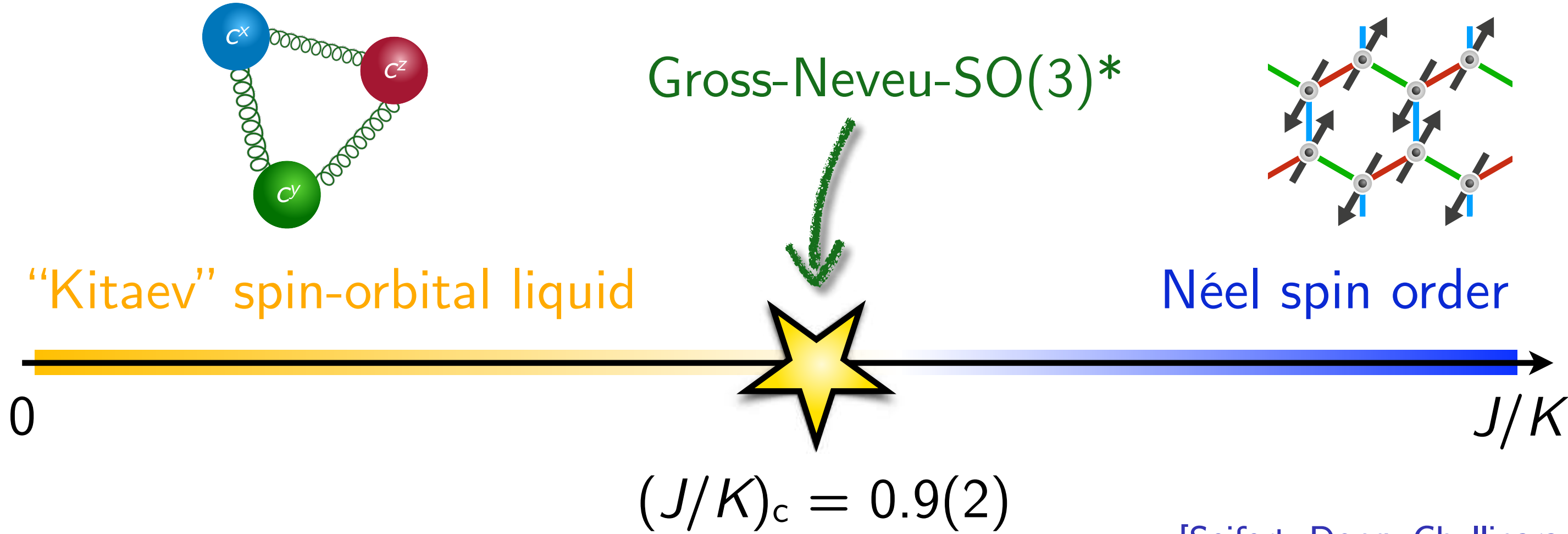


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[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, arXiv:2009.05051]

Finite-size spectroscopy: Ising vs Ising*

Transverse-field Ising:

$$H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

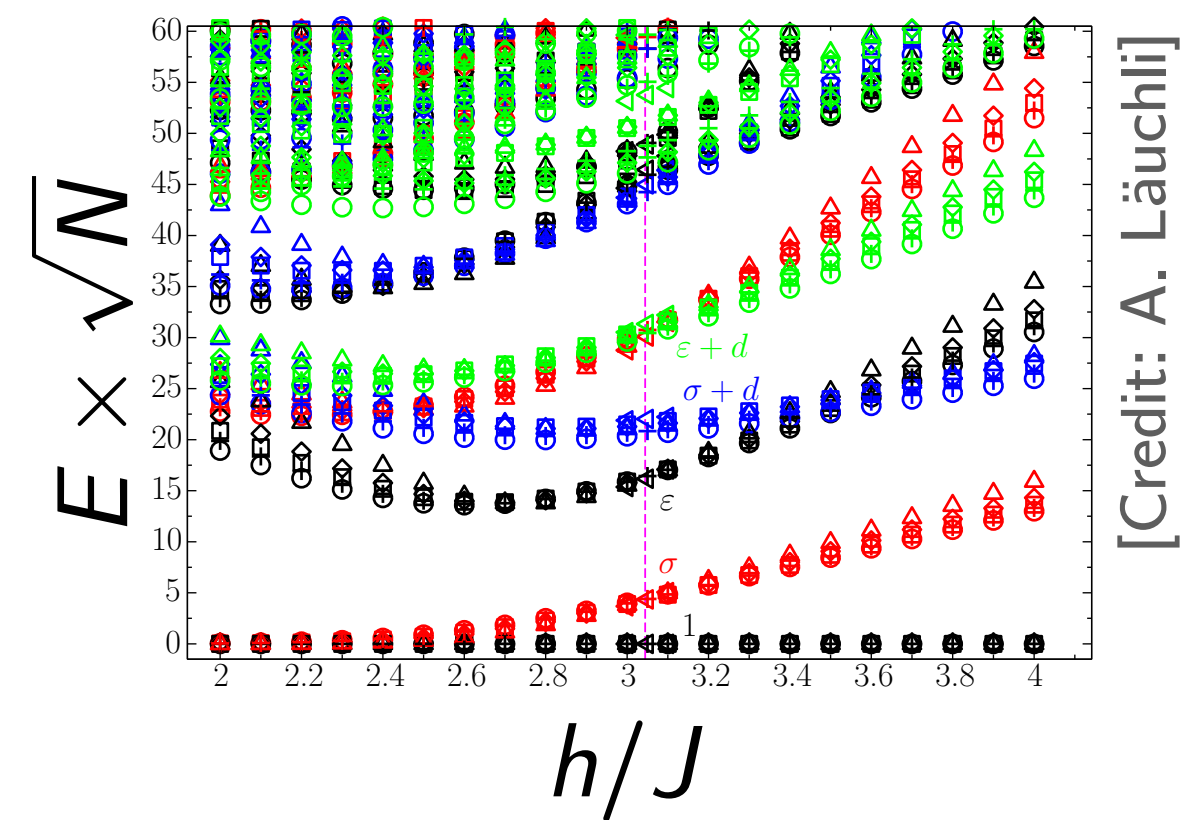
Transverse-field toric code:

$$H = -J \sum_s \prod_{i \in s} \sigma_i^x - J \sum_p \prod_{i \in p} \sigma_i^z - h \sum_i \sigma_i^x$$

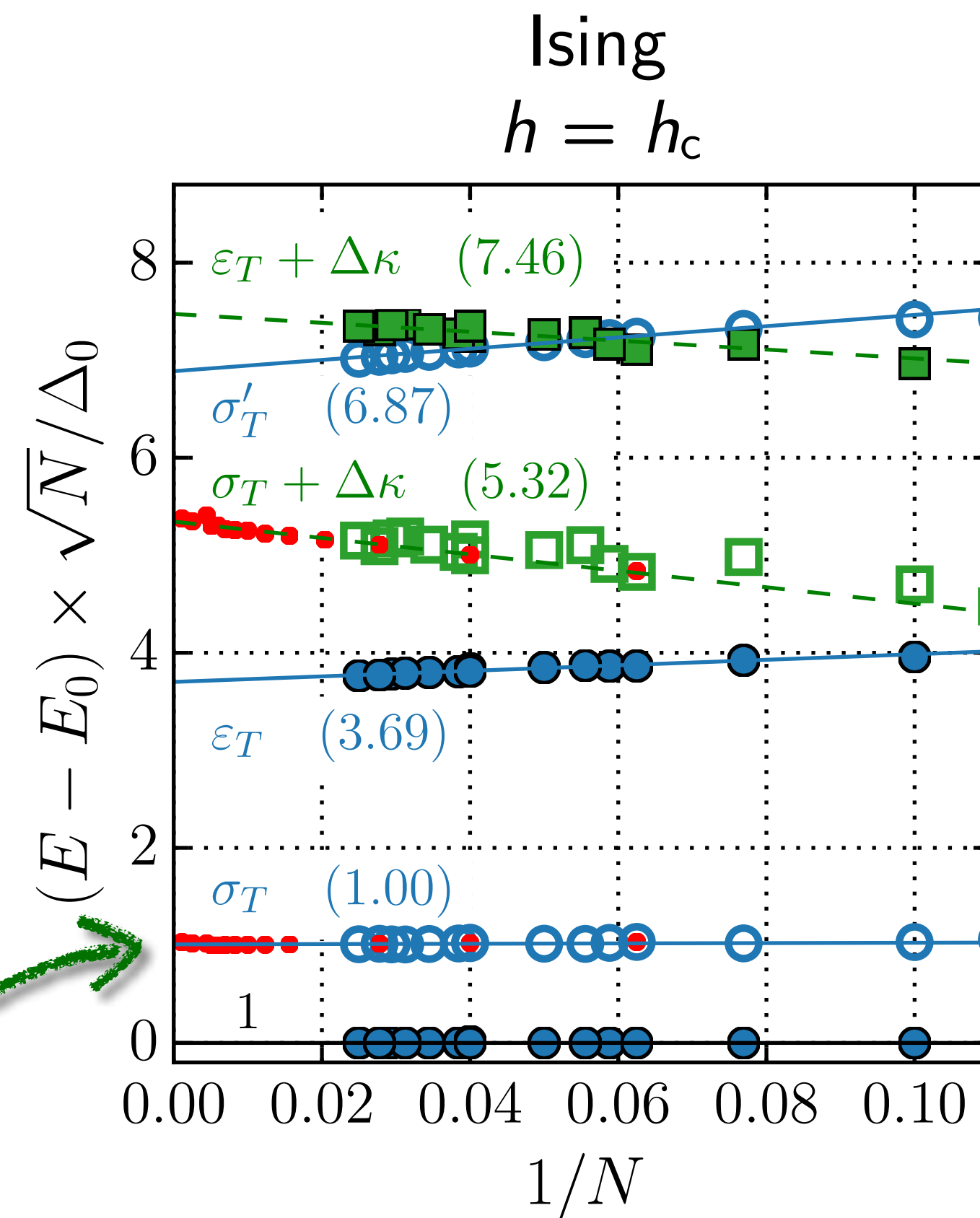
Finite-size spectroscopy: Ising vs Ising*

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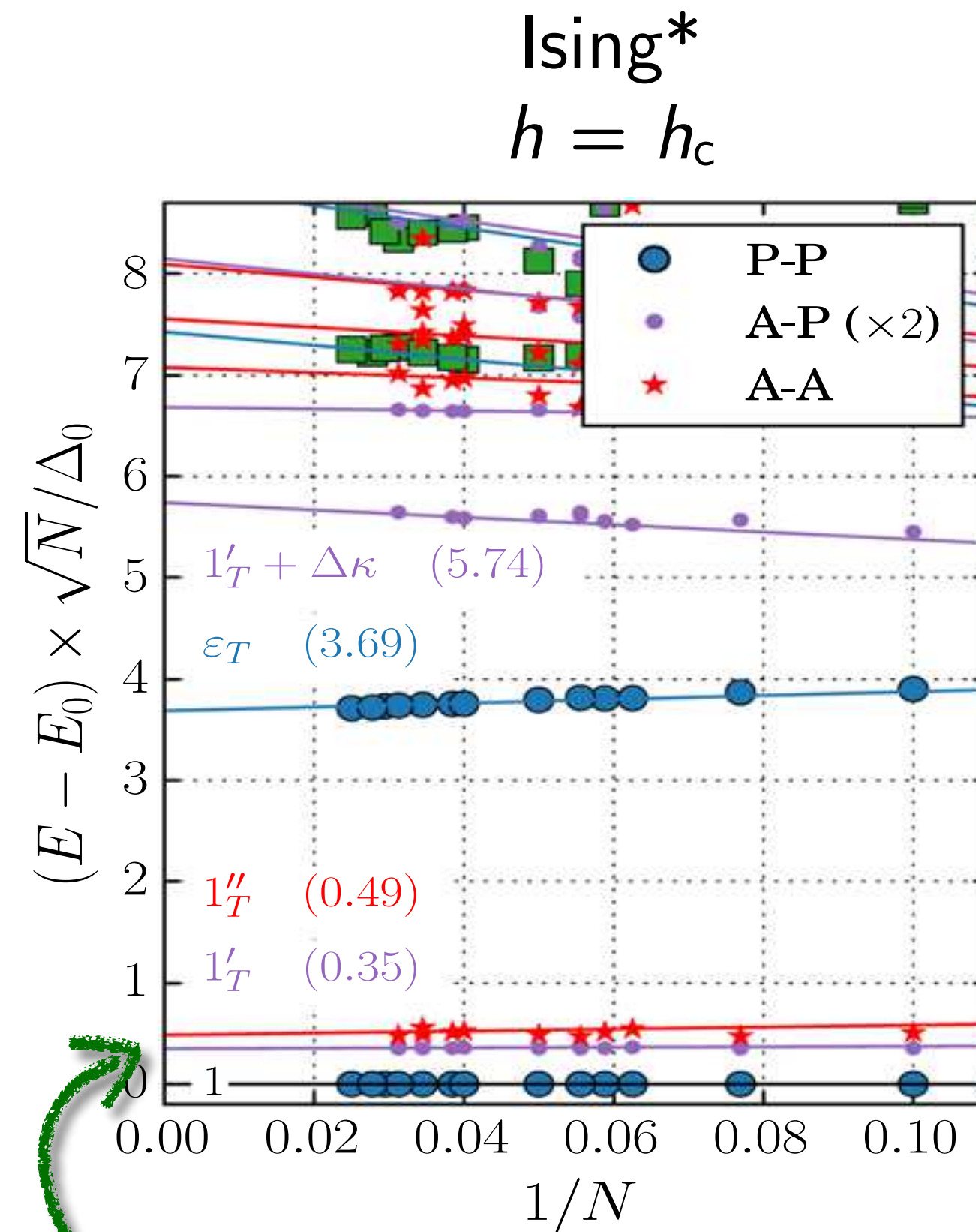
[Credit: A. Läuchli]



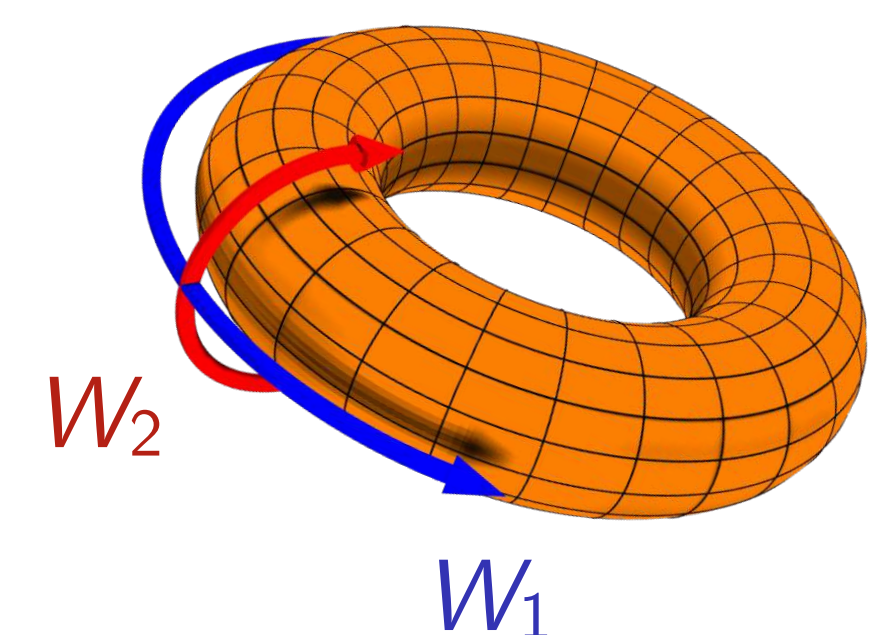
missing in Ising*

Transverse-field toric code:

$$H = -J \sum_s \prod_{i \in s} \sigma_i^x - J \sum_p \prod_{i \in p} \sigma_i^z - h \sum_i \sigma_i^x$$



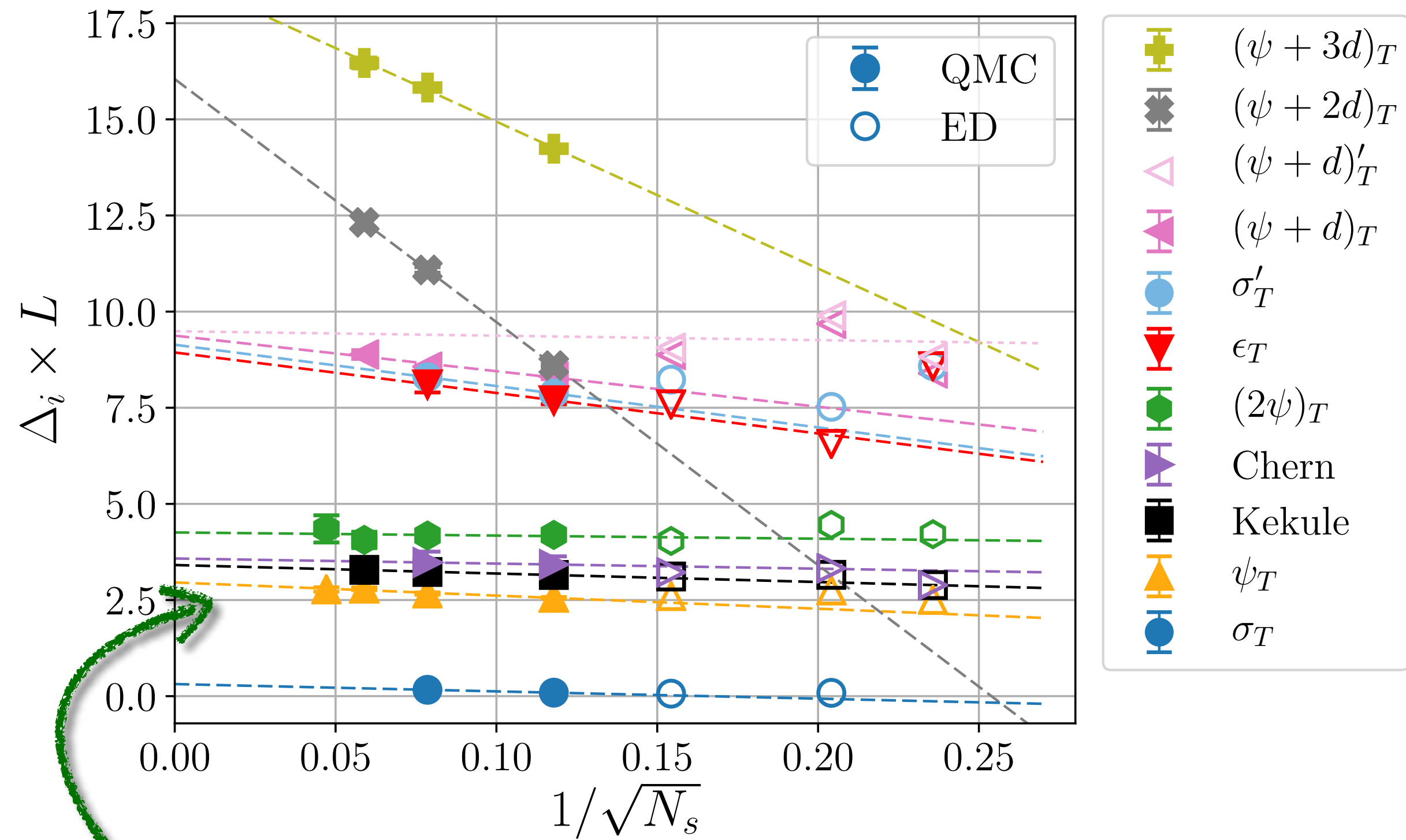
topological "copies"



[Schuler, Whitsitt, Henry, Sachdev, Läuchli, PRL '16]

Gross-Neveu vs Gross-Neveu*

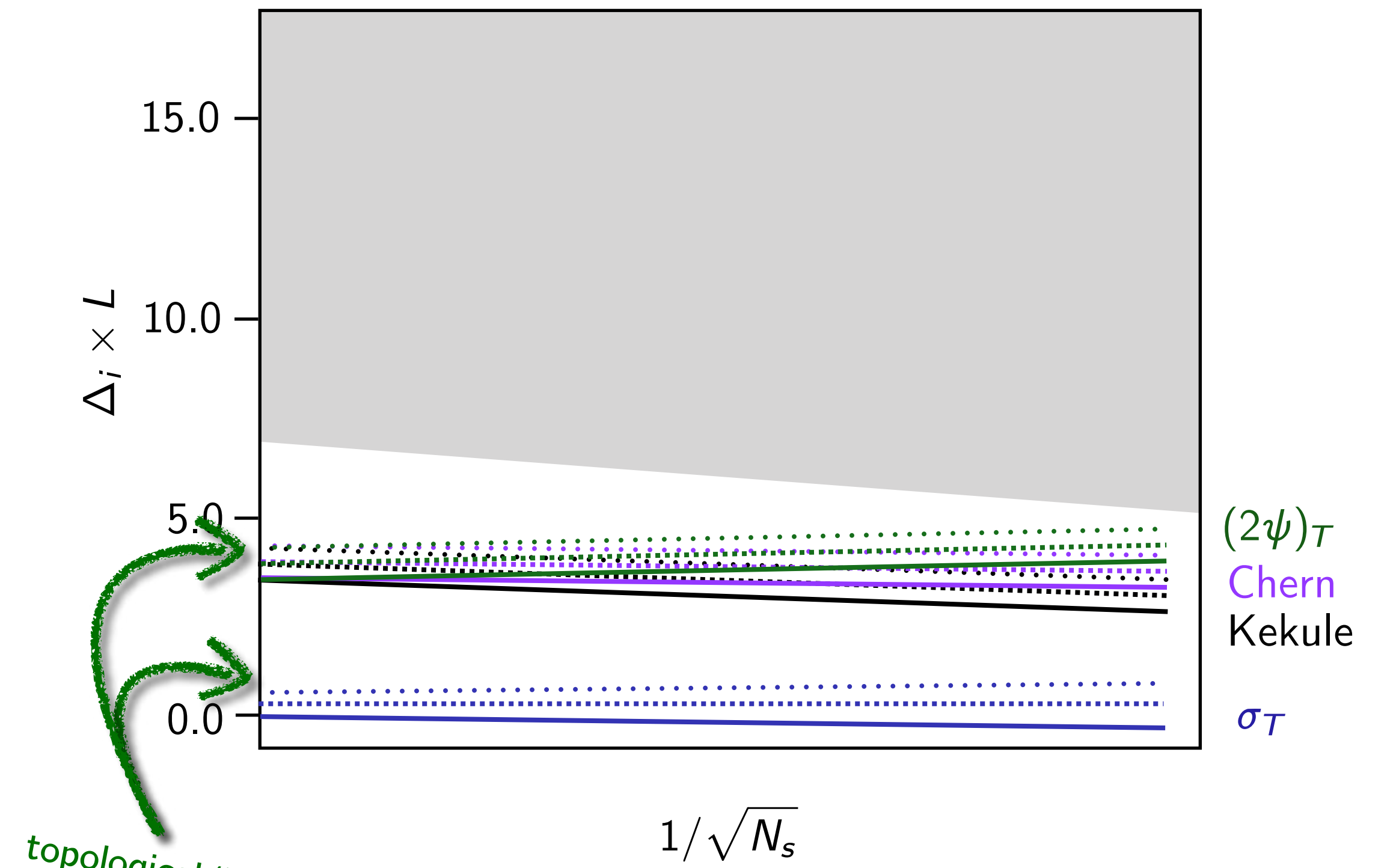
Gross-Neveu- \mathbb{Z}_2



missing in GN*

[Schuler et al., arXiv:1907.05373]

Gross-Neveu- \mathbb{Z}_2^* (schematic)



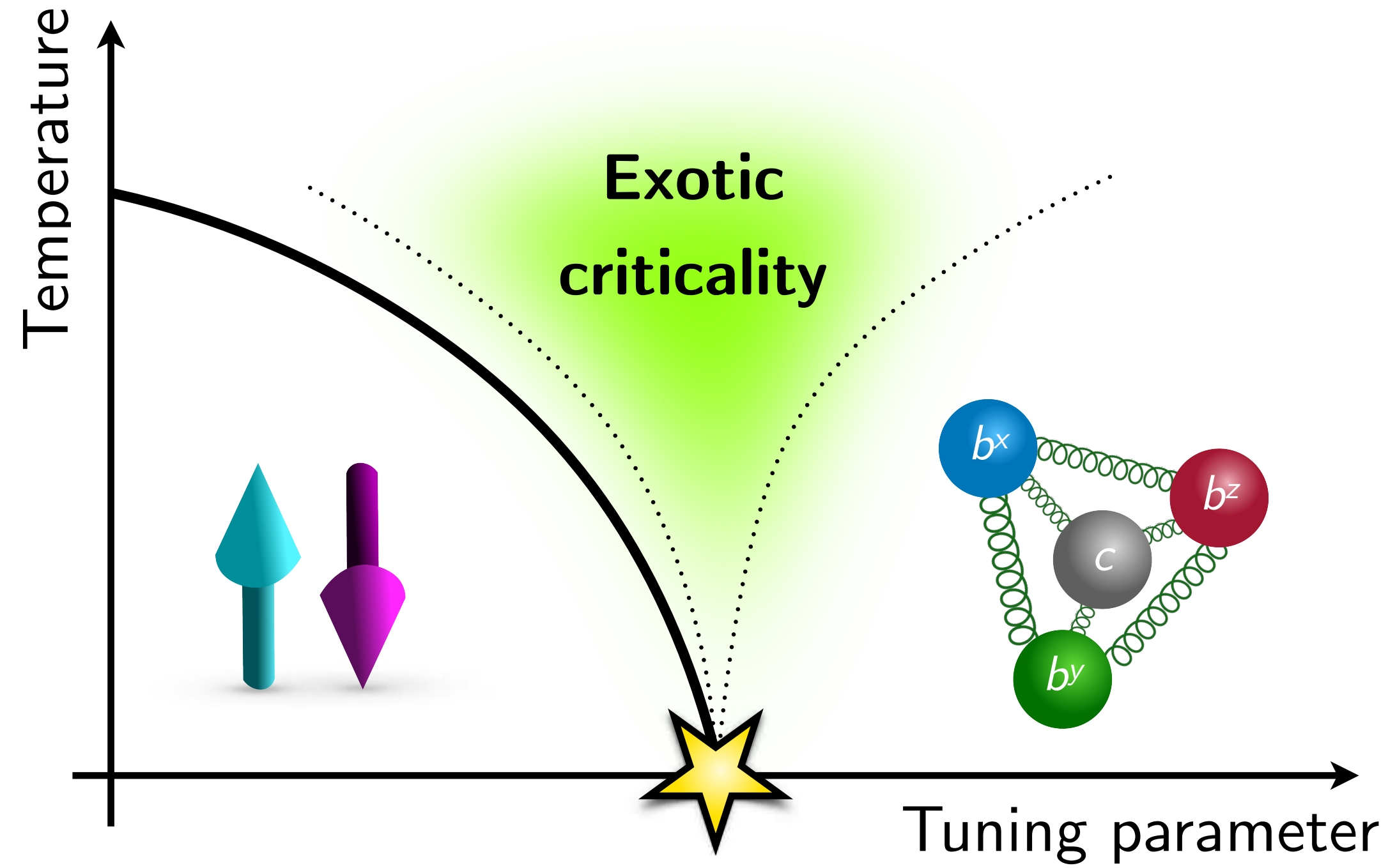
topological "copies"

... testable in future simulations

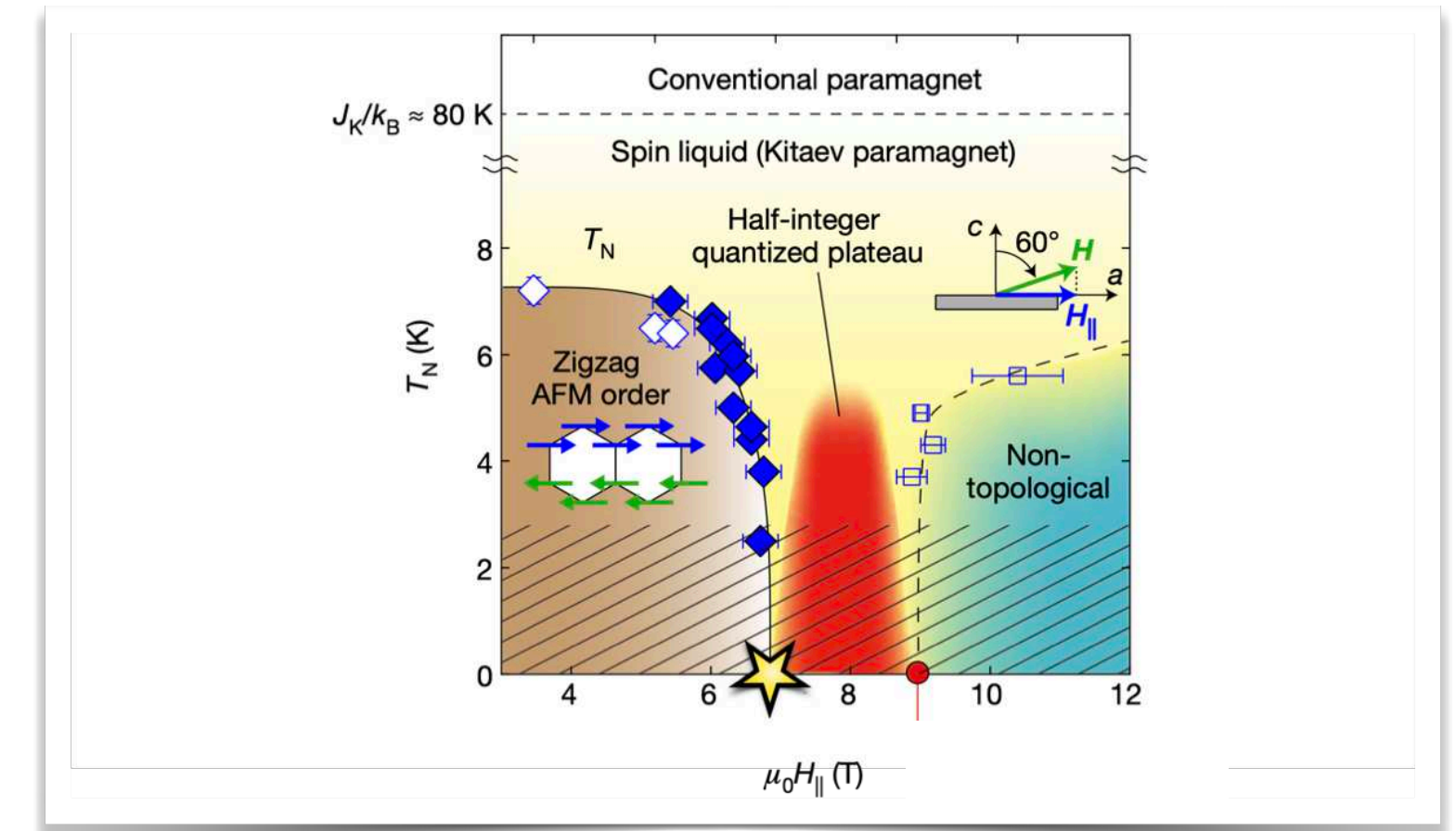
Outline

- (1) Introduction: *“Beyond-Landau” quantum criticality*
- (2) Spin-1/2: *Field-induced criticality in Kitaev materials*
- (3) Spin-3/2: *Fractionalized fermionic criticality in spin-orbital models*
- (4) Conclusions

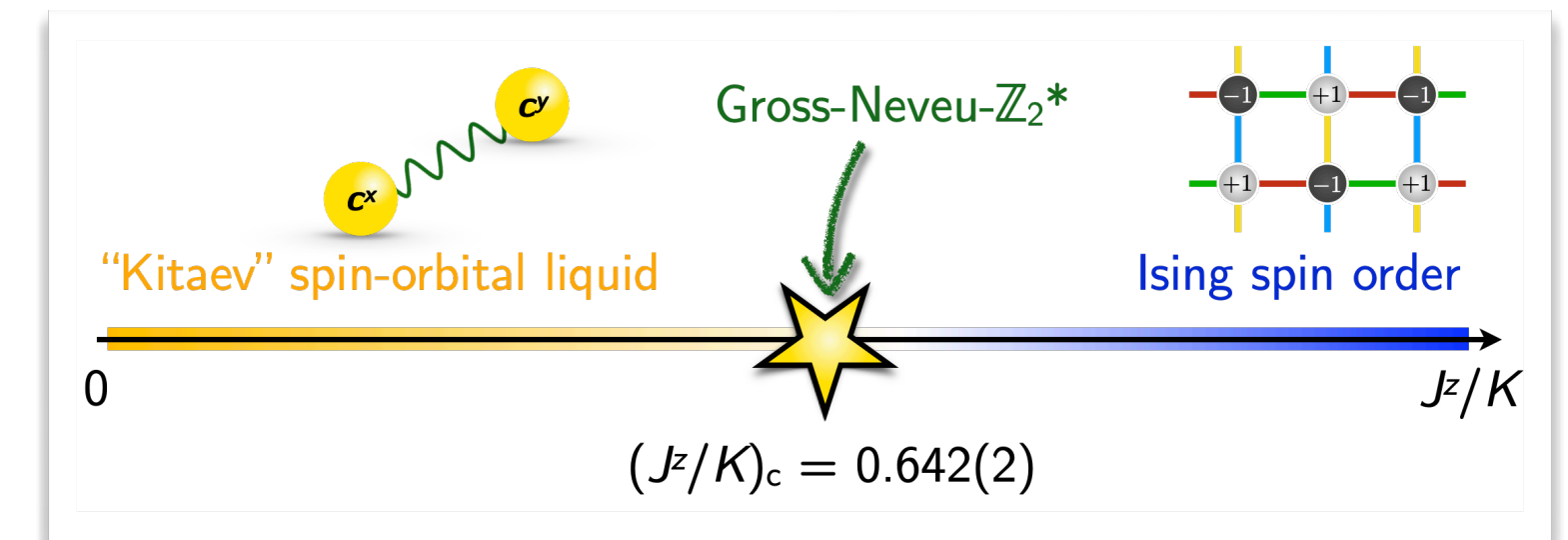
Conclusions



α -RuCl₃ in field



Square-lattice spin-orbital model



Honeycomb-lattice spin-orbital model

