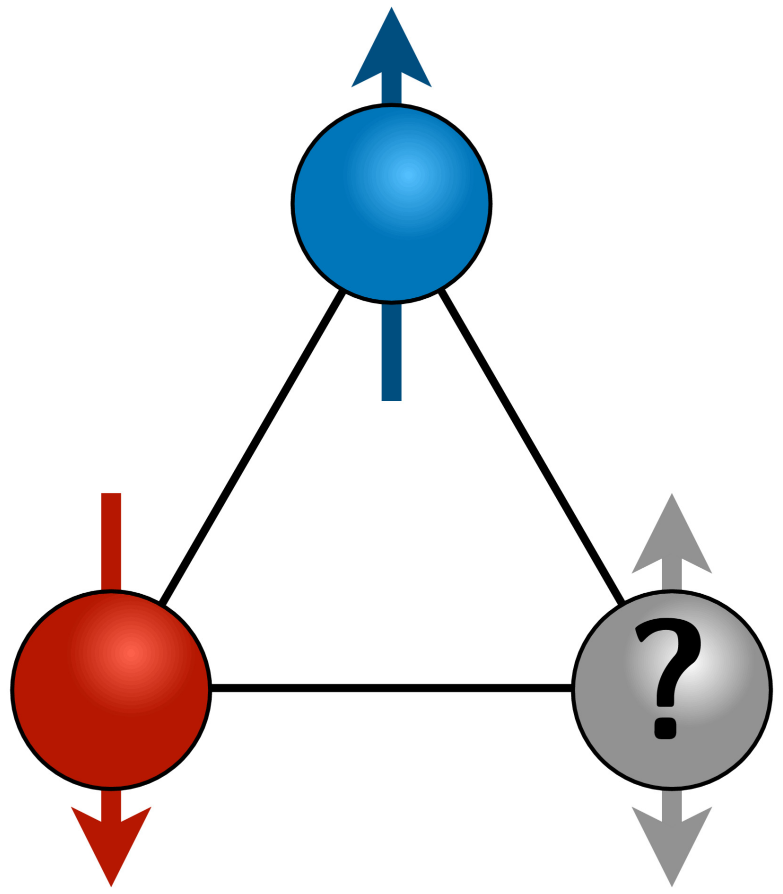
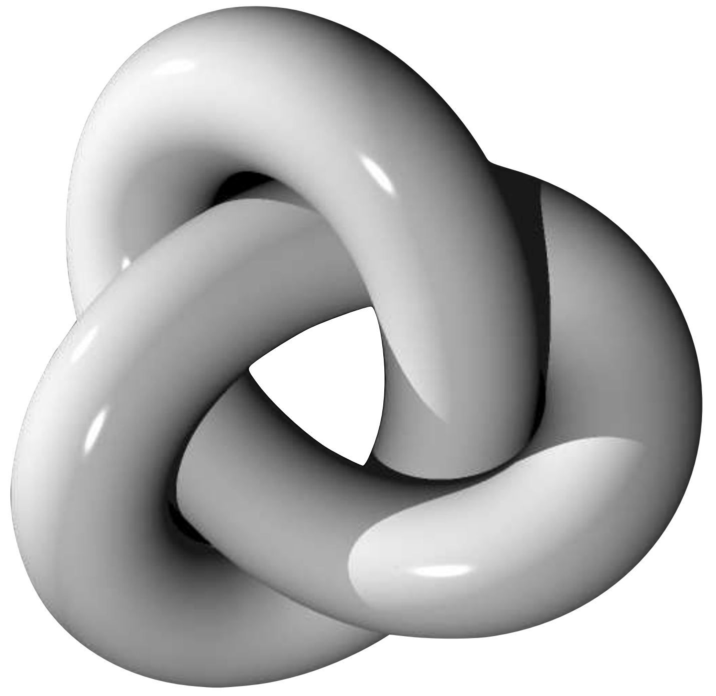
Topological phases of matter in frustrated quantum magnets

Lukas Janssen
TU Dresden



From frustration ...



... to topology

Urban Seifert (Santa Barbara)
Sreejith Chulliparambil (Dresden)

Xiao-Yu Dong (Ghent)
Matthias Vojta (Dresden)
Hong-Hao Tu (Dresden)

Shouryya Ray (Dresden)
John Gracey (Liverpool)

Bernhard Ihrig (Cologne)
Daniel Kruti (Cologne)
Michael Scherer (Cologne)

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

(1) Introduction: *Topological phases of matter*

(2) Spin-1/2: *Kitaev spin model*

(3) Spin-3/2: *Kitaev spin-orbital models*

(4) Conclusions

Slides available on https://tu-dresden.de/physik/qcm/vortraege

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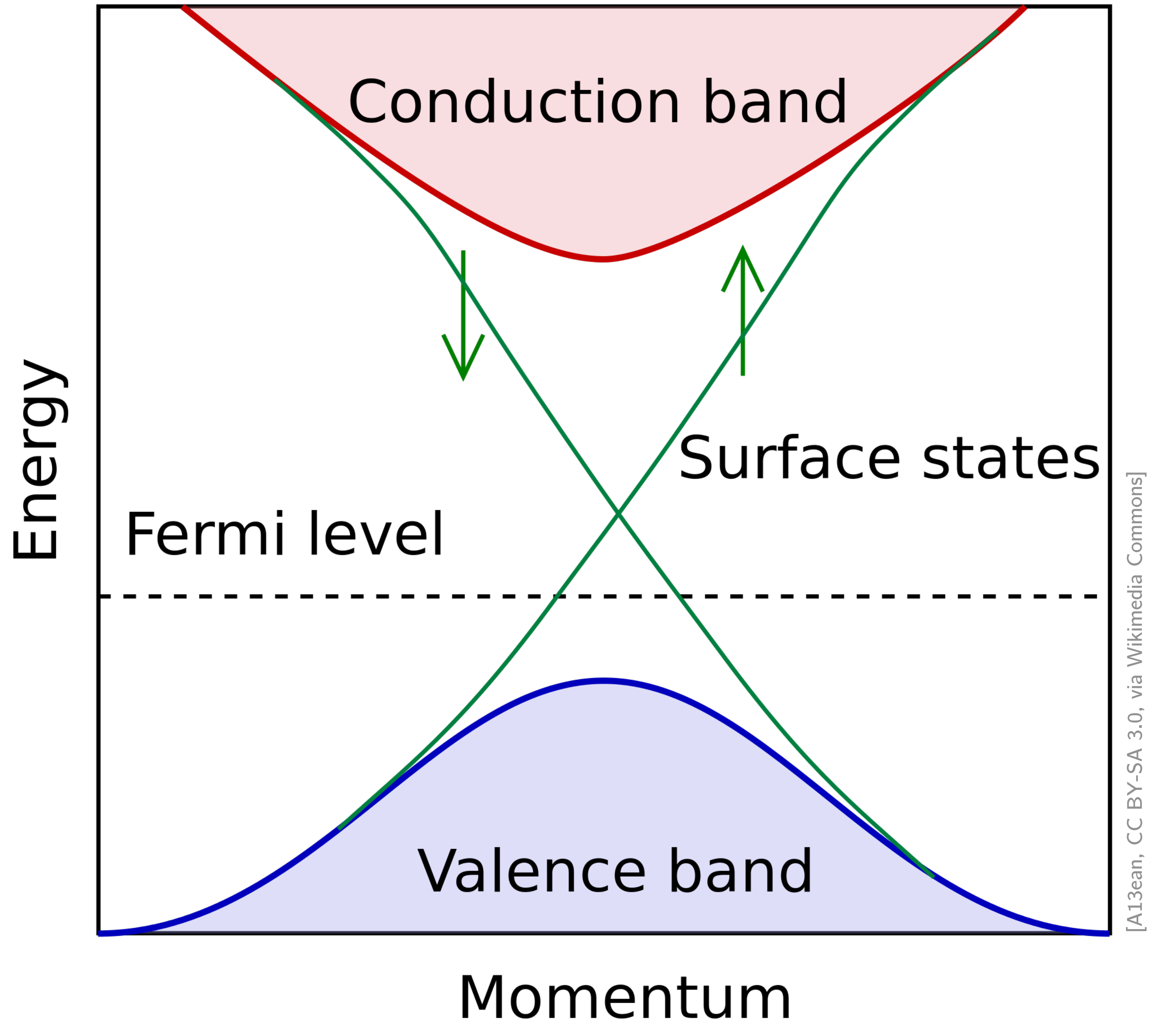
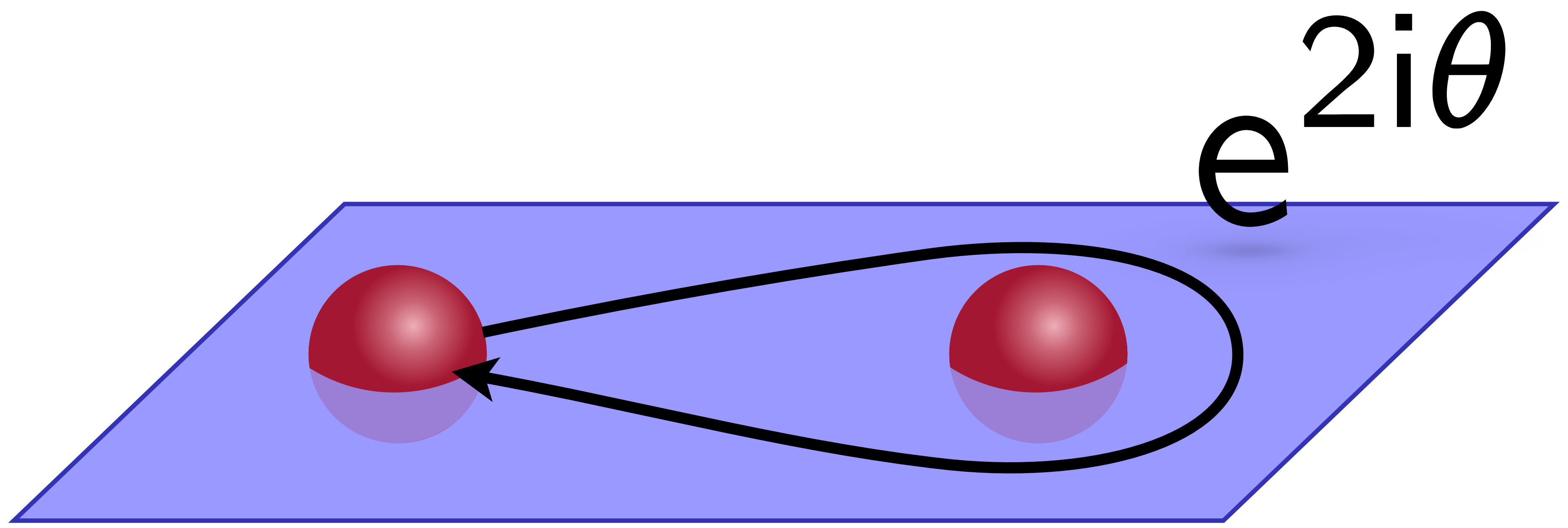
Topological phases of matter

"Phases with exotic edges"



Gapless surface states

"Phases with exotic excitations"



Exchange statistics with $\theta \notin \{0, \theta\}$

Anyons

Topological superconductors

Chiral $p + \mathrm{i}p$ superconductor:

$$\mathcal{H}_{\mathrm{BdG}} = \frac{1}{2}\sum_{\mathbf{p}} \Psi^\dagger_{\mathbf{p}}[\vec{d}(\mathbf{p},\mu)\cdot\vec{\sigma}]\Psi_{\mathbf{p}}\,, \qquad \vec{d}(\mathbf{p},\mu) = (-2|\Delta|p_y, -2|\Delta|p_x, \tfrac{p^2}{2m}-\mu)$$

[Bernevig & Neupert, arXiv:1506.0580]

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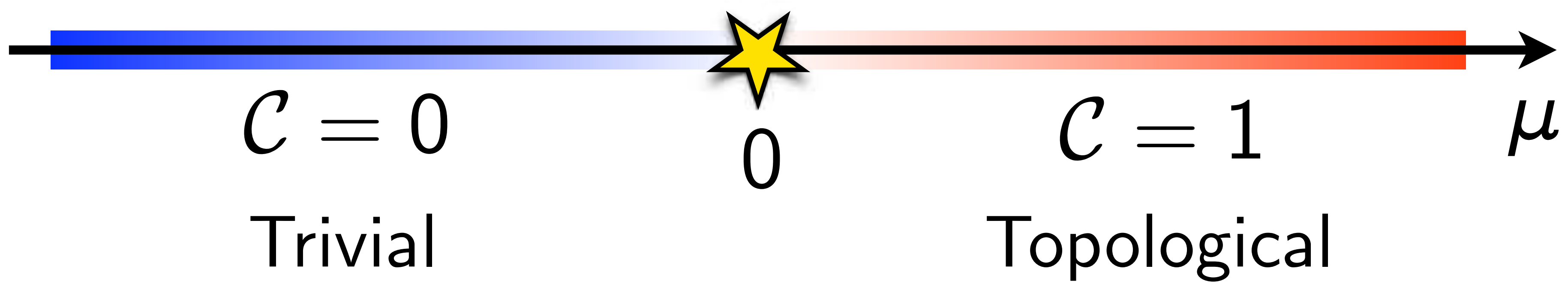
Chern number:

$$\mathcal{C} = \frac{1}{8\pi}\int \mathrm{d}^2\mathbf{p}\,\frac{\epsilon^{ij}}{|\vec{d}|^3}\vec{d}\cdot(\partial_{p_i}\vec{d}\times\partial_{p_j}\vec{d})$$

Phase diagram:



[Bernevig & Neupert, arXiv:1506.0580]

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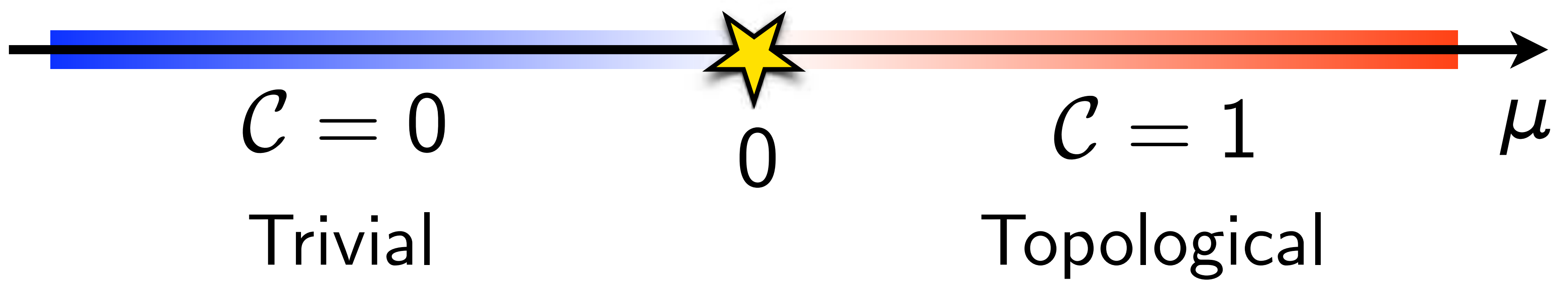
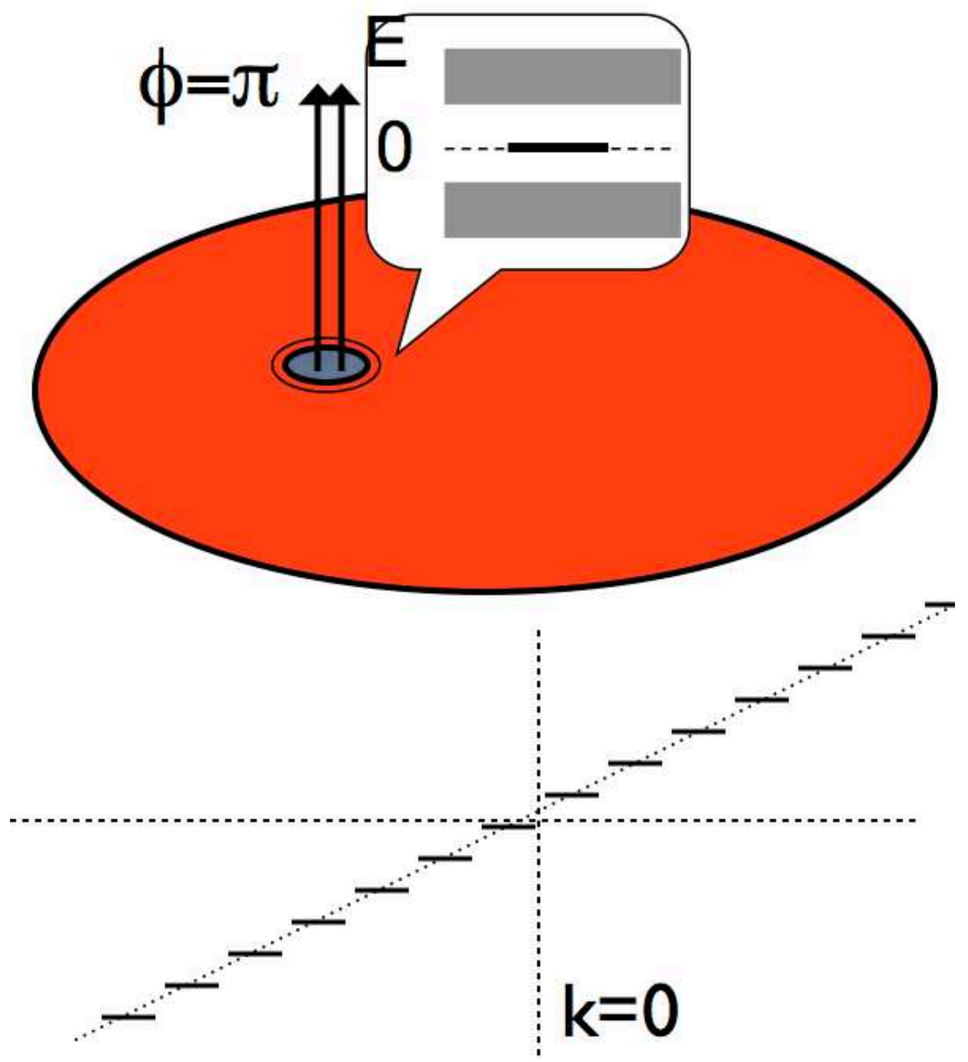


Vortices:



[Bernevig & Neupert, arXiv:1506.0580]

Topological superconductors

Chiral $p + ip$ superconductor:

$$\mathcal{H}_{\mathrm{BdG}} = \frac{1}{2} \sum_{\mathbf{p}} \Psi^{\dagger}_{\mathbf{p}} [\vec{d}(\mathbf{p}, \mu) \cdot \vec{\sigma}] \Psi_{\mathbf{p}} \, , \qquad \vec{d}(\mathbf{p}, \mu) = (-2|\Delta| p_y, -2|\Delta| p_x, \tfrac{p^2}{2m} - \mu)$$

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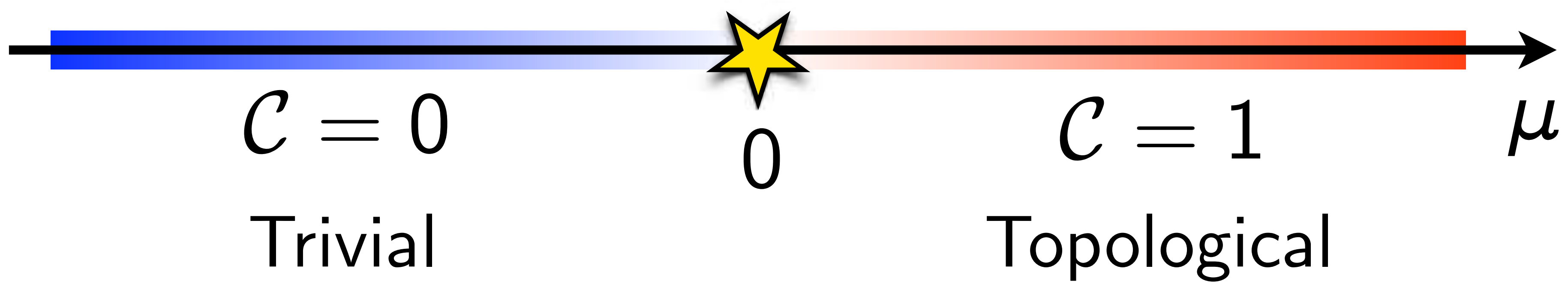
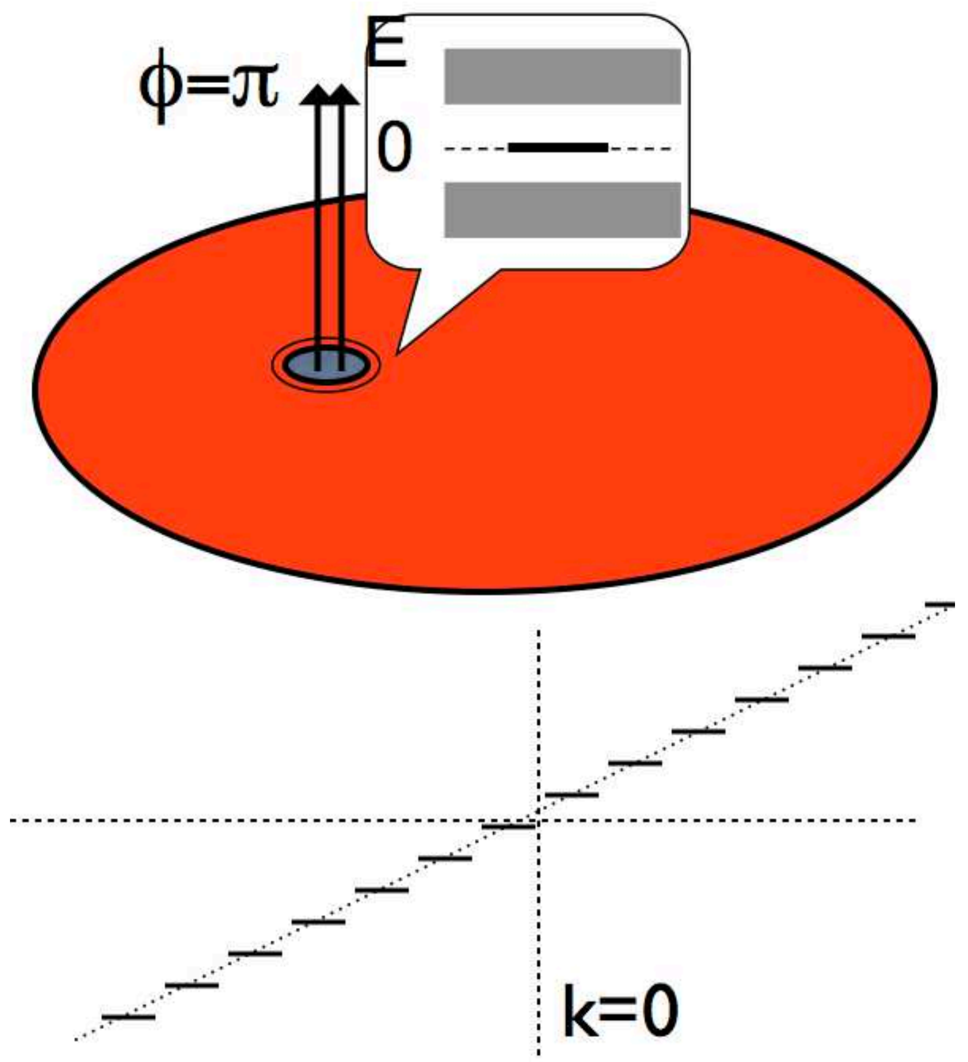
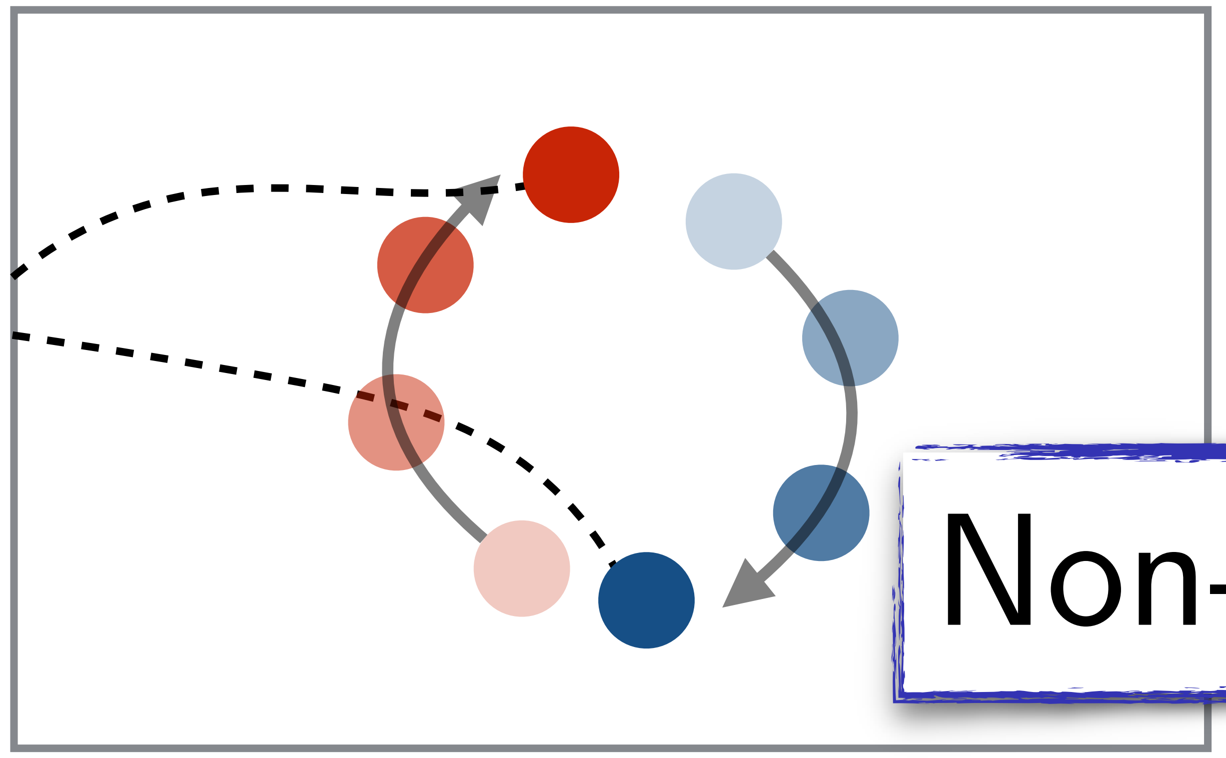


Vortices:



Exchange statistics:



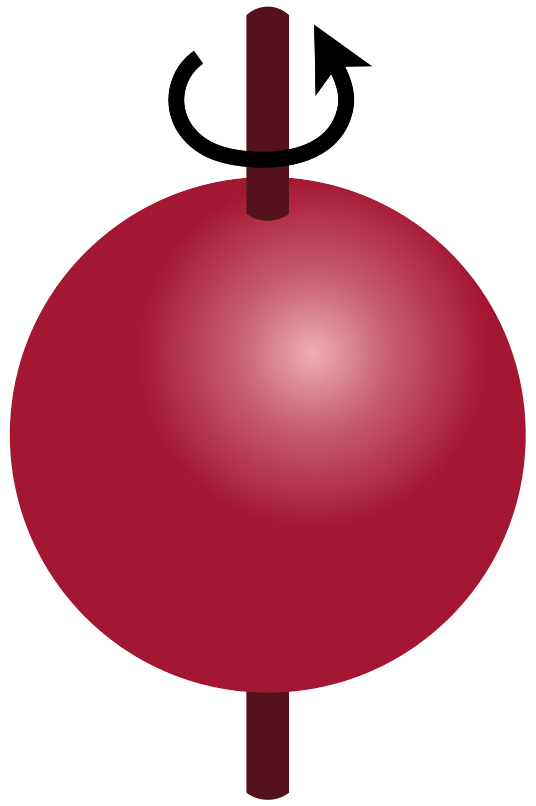
$$\tau(T_{ij}) = e^{\frac{\pi}{4} \gamma_j \gamma_i}$$

Non-Abelian anyons!

[Bernevig & Neupert, arXiv:1506.0580]

Kitaev's 16-fold way

Topological spin:

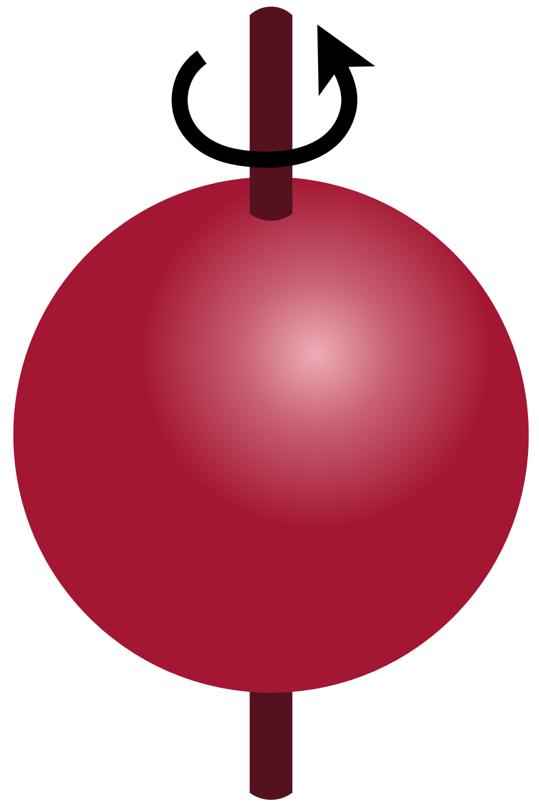


$$e^{2\pi i \frac{\mathcal{C}}{16}}$$

16 classes of topological SCs!

Kitaev's 16-fold way

Topological spin:



$$e^{2\pi i \frac{\mathcal{C}}{16}}$$

16 classes of topological SCs!

Q1. How to realize them?

Q2. How to detect them?

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(4) Conclusions

Frustrated magnets

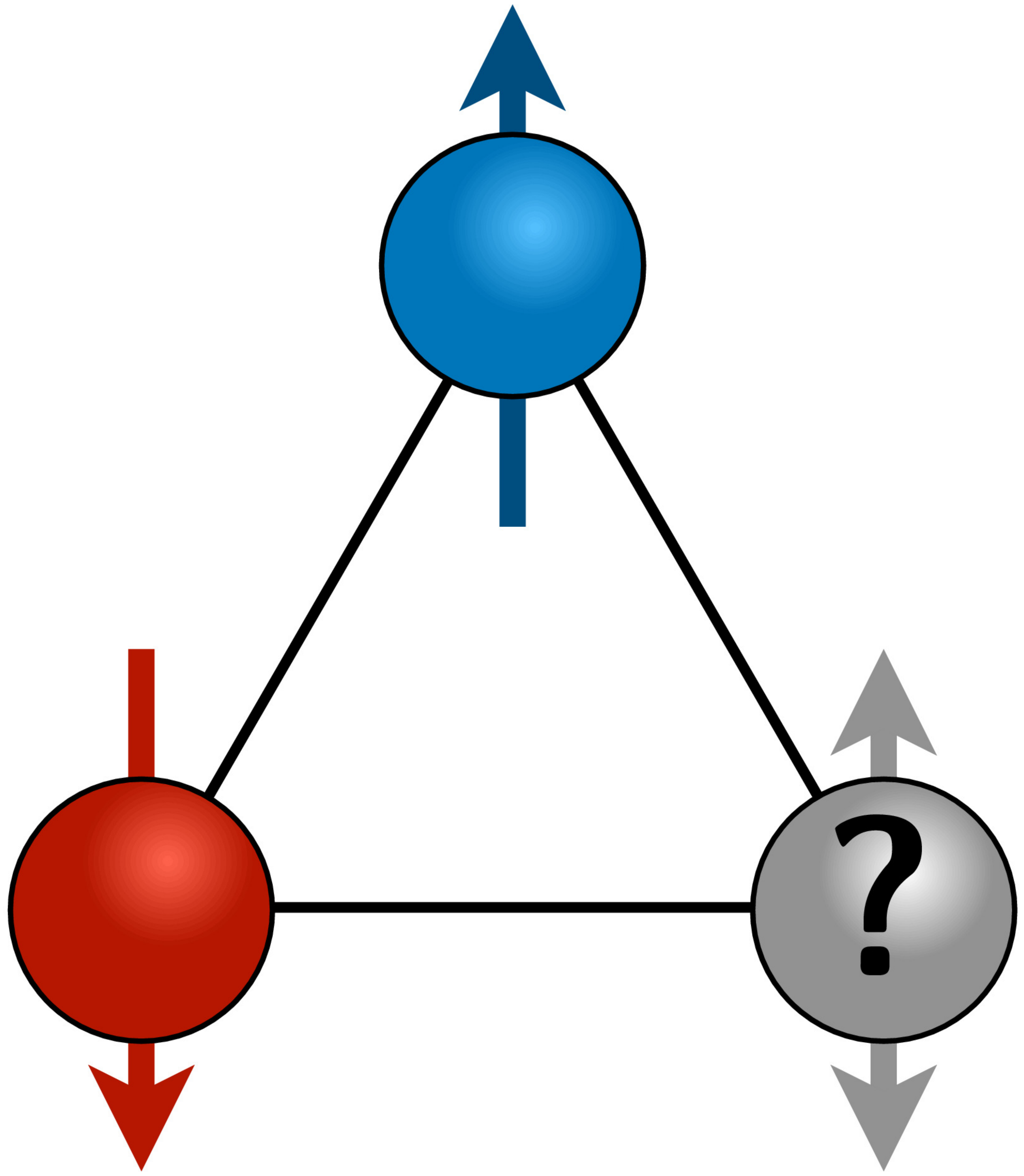
Frustration:

Not all local constraints can be simultaneously satisfied

Consequences:

Classical: Exponentially large ground-state manifold

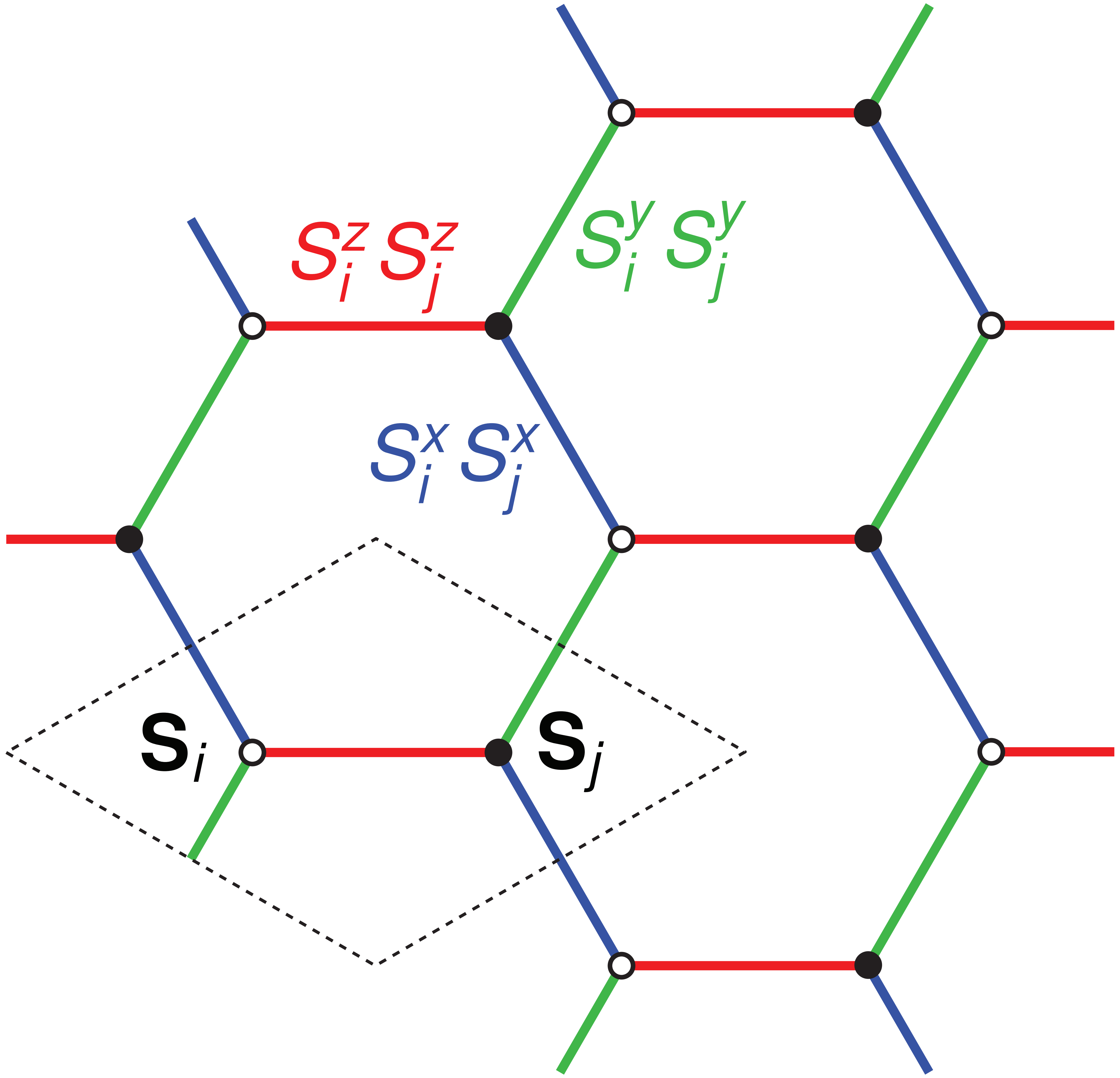
Quantum: New phases of matter?



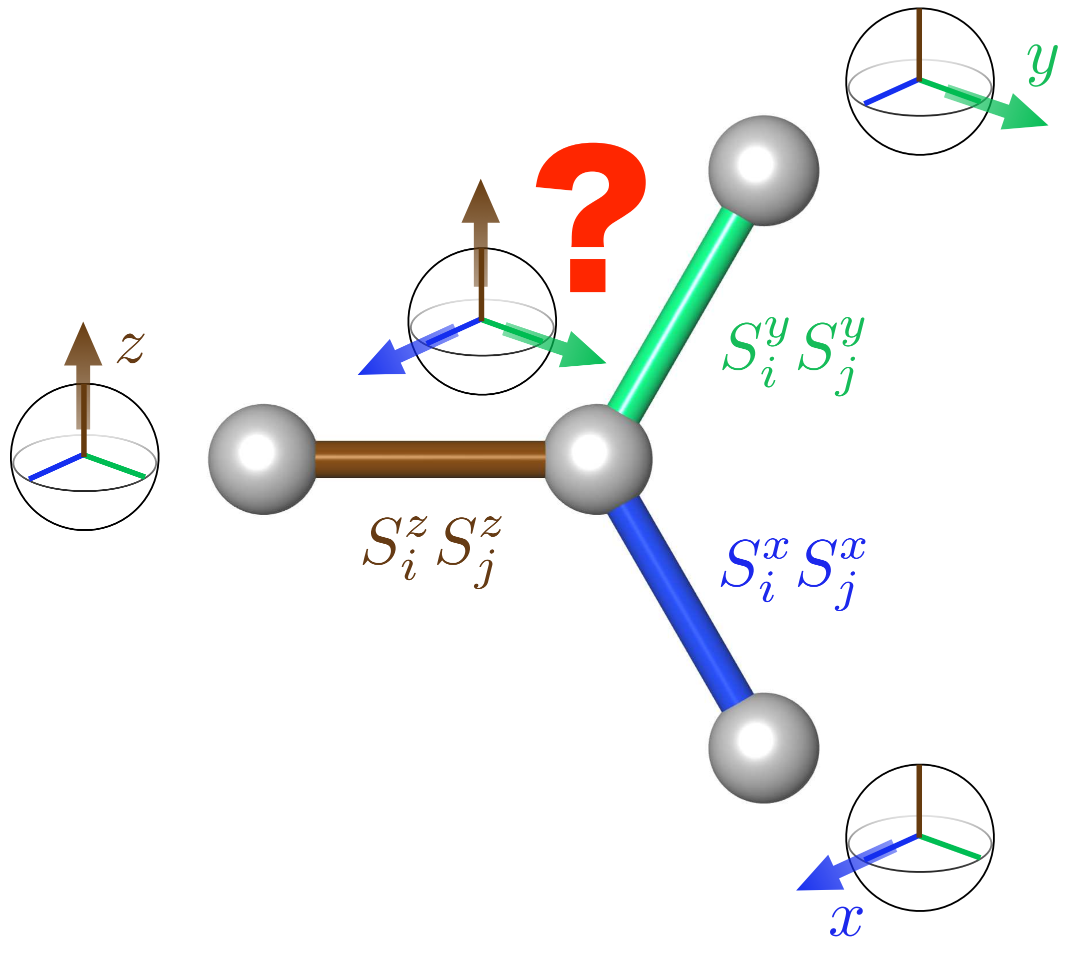
Antiferromagnetic coupling of 3 Ising spins

Kitaev honeycomb model

Spin-1/2 on honeycomb lattice:



Alexei Kitaev



Exchange frustration

Hamiltonian:

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

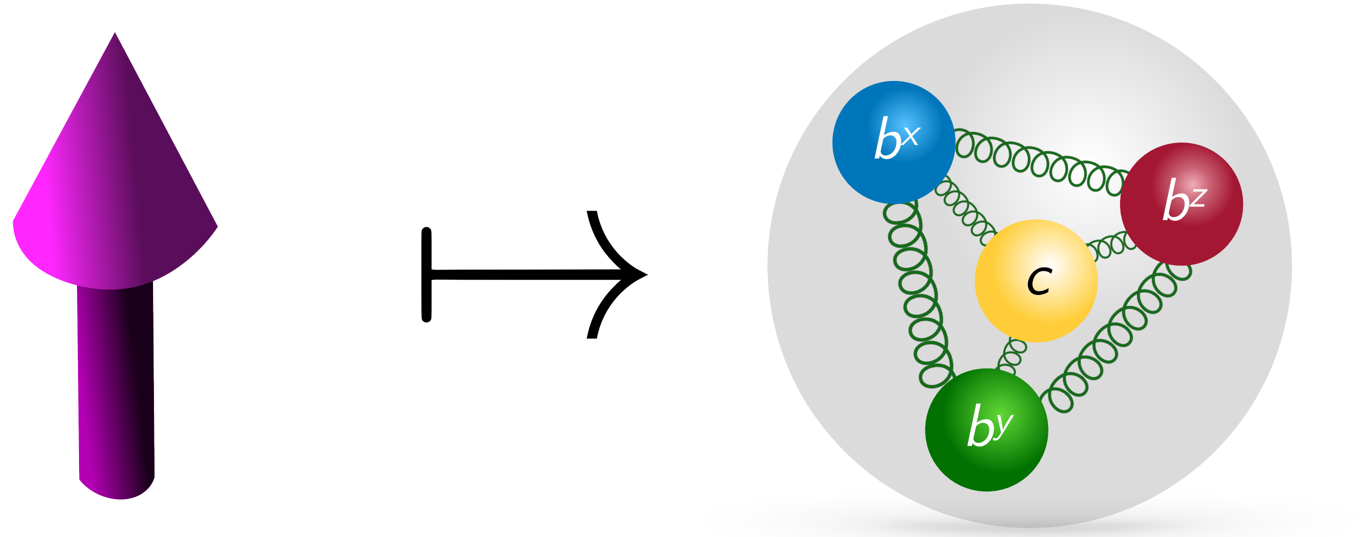
[Kitaev, Ann. Phys. '06]

Review: [Trebst, arXiv:1701.07056]

Parton construction

Majorana representation:

$$\sigma^x \mapsto \tilde{\sigma}^x = i b^x c$$
$$\sigma^y \mapsto \tilde{\sigma}^y = i b^y c$$
$$\sigma^z \mapsto \tilde{\sigma}^z = i b^z c$$



1 spin

4 Majoranas
with gauge constraint

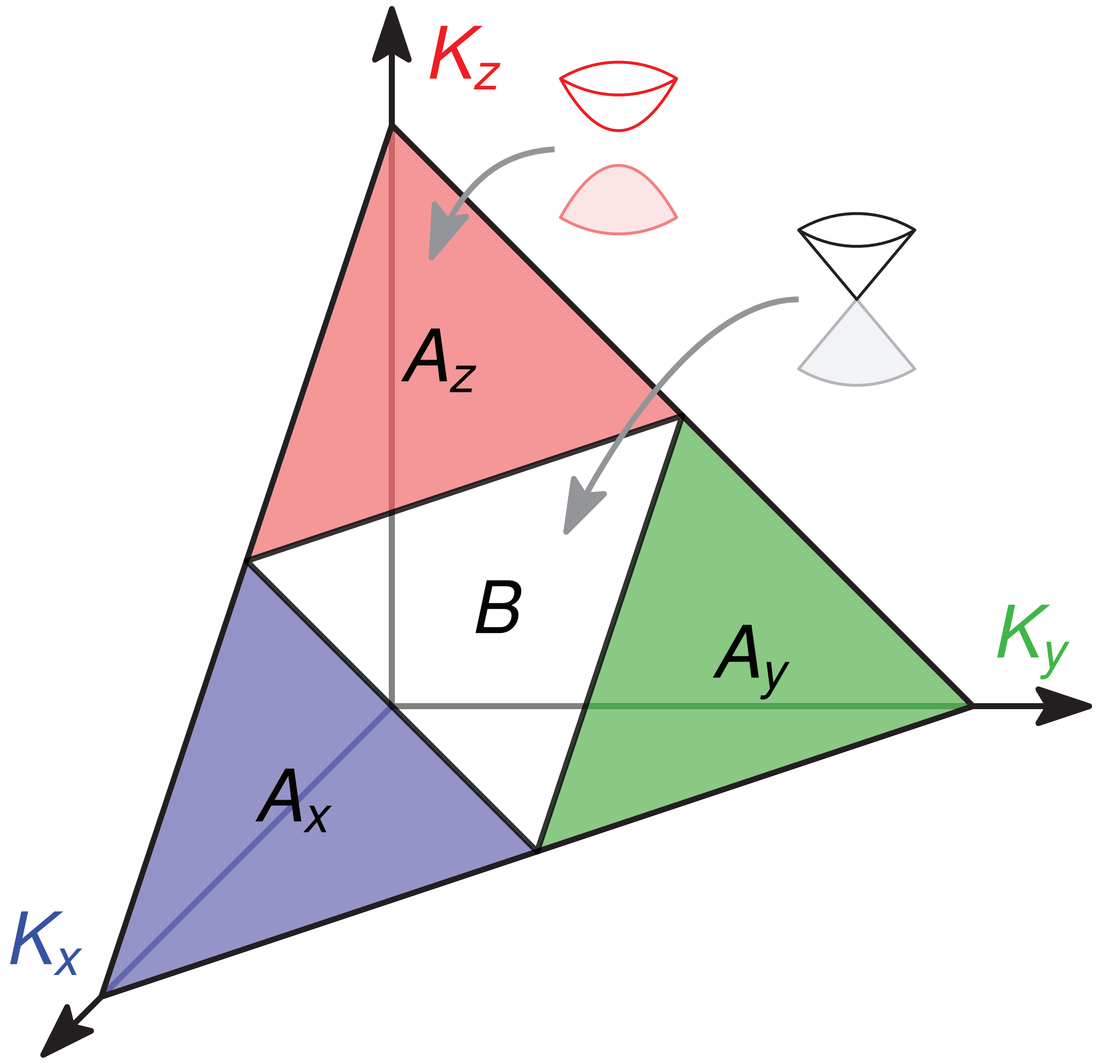
Fractionalization:

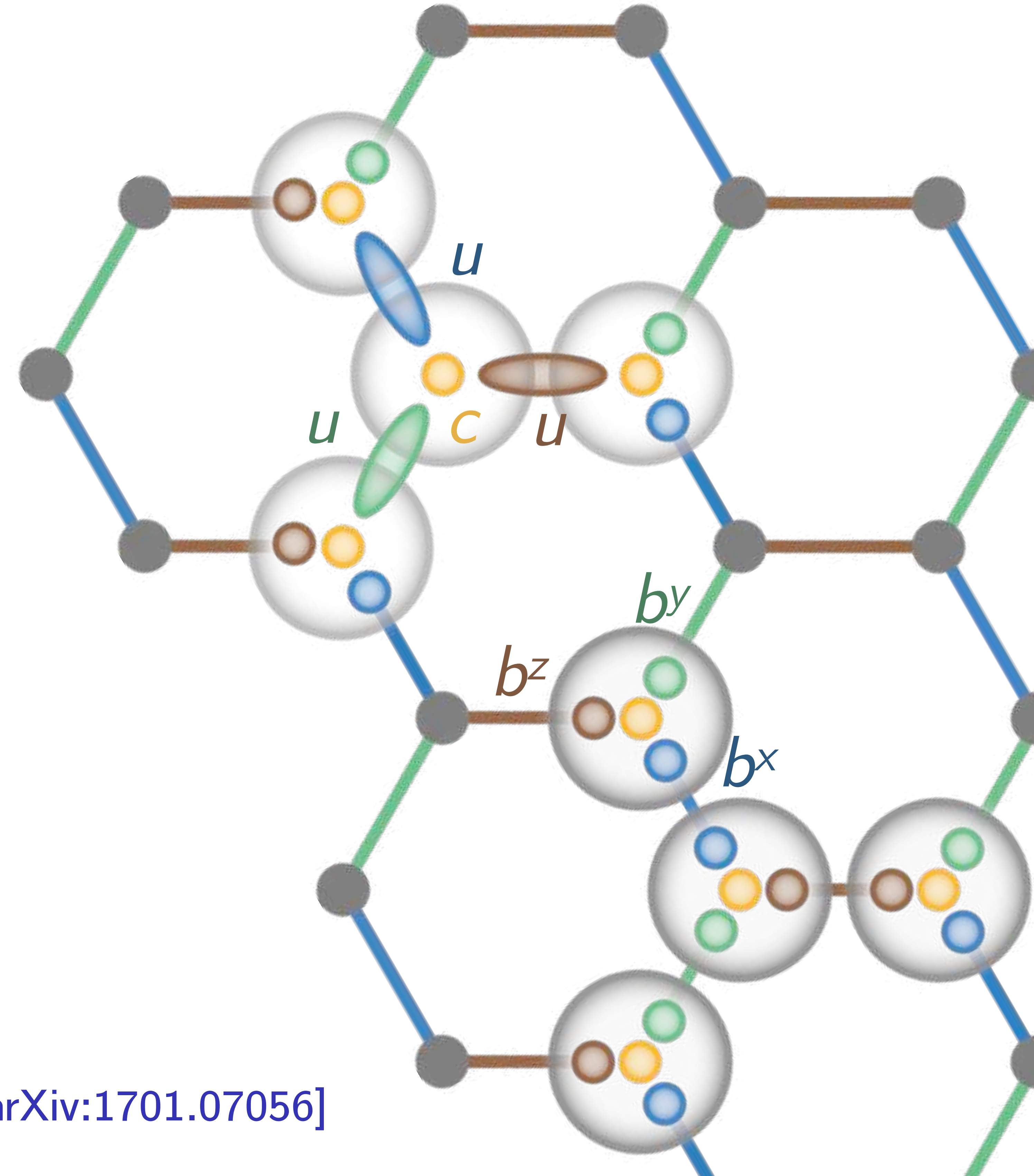
$$H \mapsto \tilde{H} = -i \sum_{\langle ij \rangle_\gamma} K_\gamma \underbrace{(i b_i^\gamma b_j^\gamma)}_{\equiv \hat{u}_{ij} = \hat{u}_{ij}^\dagger} c_i c_j$$

static!

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

Fermion spectrum:

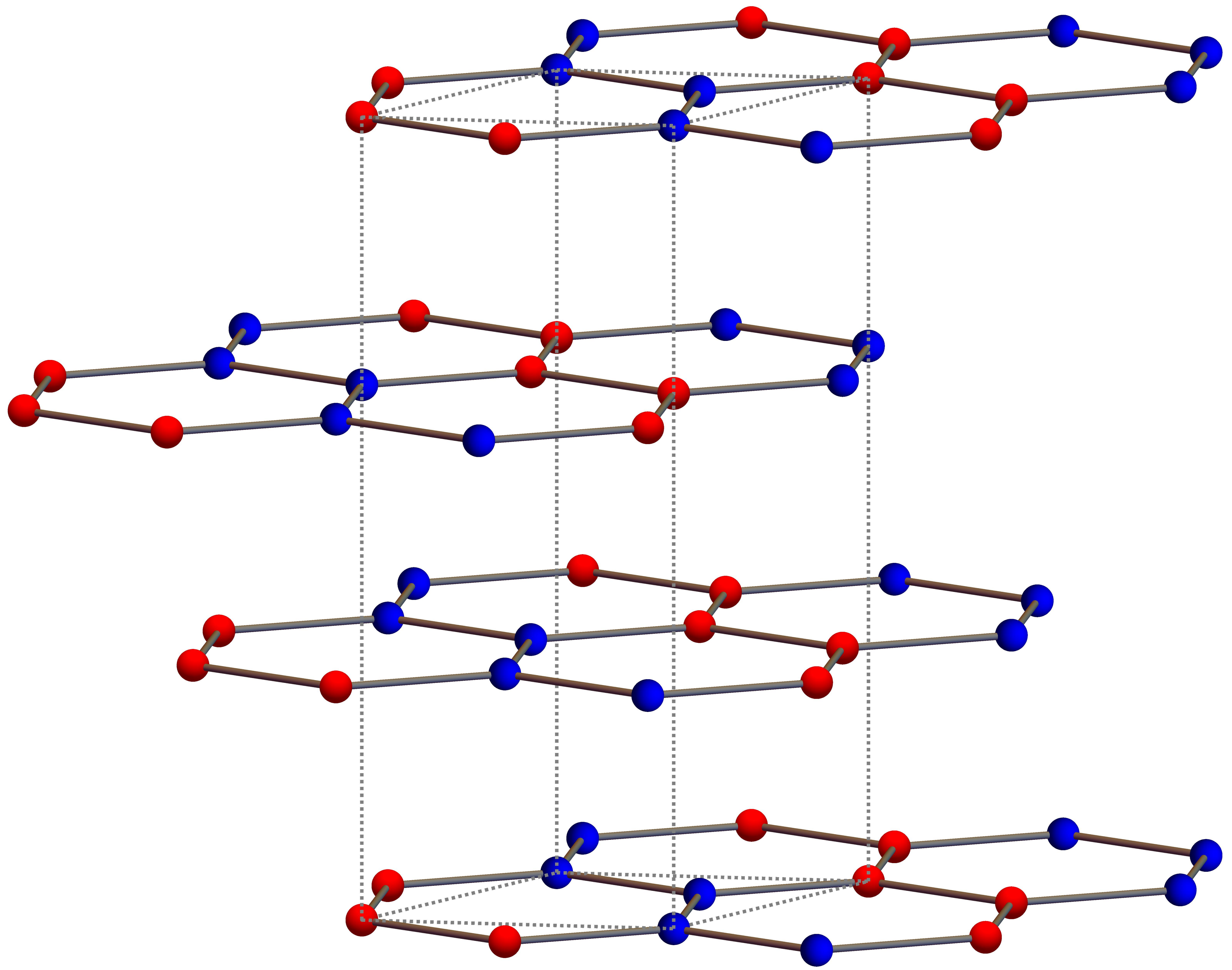




Review: [Trebst, arXiv:1701.07056]

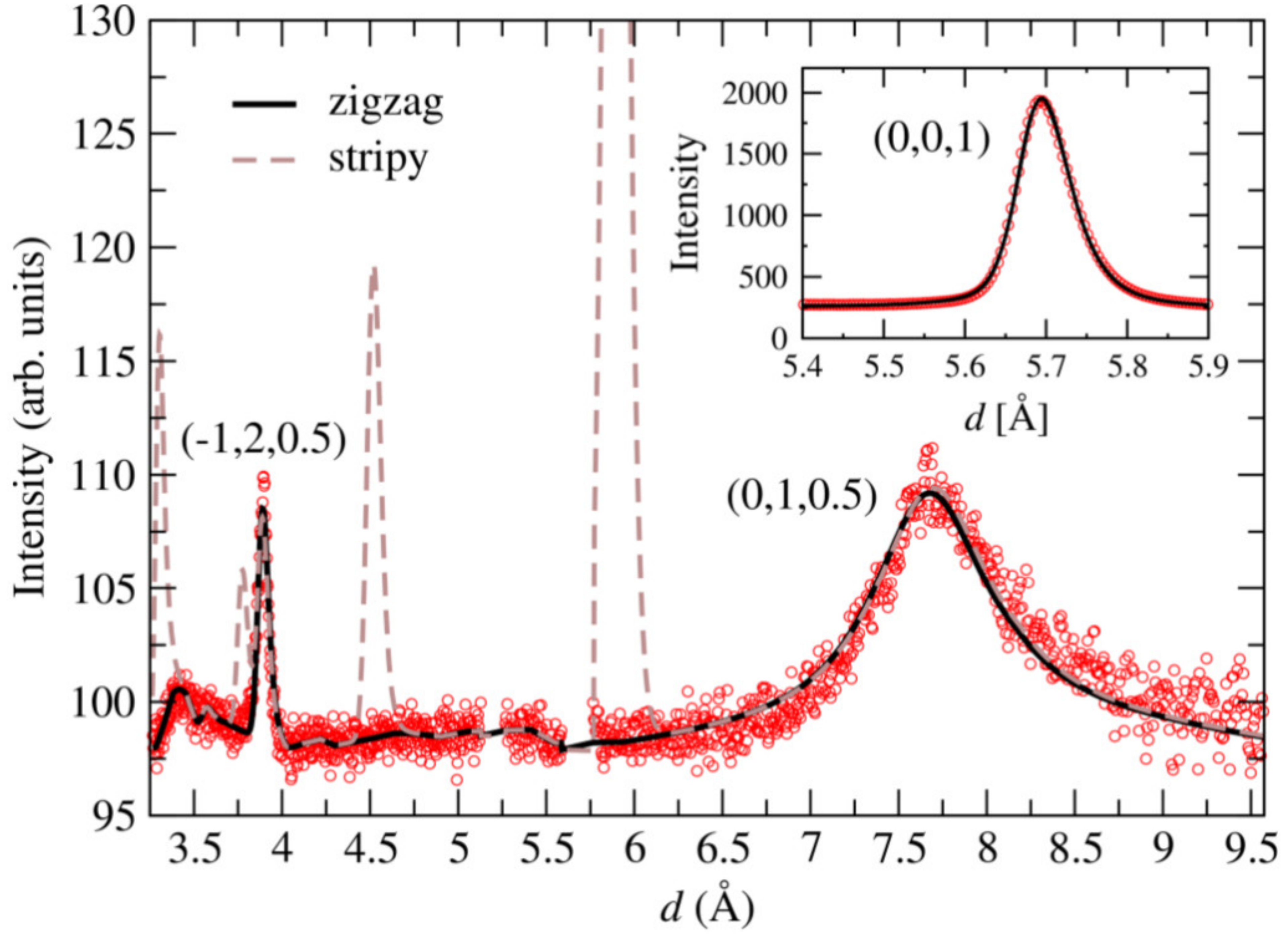
α-$RuCl_3$ in zero field: Zigzag antiferromagnet

Zigzag order:



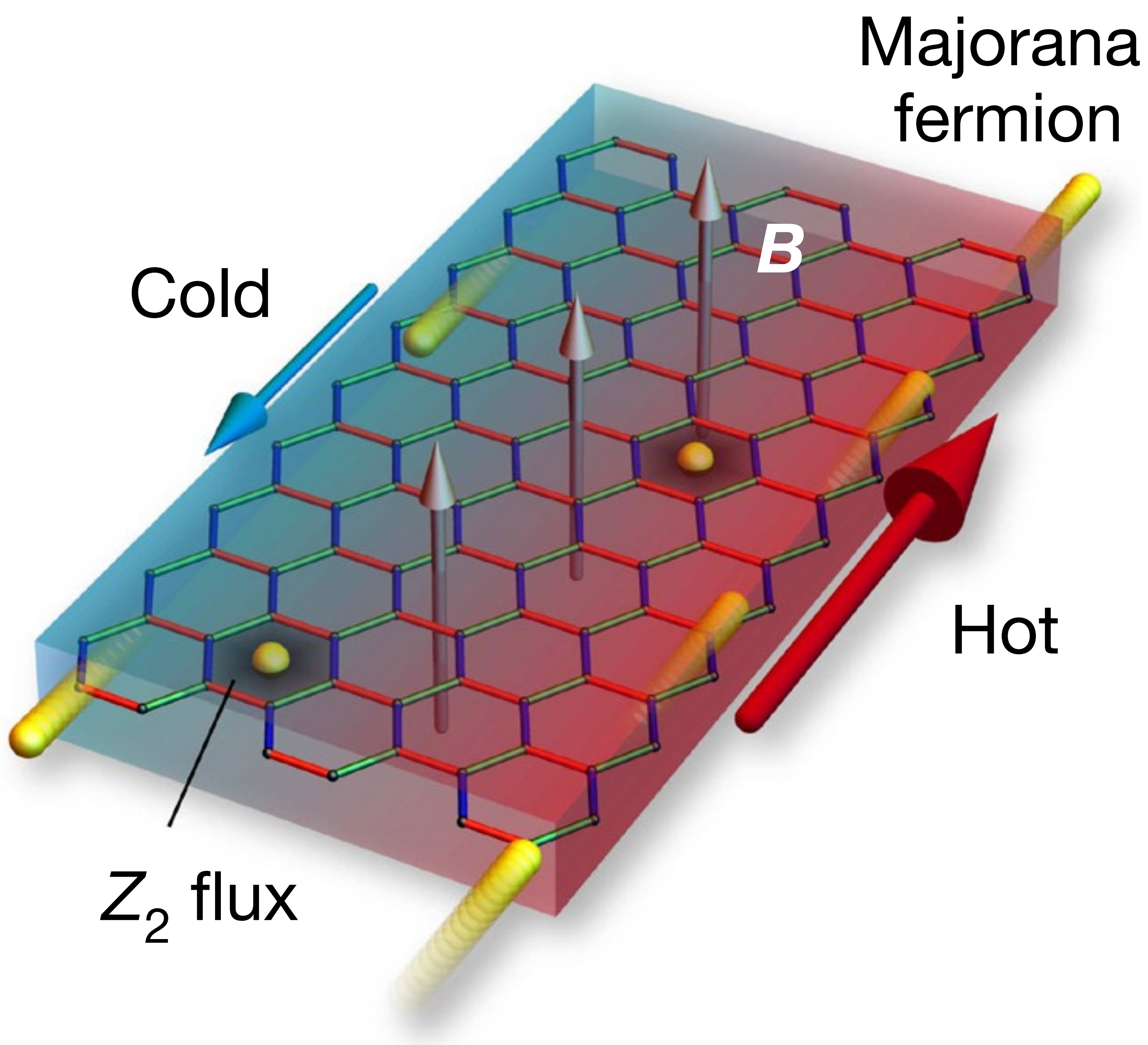
Neutron diffraction:

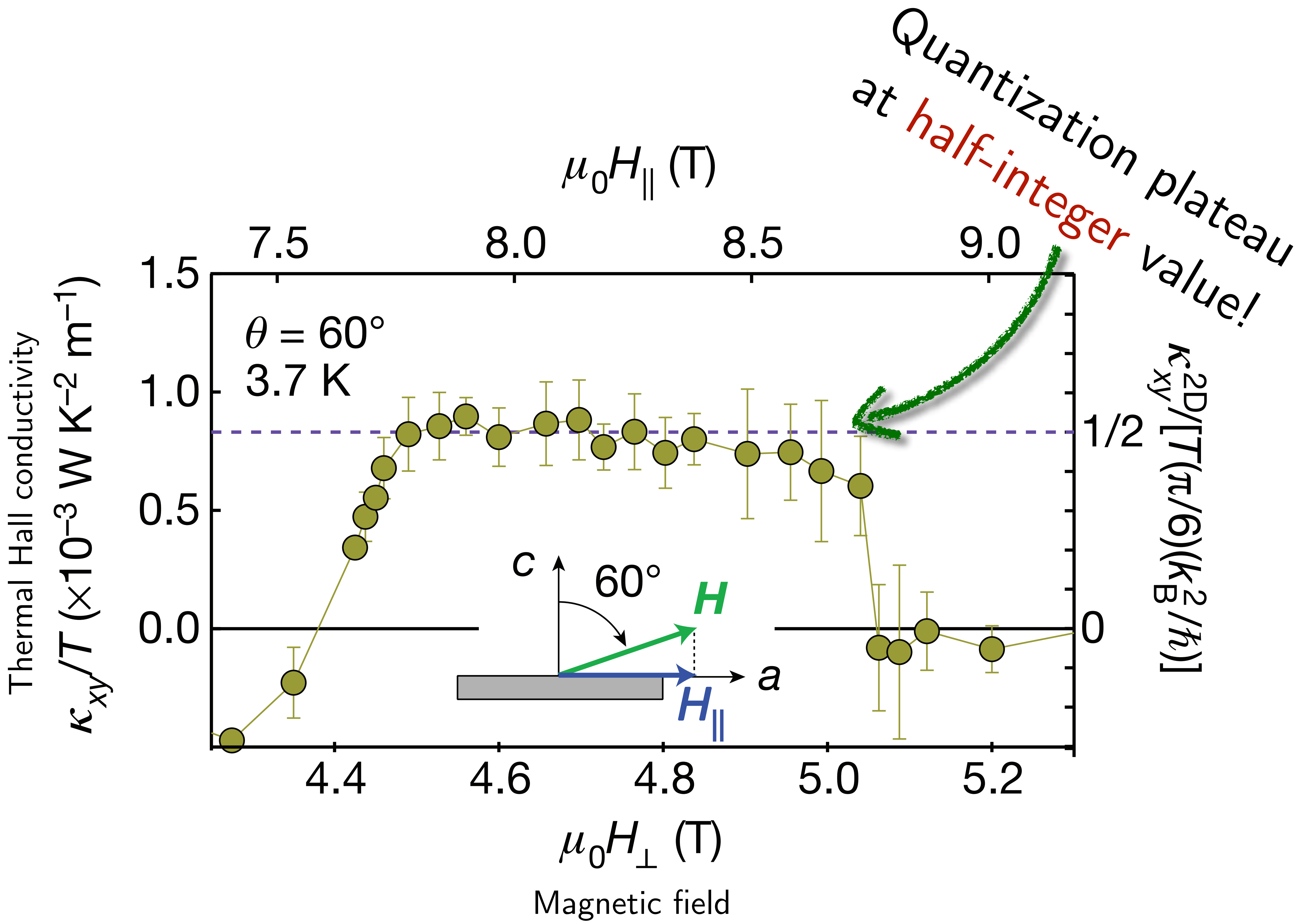
[Johnson *et al.*, PRB '15]



Experimental search: α-$RuCl_3$ in field

Half-integer thermal Quantum Hall effect:



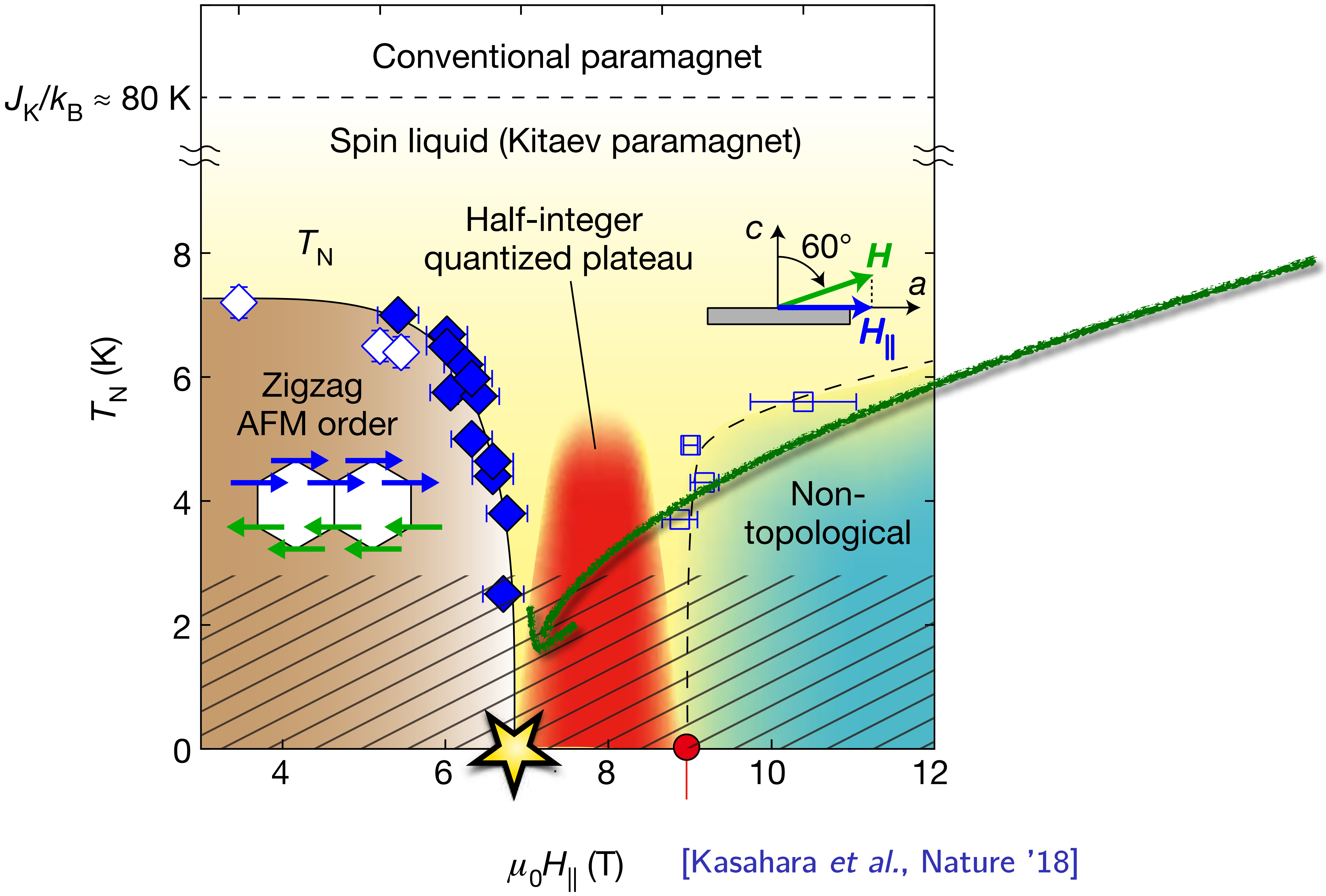


[Kasahara *et al.*, Nature '18]

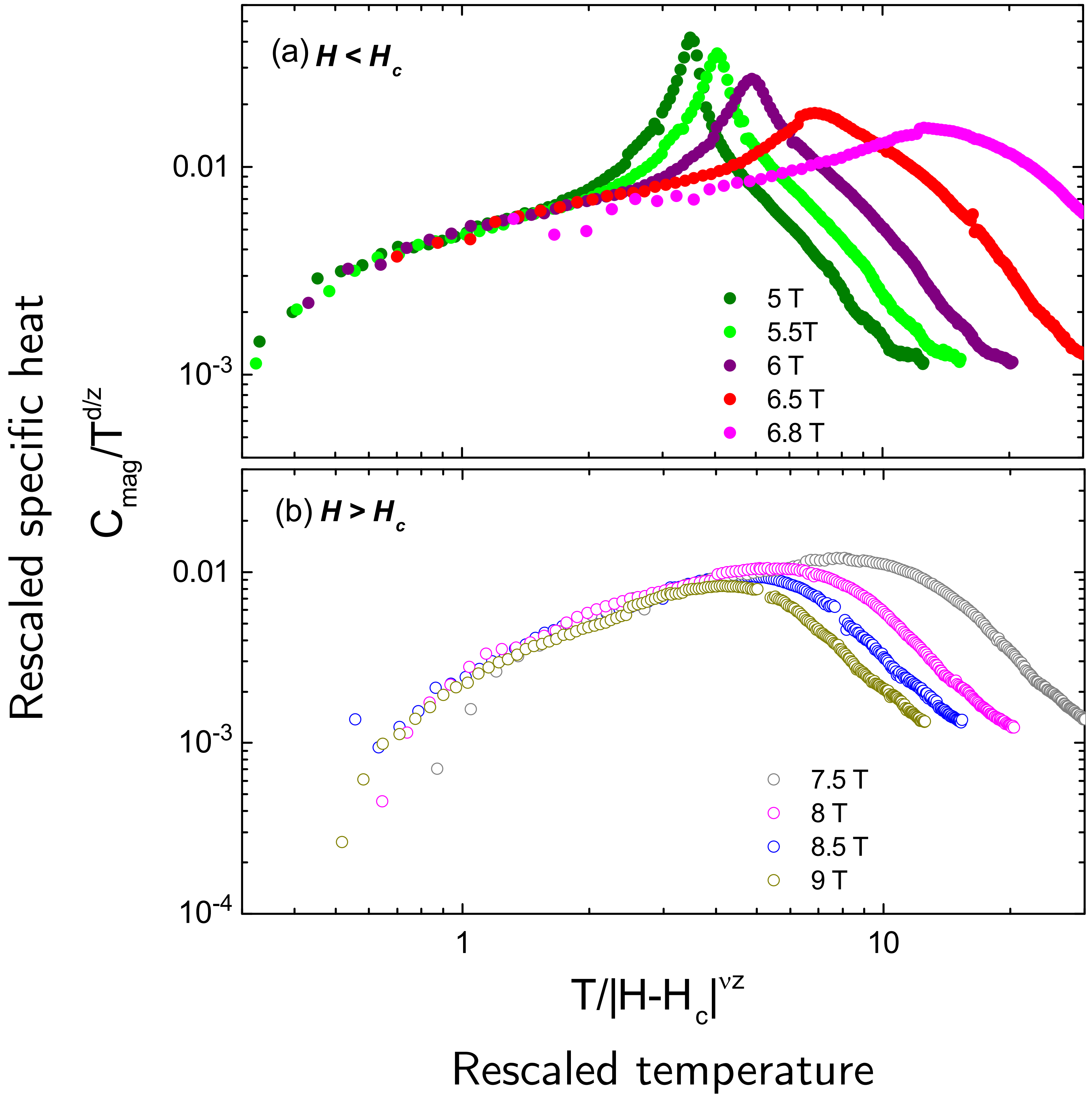
Topical Review: [LJ & Vojta, JPCM '19]

Smoking-gun signature of Majorana edge states?

α-$RuCl_3$: Field-induced quantum criticality



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



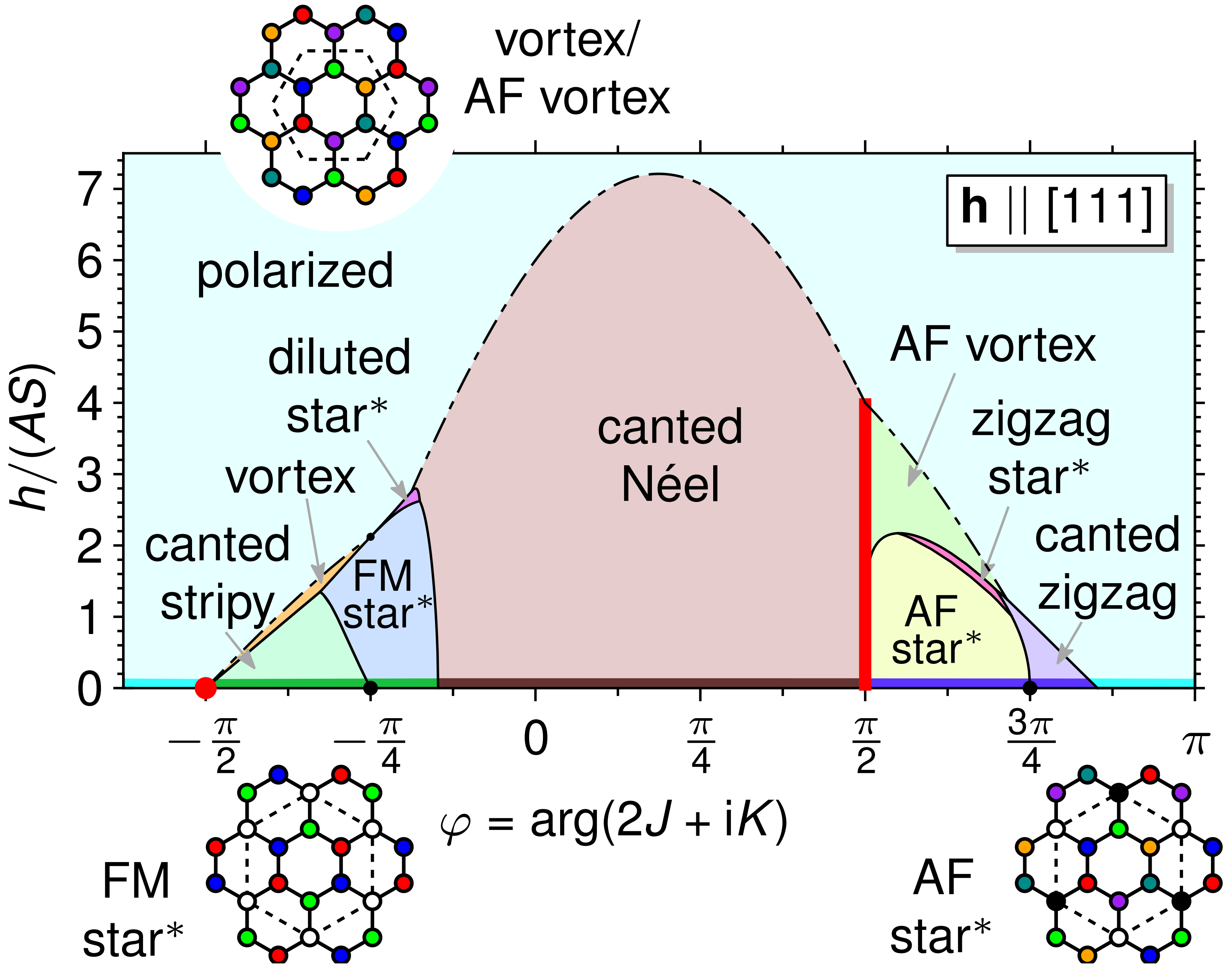
... with $z \approx 1$ and $\nu \approx 0.7$

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

Fractionalized transition?

Kitaev-Heisenberg models in field

Classical ($S \to \infty$)



[LJ, Andrade, Vojta, PRL '16]

... linear spin-wave theory
& classical Monte Carlo

Kitaev-Heisenberg models in field

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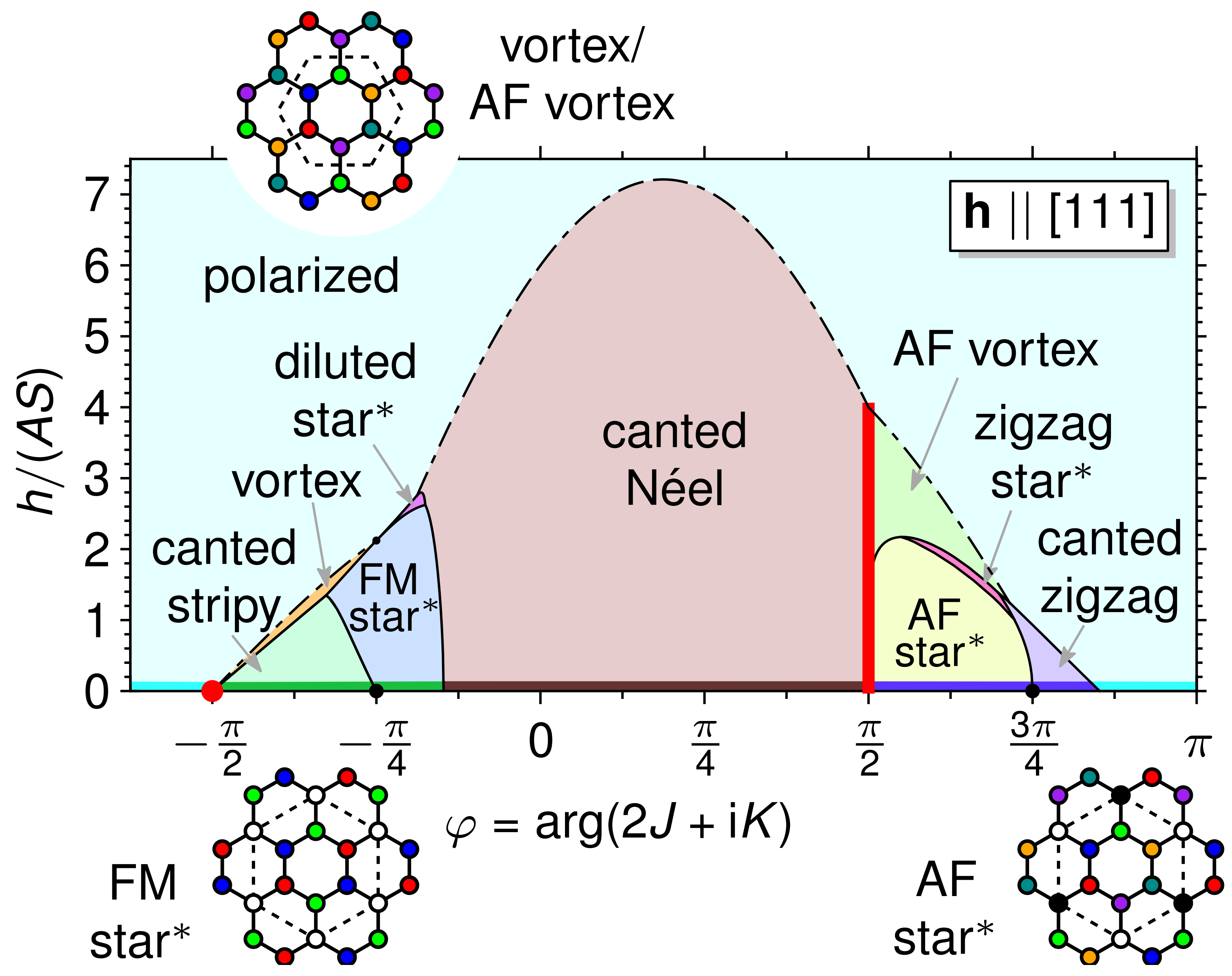

[LJ, Andrade, Vojta, PRL '16]

... linear spin-wave theory
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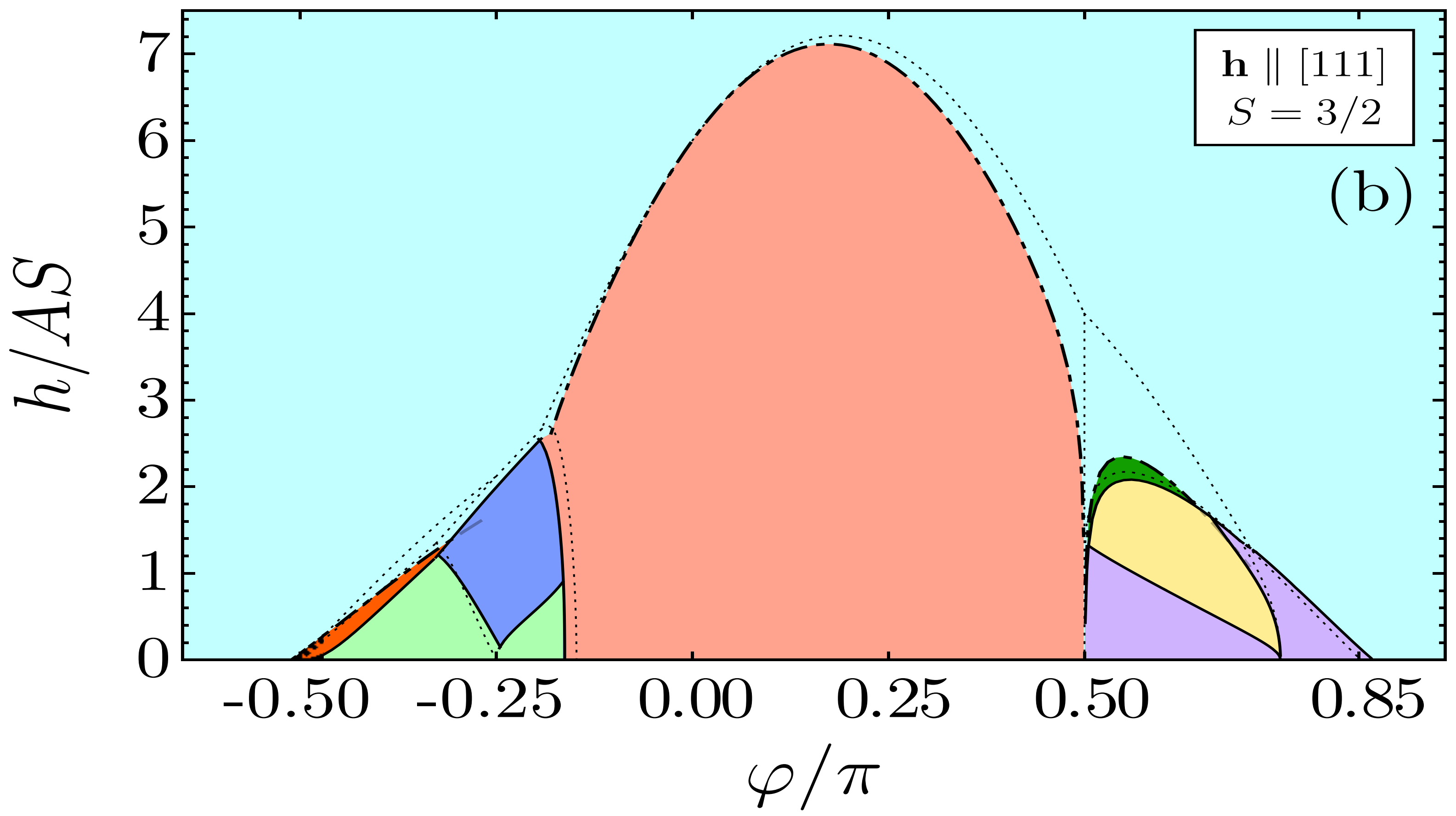
Semiclassical ($S = 3/2$)

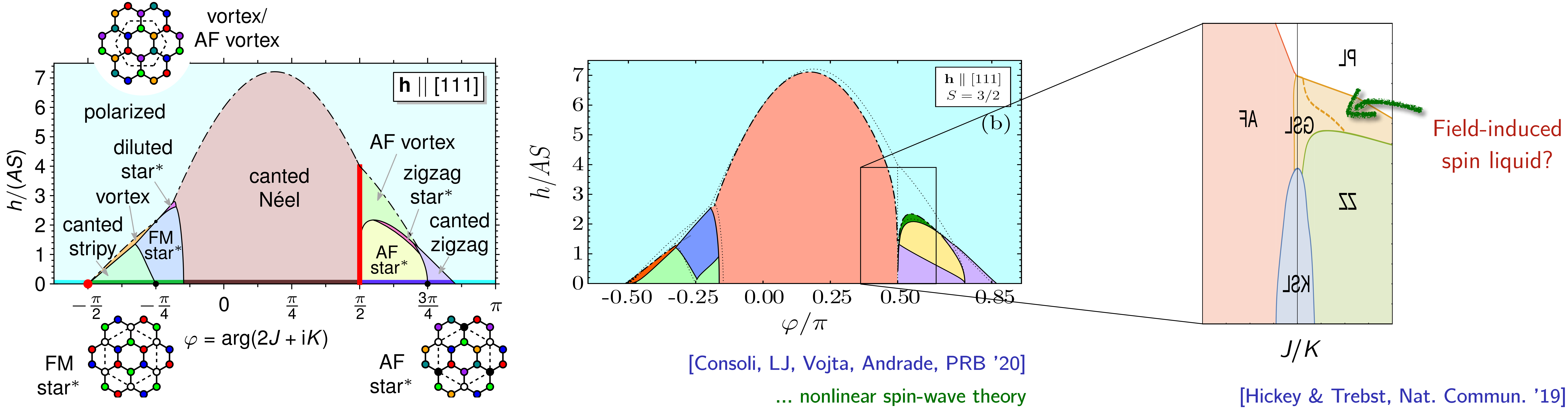


[Consoli, LJ, Vojta, Andrade, PRB '20]

... nonlinear spin-wave theory

Kitaev-Heisenberg models in field

Classical ($S \to \infty$) | Semiclassical ($S = 3/2$) | Quantum ($S = 1/2$)



[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: [Sato & Assaad, PRB '21]

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Generalizations of Kitaev model: Spin-orbital liquids

Spin + orbital + ... degrees of freedom:

...

$\sigma^\alpha \quad 2 \times 2$ $\qquad$ $\sigma^\alpha \otimes \tau^\beta = \gamma^i \quad 4 \times 4$ $\qquad$ $\Gamma^\mu \quad 8 \times 8$

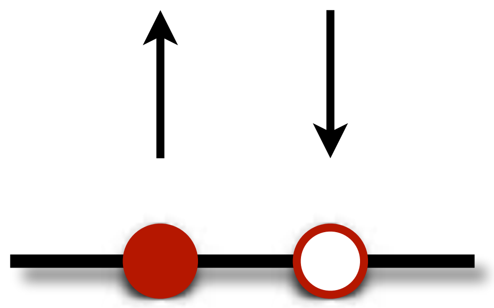
$\mathcal{C} = 0, 1$ $\qquad$ $\mathcal{C} = 2, 3$ $\qquad$ $\mathcal{C} = 4, 5$

... can realize all 16 topological superconductors

[Chulliparambil, ..., LJ, Tu, PRB '20]

Generalizations of Kitaev model: Spin-orbital liquids

Spin + orbital + ... degrees of freedom:



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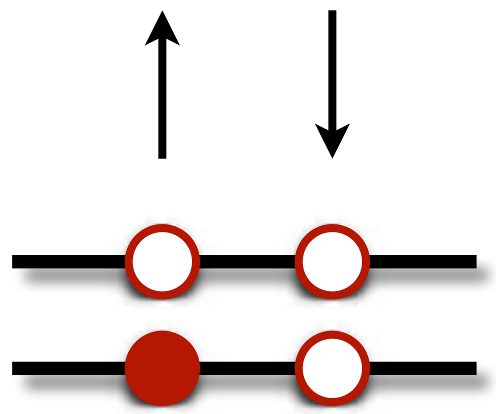

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$\mathcal{C} = 2, 3$

...

$\Gamma^\mu \quad 8 \times 8$

$\mathcal{C} = 4, 5$

... can realize all 16 topological superconductors

[Chulliparambil, ..., LJ, Tu, PRB '20]

Example #1 (square lattice):

XY spin

Kitaev orbital

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

Majorana representation:

$\sigma^y \otimes \tau^x = i b^1 c^x$

$\sigma^y \otimes \tau^y = i b^2 c^x$

$\sigma^y \otimes \tau^z = i b^3 c^x$

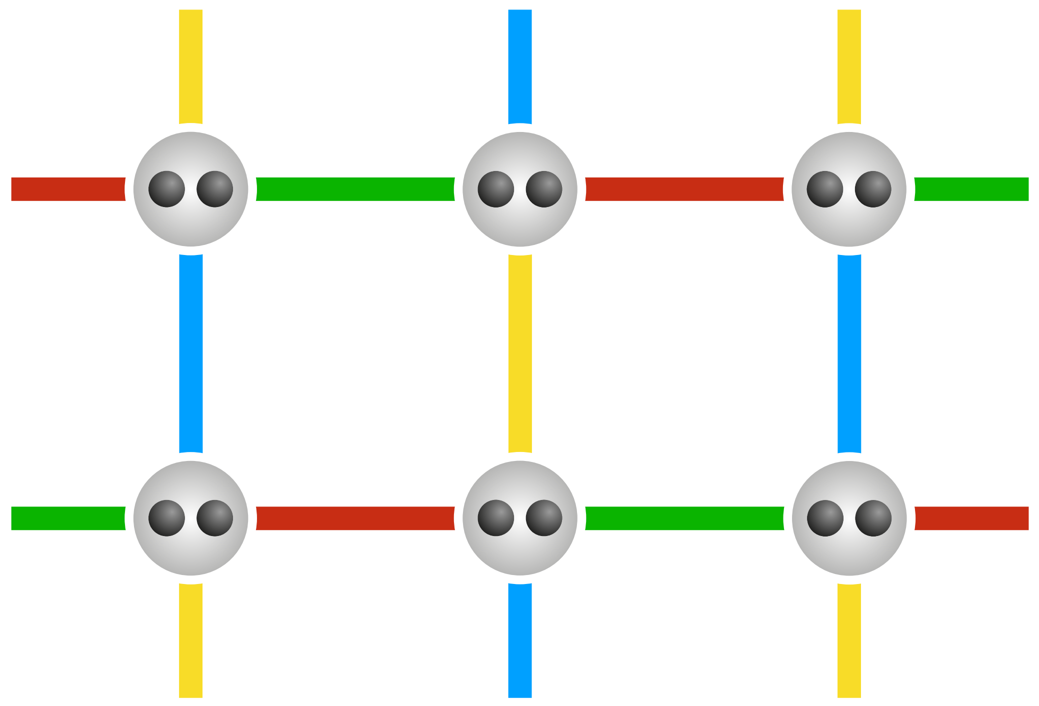
$\sigma^x \otimes \mathbb{1} = i b^4 c^x$

$\sigma^z \otimes \mathbb{1} = i c^y c^x$

... recover known model for $j = 3/2$ spin liquid:

[Yao, Zhang, Kivelson, PRL '09]

[Nakai, Ryu, Furusaki, PRB '12]



2 itinerant fermions

$\mathcal{C} = 2$

Kitaev-Ising spin-orbital model

Ising perturbation:

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

Kitaev-Ising spin-orbital model

Ising perturbation:

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

Parton representation:

hopping parameter $t = 2K$

π flux

nearest-neighbor repulsion $V = 4J^z$

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

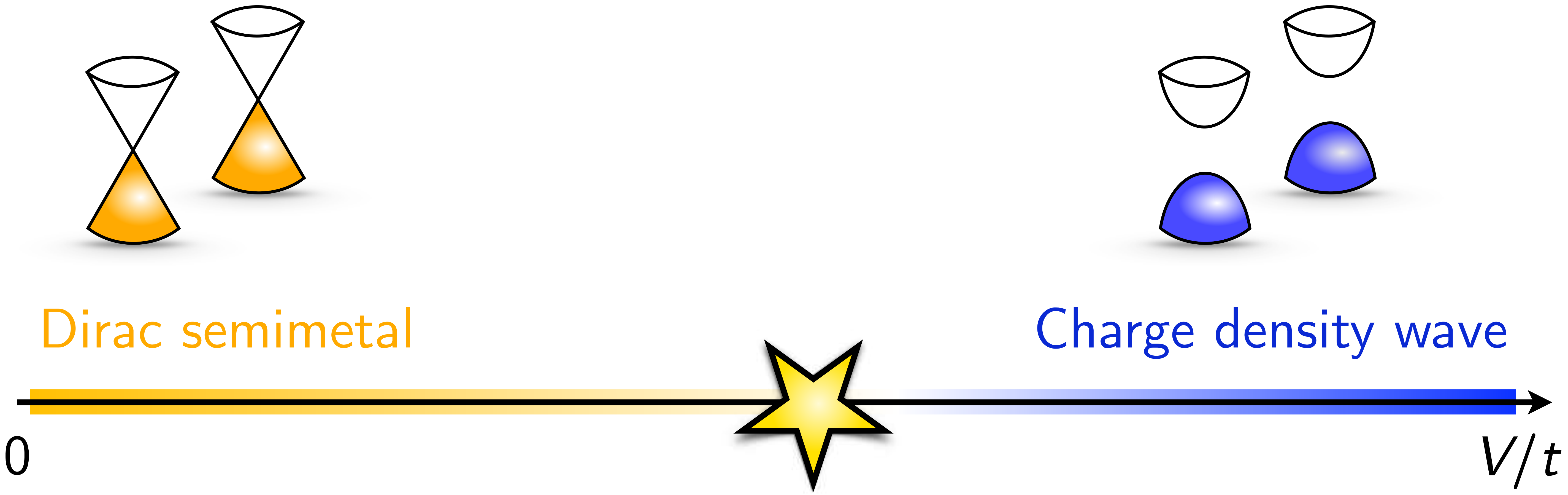
$f = \frac{1}{2}(c^x + i c^y)$

electron density $f^\dagger f$

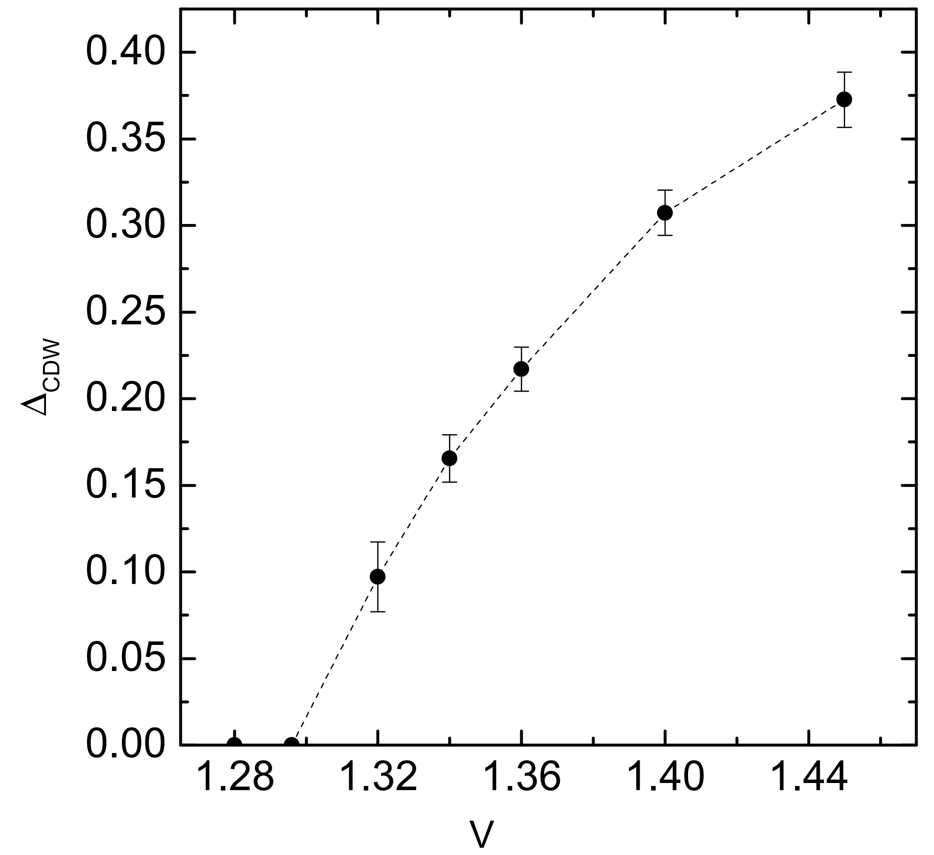
Ground-state flux pattern: [Lieb, PRL '94]

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

Spinless fermions on π-flux lattice: QMC



$(V/t)_c = 1.281(2)$

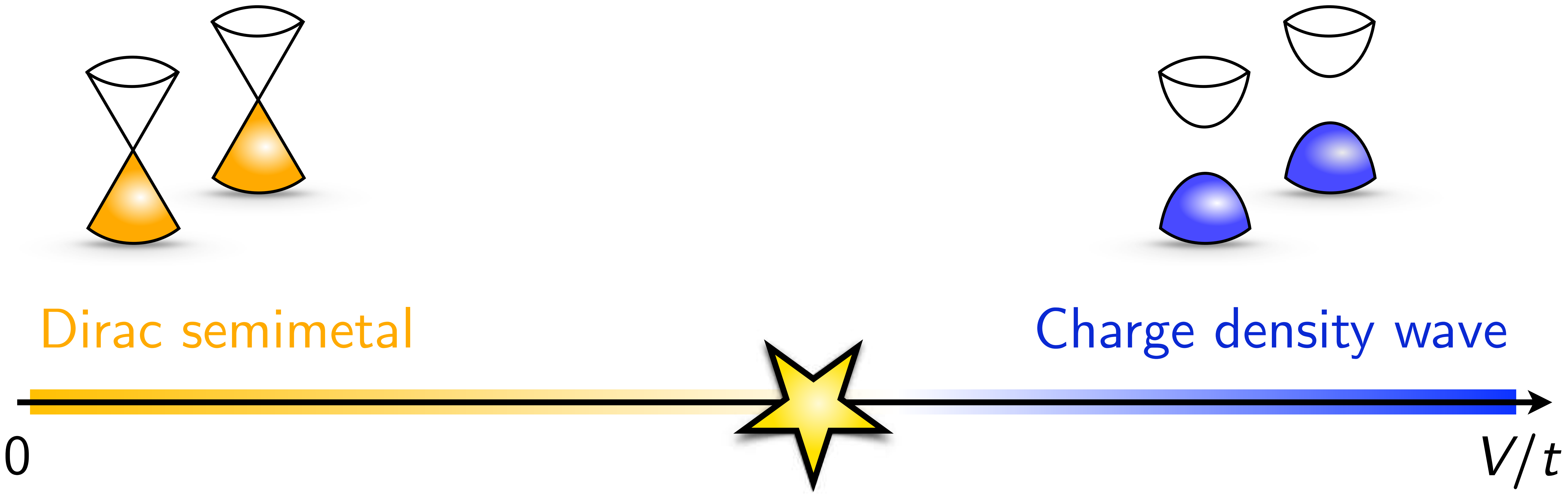


[Wang, Corboz, Troyer, NJP '14]
[Li, Jiang, Yao, NJP '15]
[Huffman & Chandrasekharan, PRD '17; PRD '20]

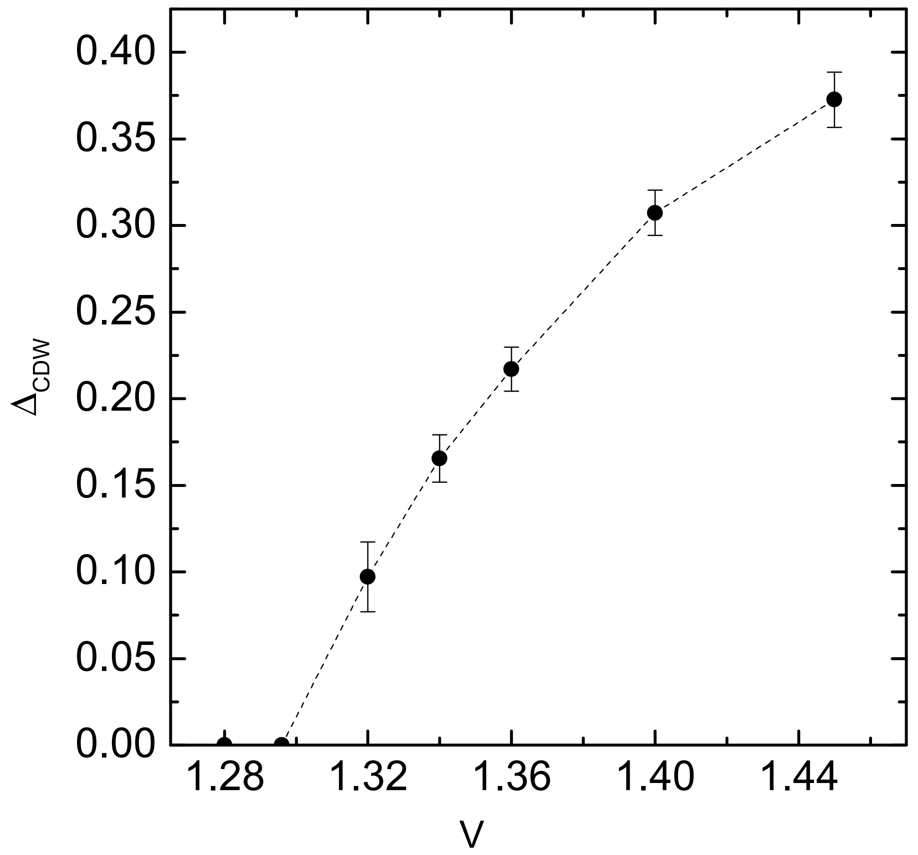
Gross-Neveu-$\mathbb{Z}_2$ universality: $1/\nu = 1.12(1)$, $\eta_\phi = 0.51(3)$

[Gracey, IJMP '94]
[LJ & Herbut, PRB '14]
[Iliesiu *et al.*, JHEP '18]
[Ihrig, Mihaila, Scherer, PRB '18]
...

Spinless fermions on π-flux lattice: QMC



$(V/t)_c = 1.281(2)$



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

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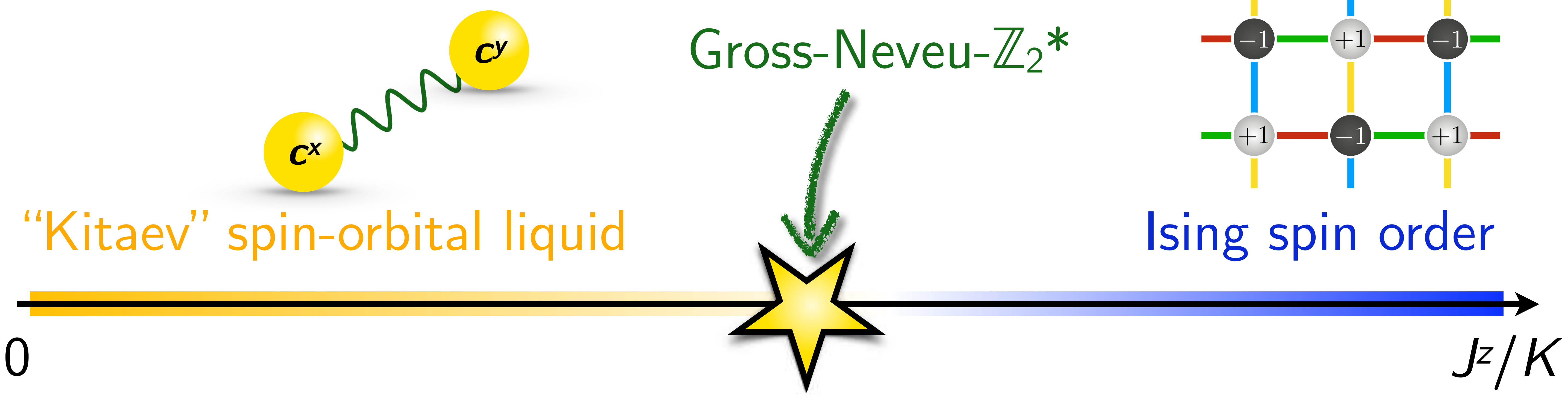
[Ihrig, Mihaila, Scherer, PRB '18]
...

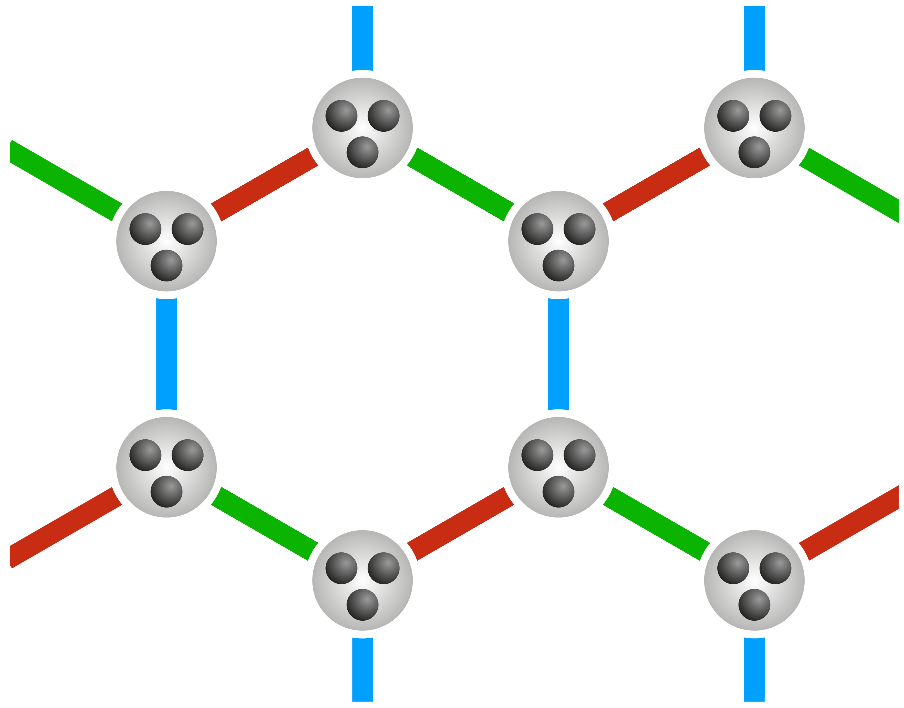
Spin-orbital model:



$(J^z/K)_c = 0.642(2)$

[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]

Kitaev-Heisenberg spin-orbital model



Example #2 (honeycomb lattice):

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

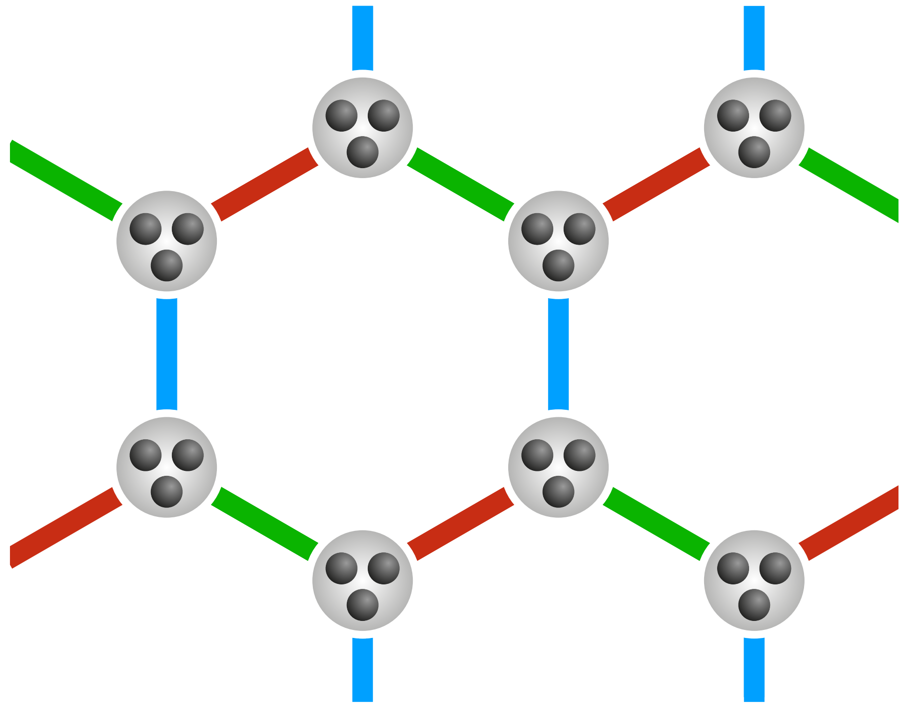
... for $J = 0$ equivalent to known models:

[Yao & Lee, PRL '11]

[Natori & Knolle, PRL '20]

Kitaev-Heisenberg spin-orbital model

Example #2 (honeycomb lattice):



3 itinerant fermions

$\mathcal{C} = 3$

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

... for $J = 0$ equivalent to known models:

[Yao & Lee, PRL '11]

[Natori & Knolle, PRL '20]

Majorana representation:

$c \equiv \begin{pmatrix} c^x \\ c^y \\ c^z \end{pmatrix}$

spin-1 matrices

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

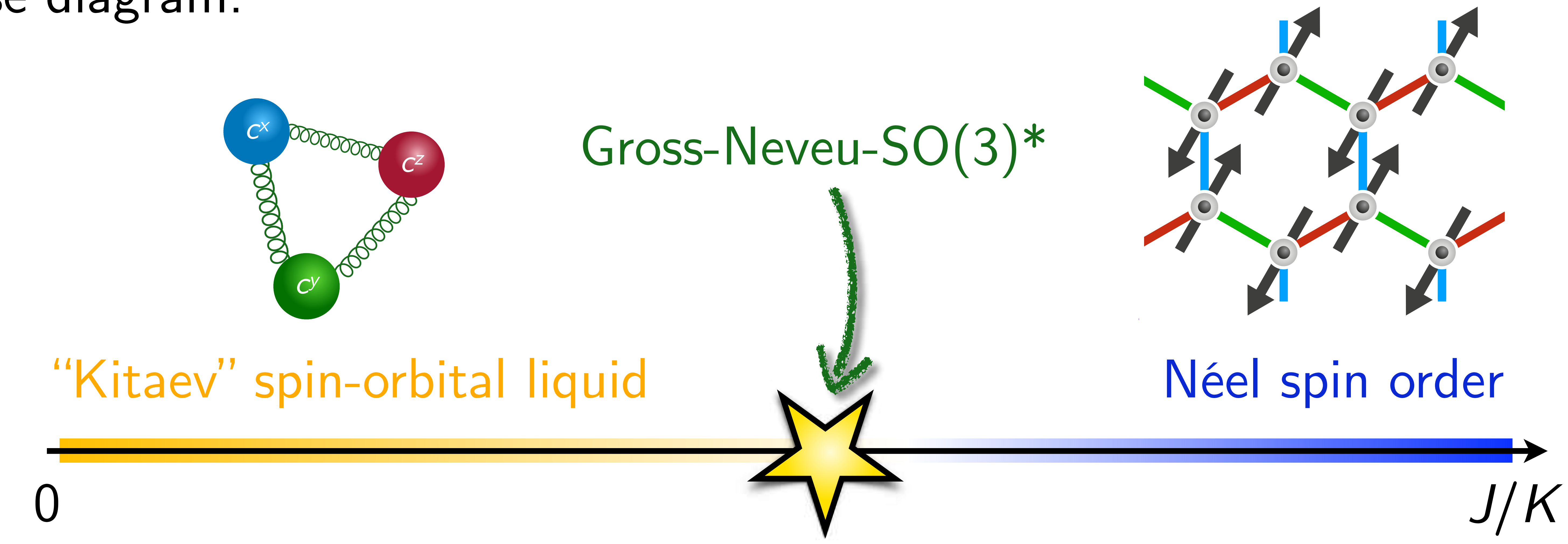
0 flux

Ordered state:

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

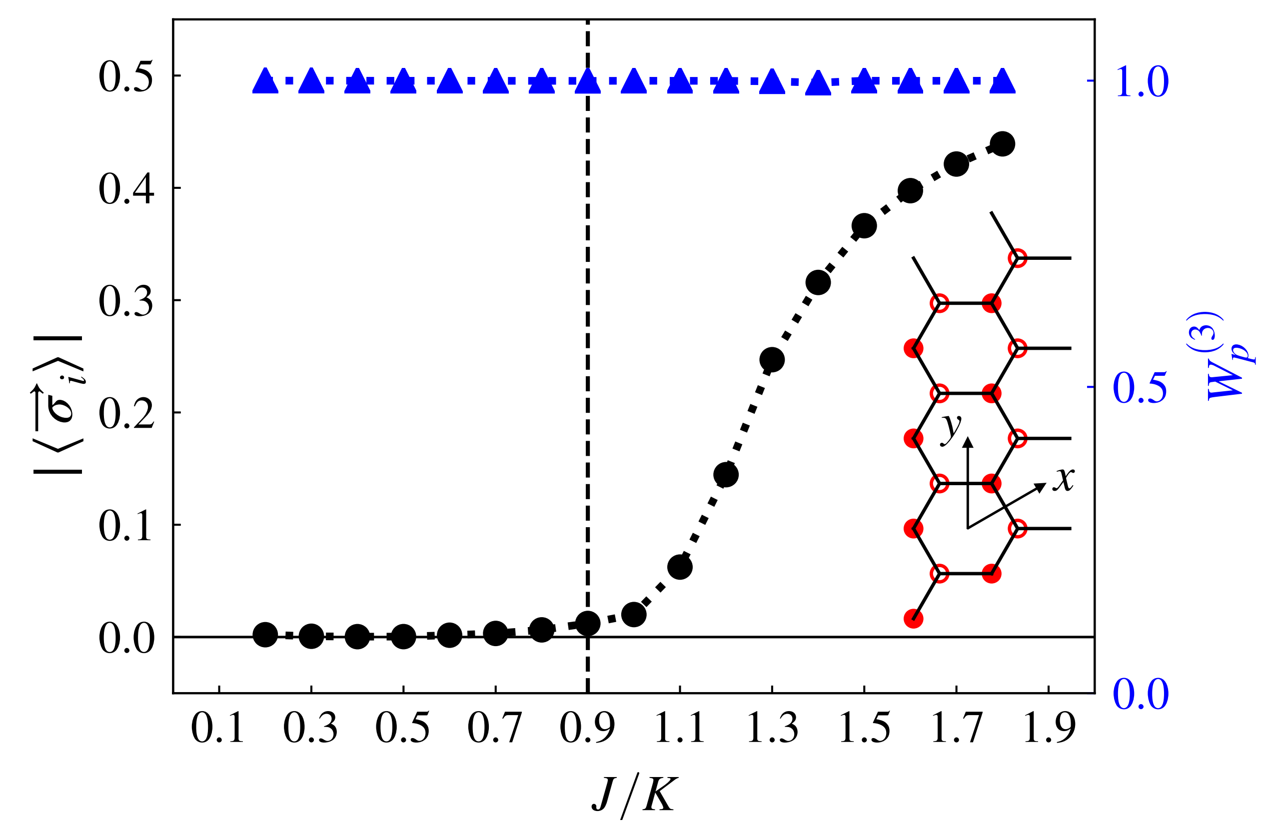
Gross-Neveu-SO(3)* quantum criticality

Phase diagram:



$(J/K)_c = 0.9(2)$

iDMRG:



[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]

Gross-Neveu-SO(3)* quantum criticality

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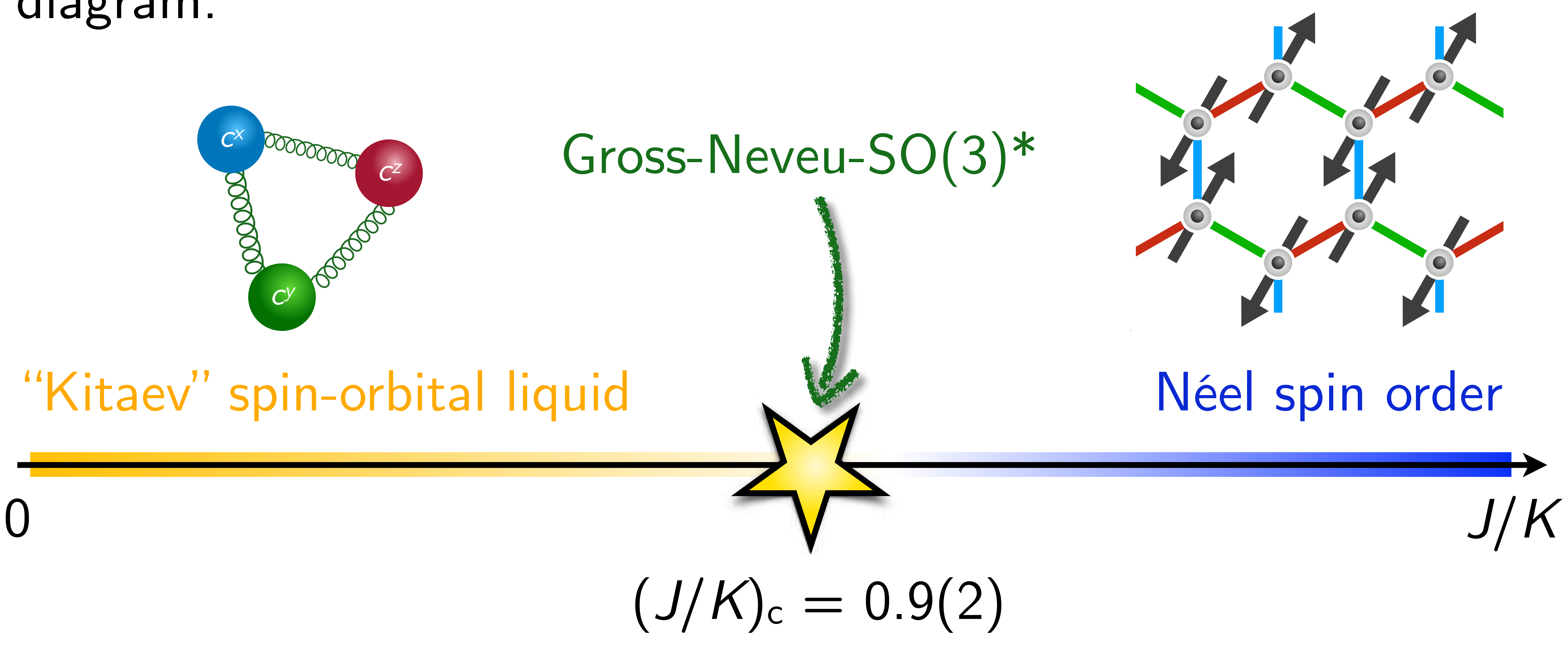
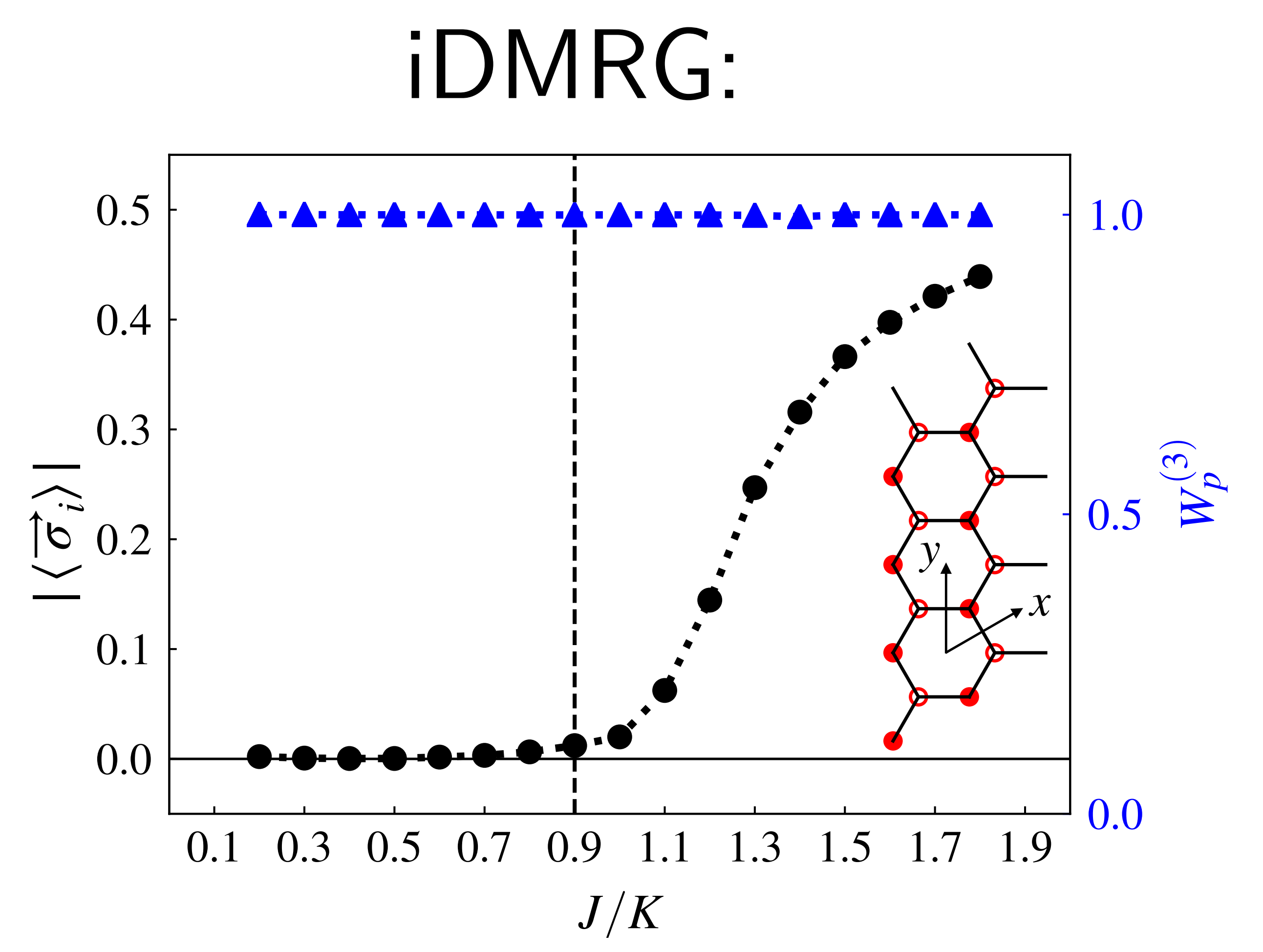




[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]

Effective field theory:

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

"Gross-Neveu-SO(3)"

Critical exponents:

$$1/\nu = 1.03(15)$$
$$\eta_\phi = 0.42(7)$$

... from:

- large-N expansion @ $O(1/N^2)$
- 4-ε expansion @ 3-loop
- functional RG @ LPA'

[Ray, Ihrig, Gracey, Scherer, LJ, PRB '21]

Sign-problem-free QMC: [Liu, Vojta, Assaad, LJ, arXiv:2108.06346]

Outline

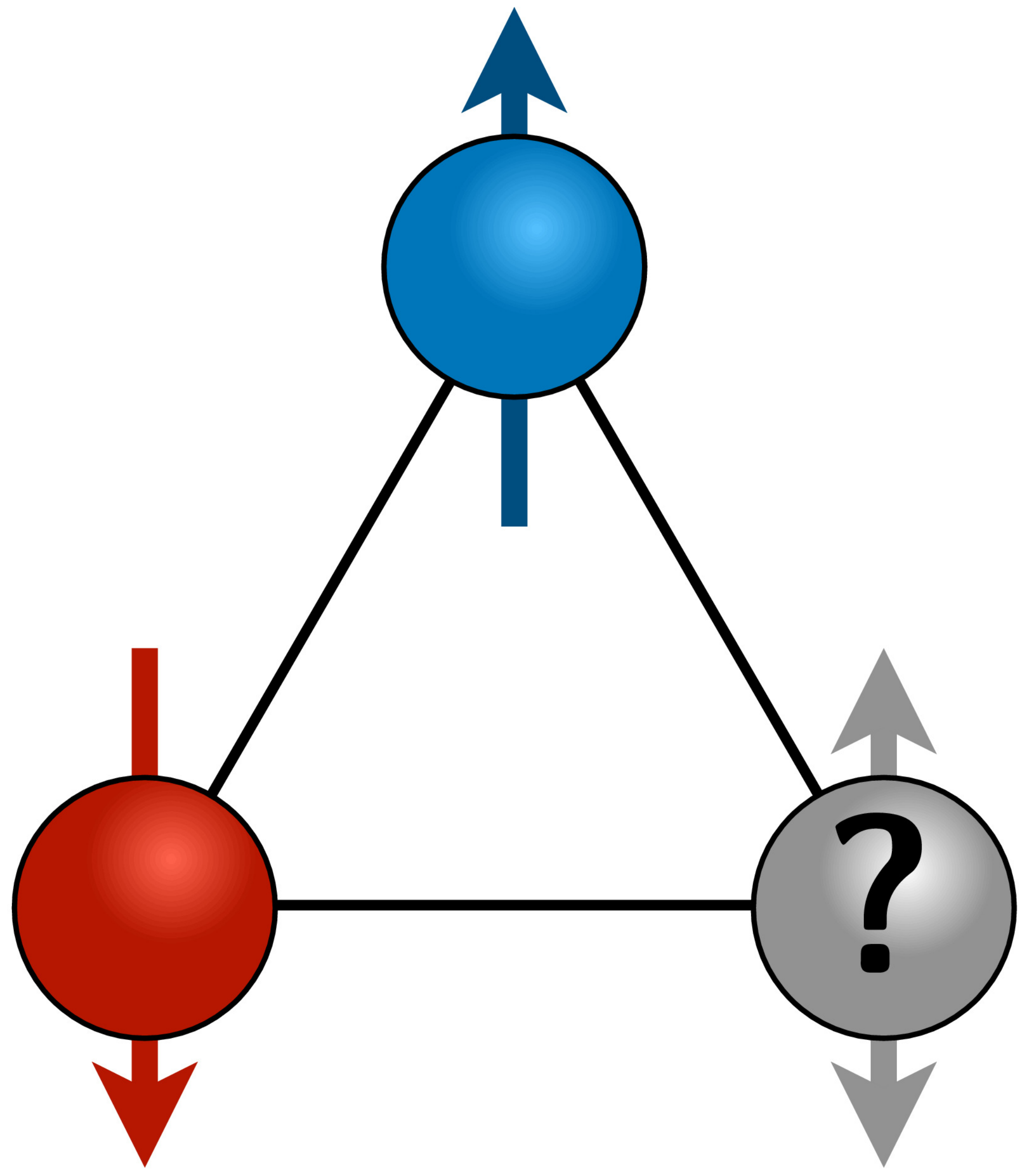
(1) Introduction: *Topological phases of matter*

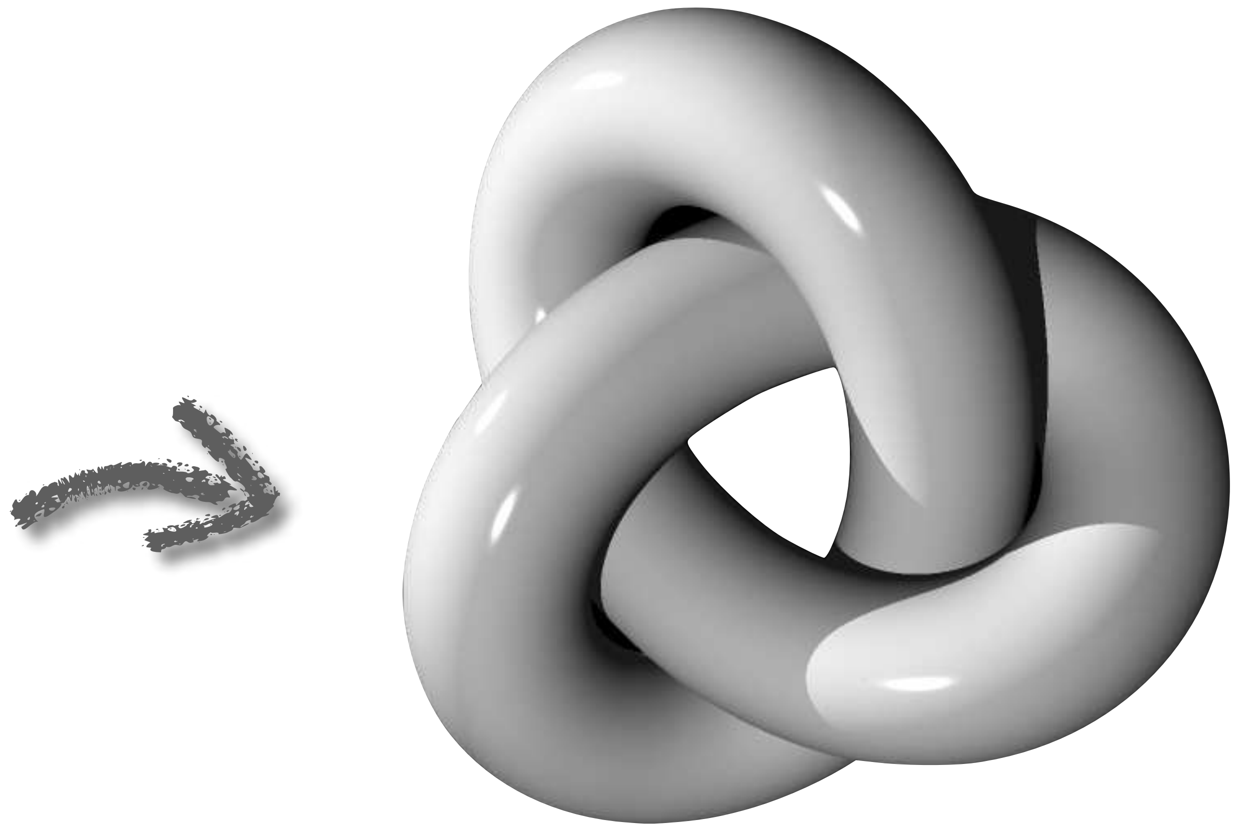
(2) Spin-1/2: *Kitaev honeycomb model*

(3) Spin-3/2: *Generalized Kitaev models*

(4) Conclusions

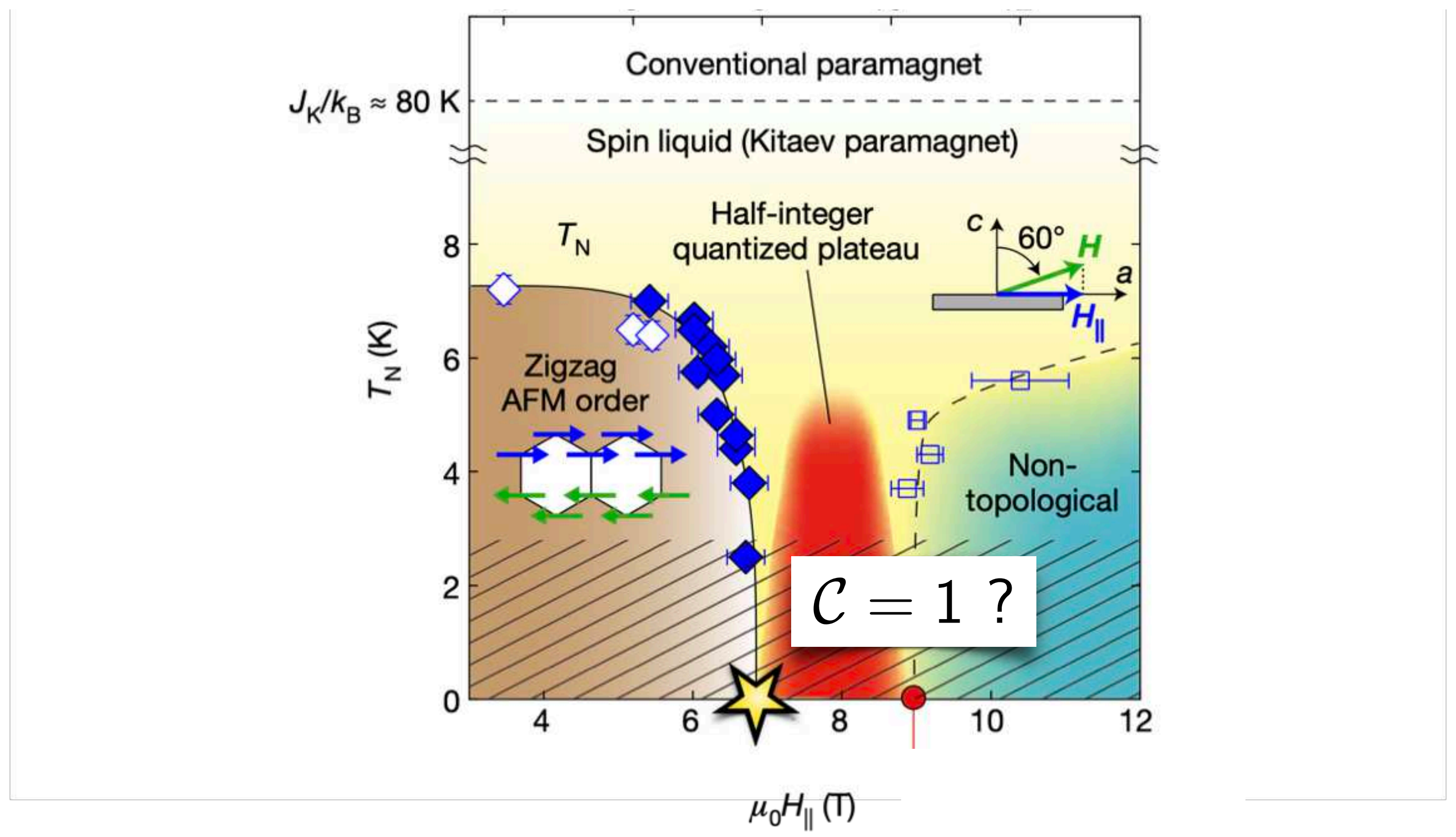
Conclusions



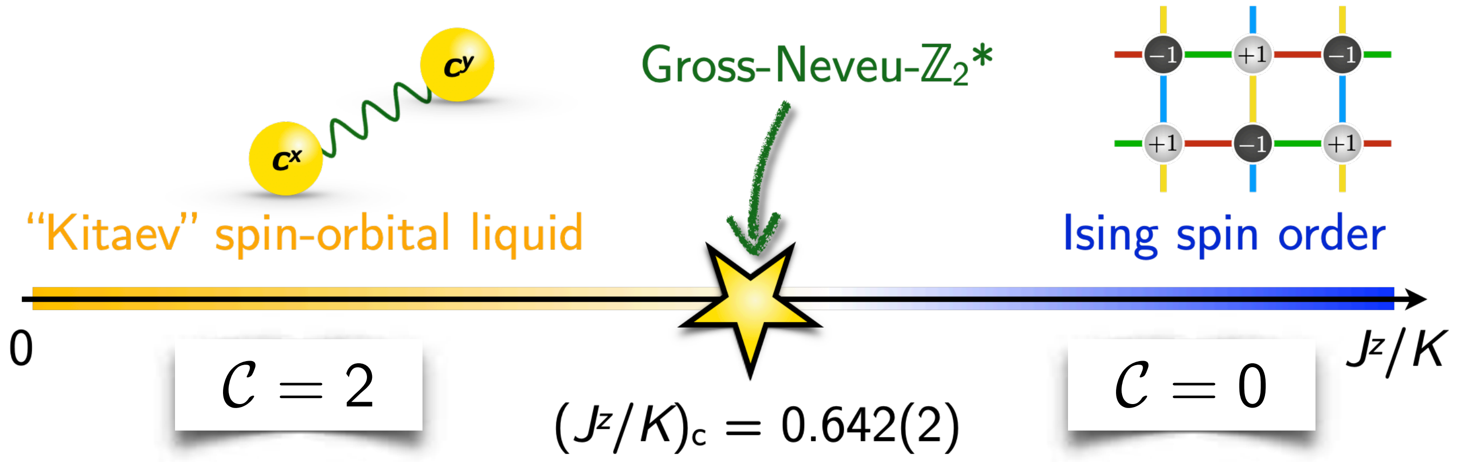


From frustration ... *... to topology*

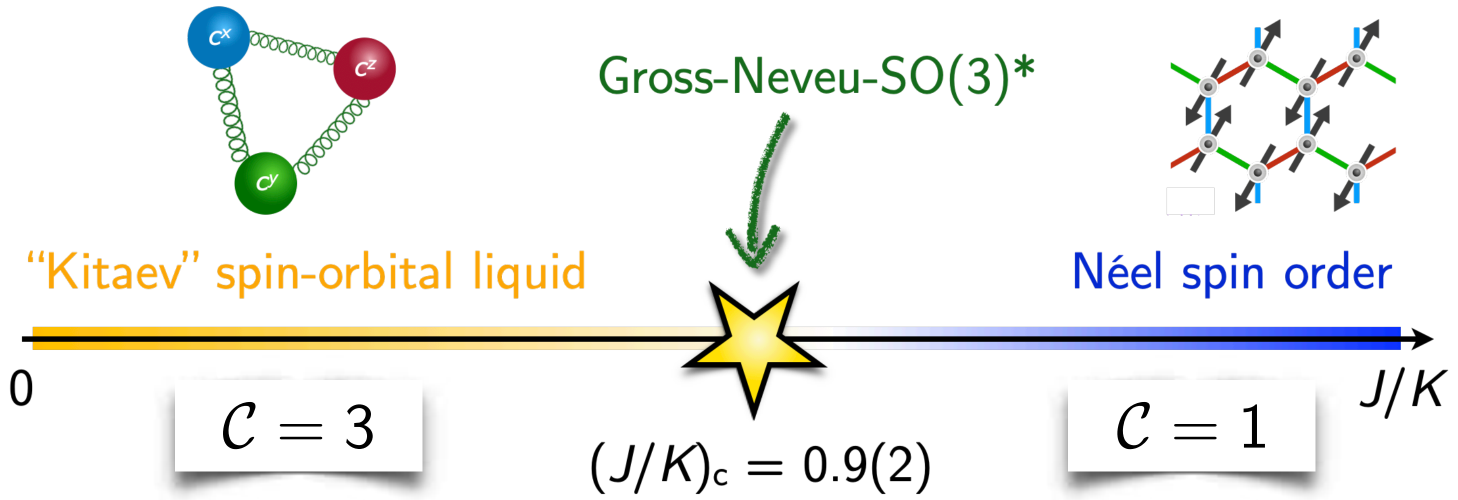
α-$RuCl_3$ in field



Kitaev-Ising spin-orbital model



Kitaev-Heisenberg spin-orbital model

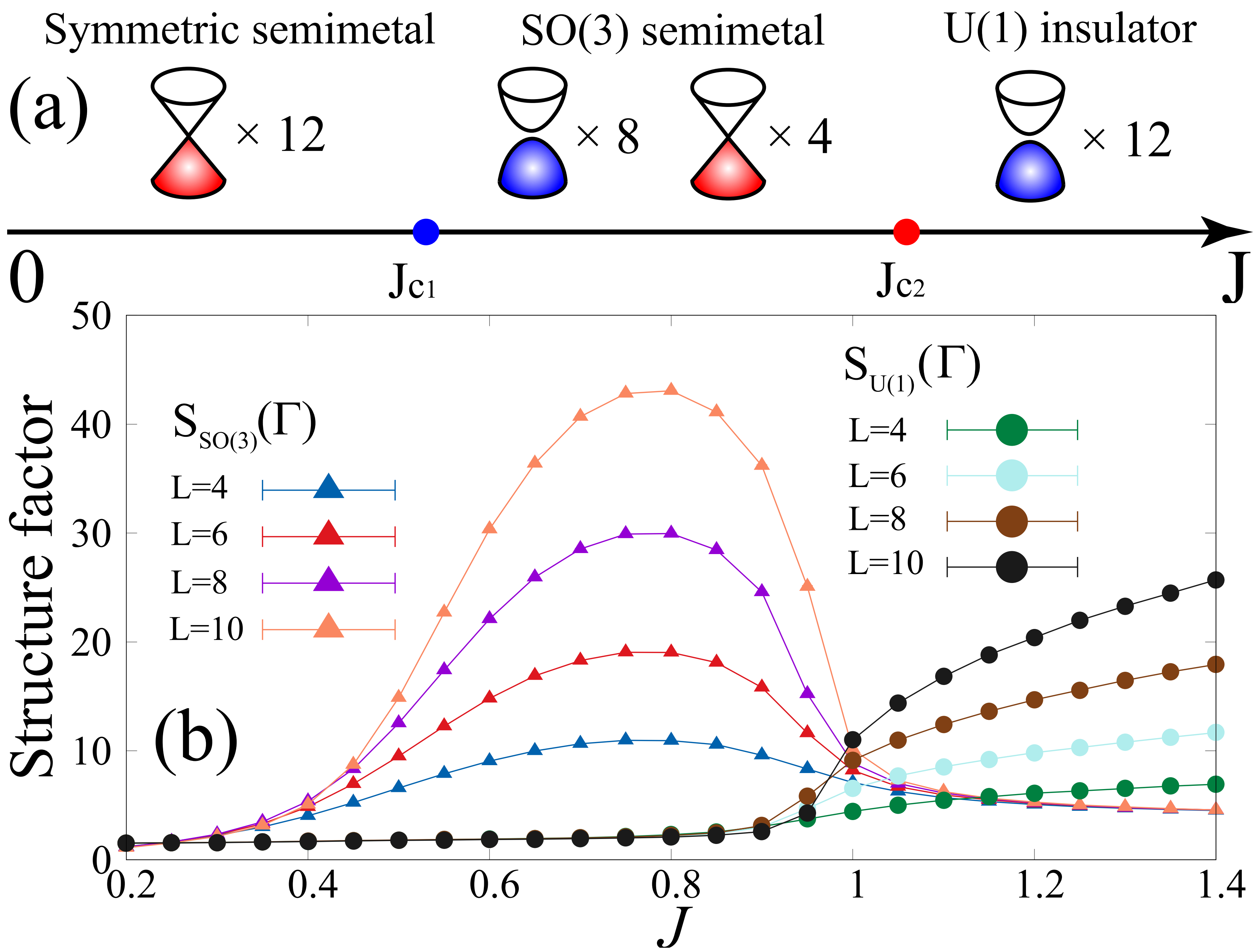


Gross-Neveu-SO(3): Sign-problem-free QMC

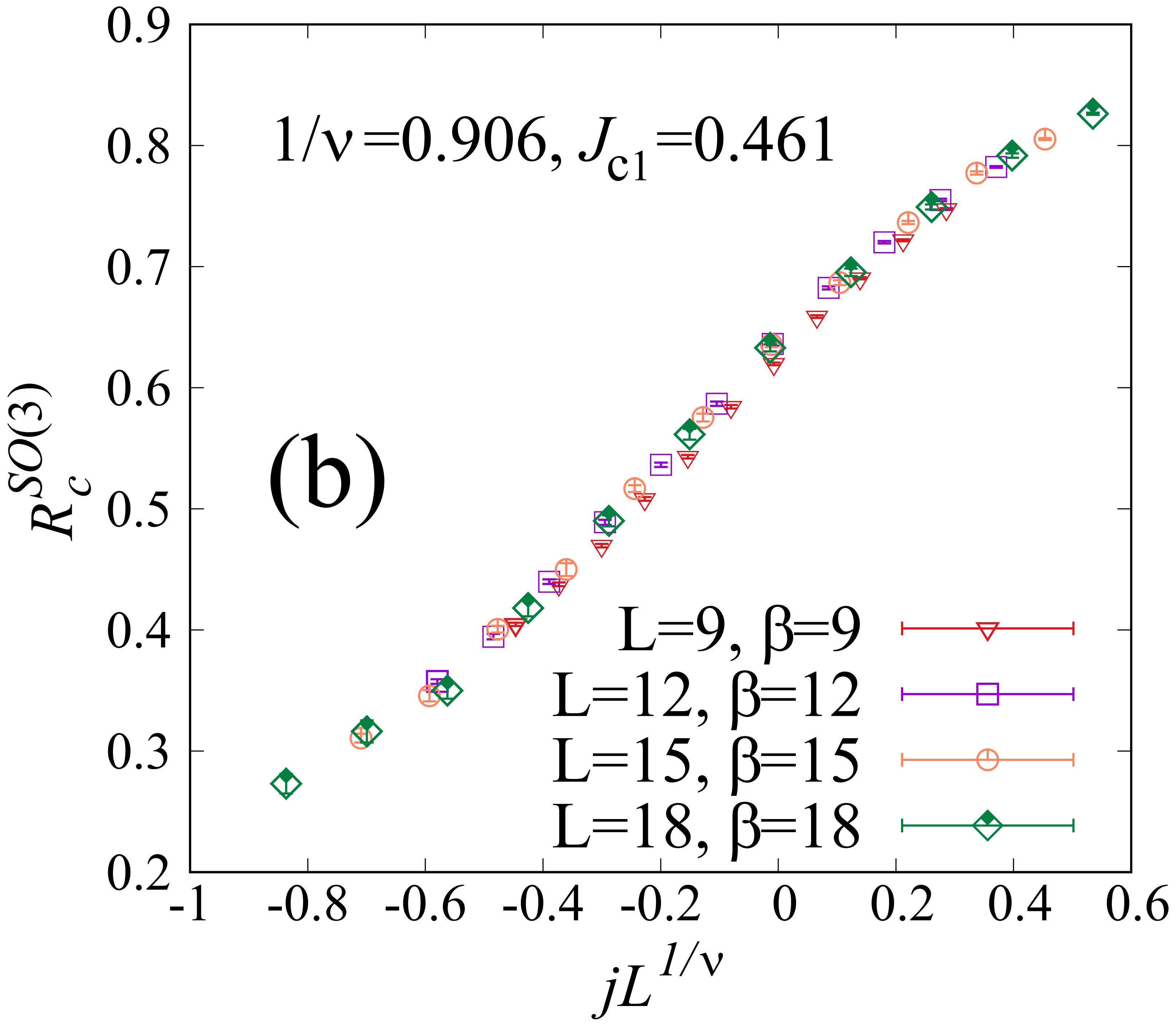
Hamiltonian:

$$H = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} c^{\dagger}_{\boldsymbol{i}\sigma\lambda} c_{\boldsymbol{j}\sigma\lambda} - J \sum_{\boldsymbol{i}\alpha} \left(c^{\dagger}_{\boldsymbol{i}\sigma\lambda} K^{\alpha}_{\sigma\sigma'} \tau^{z}_{\lambda\lambda'} c_{\boldsymbol{i}\sigma'\lambda'} \right)^2$$

Phase diagram:



Finite-size scaling collapse:



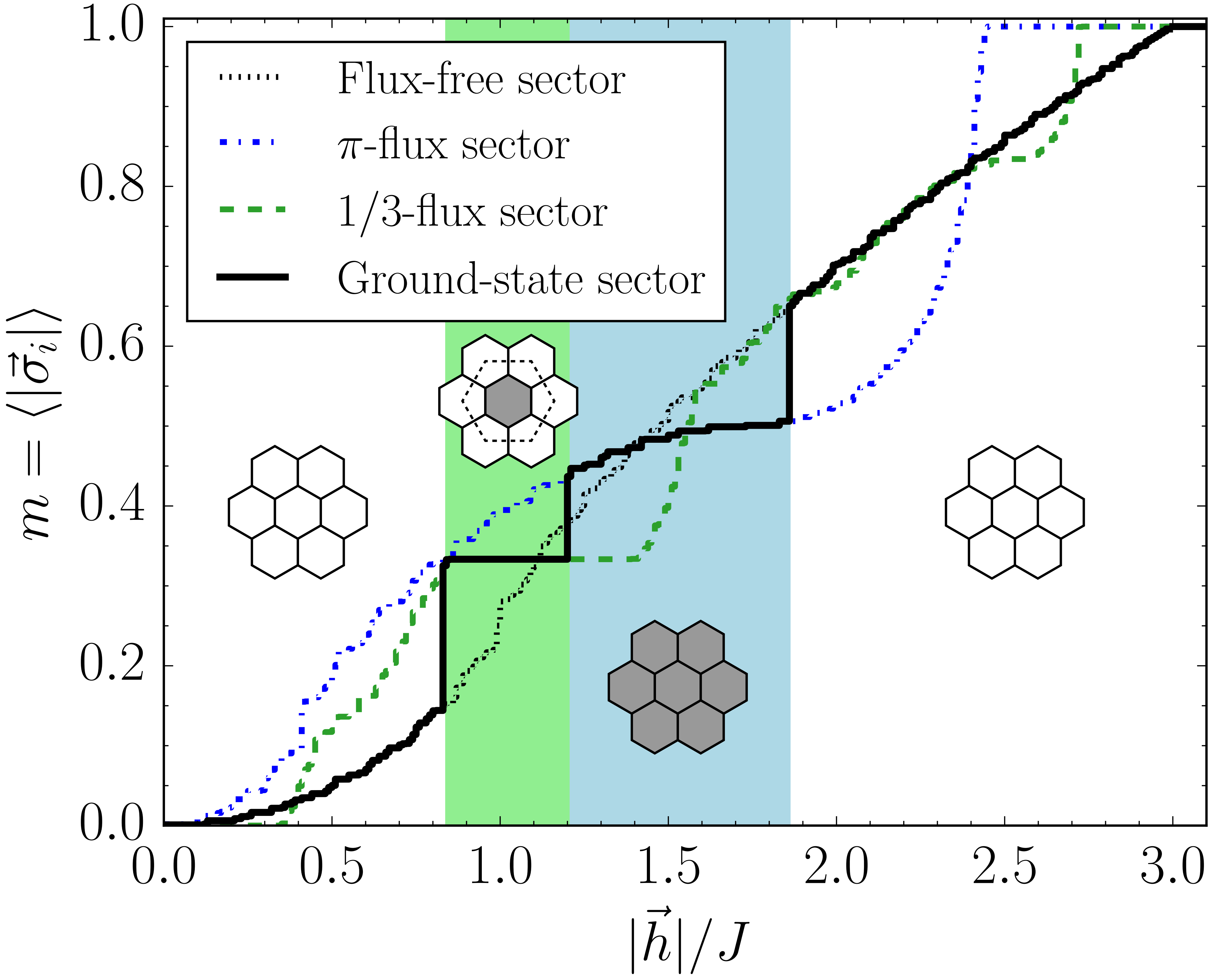
[Liu, Vojta, Assaad, LJ, arXiv:2108.06346]

Spin-orbital model in external magnetic field

Hamiltonian:

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

Magnetization:



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*

Transverse-field Ising:

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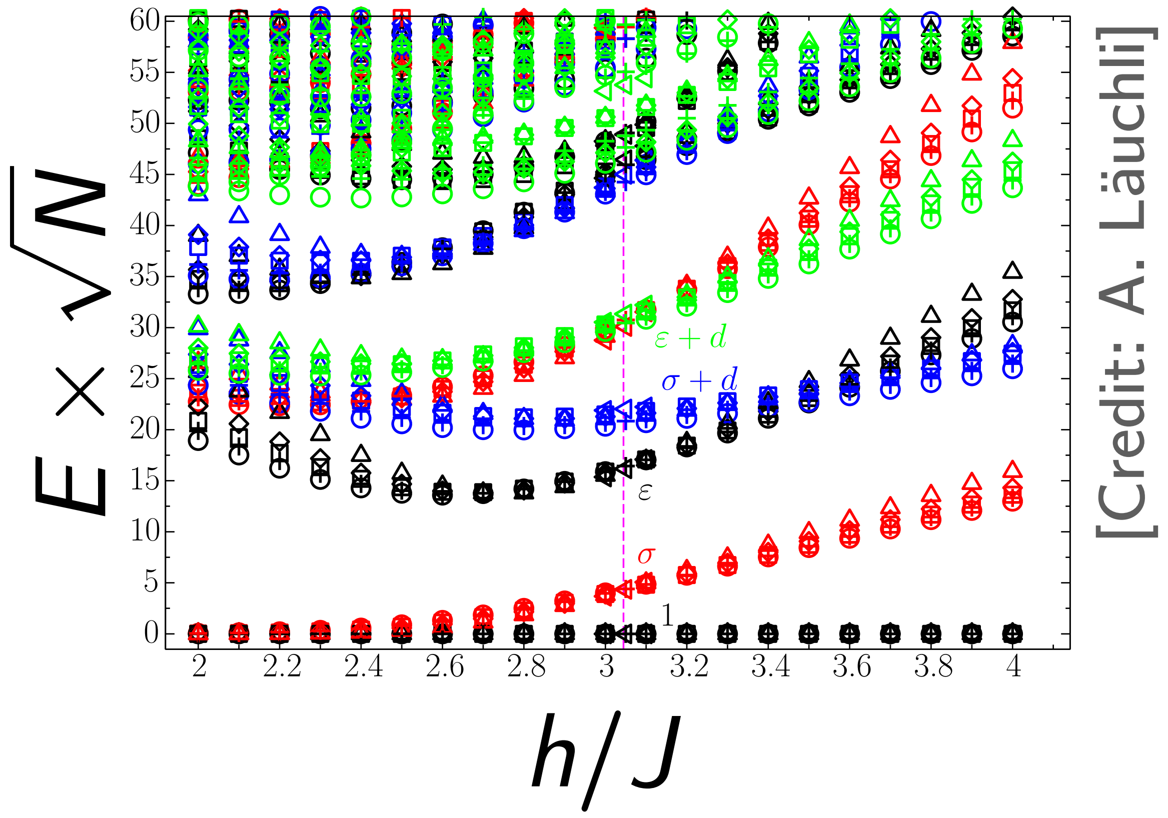
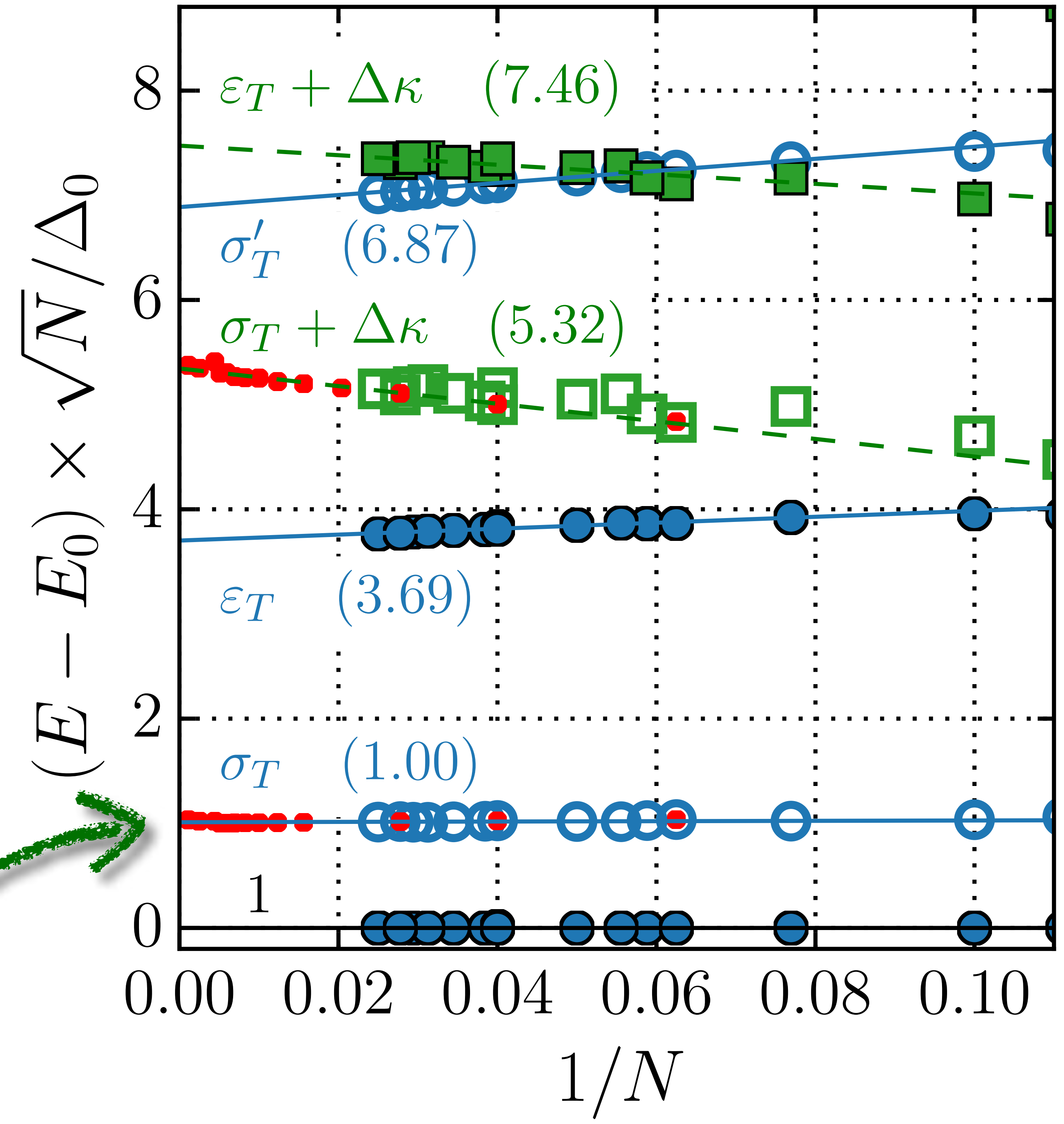
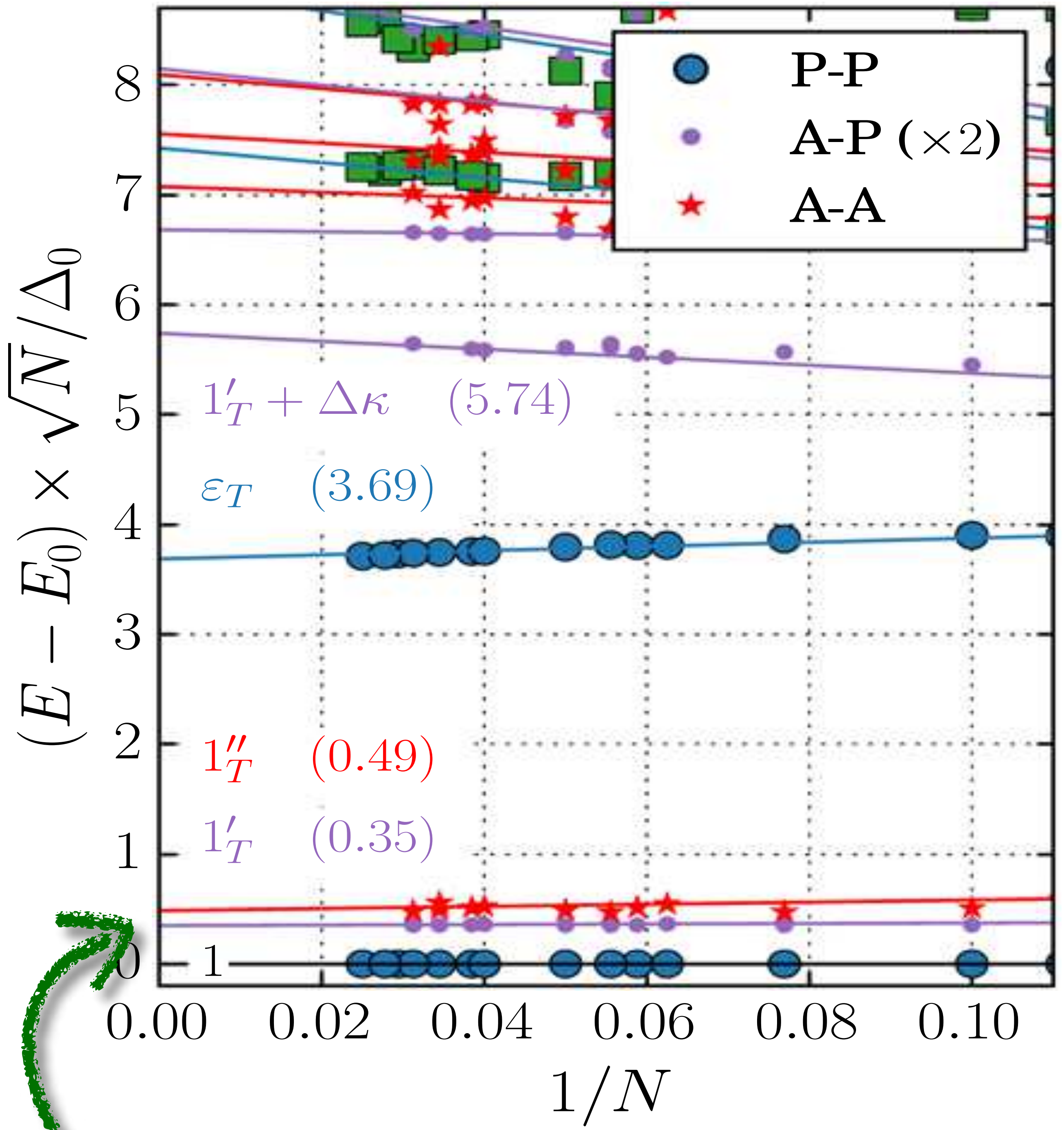


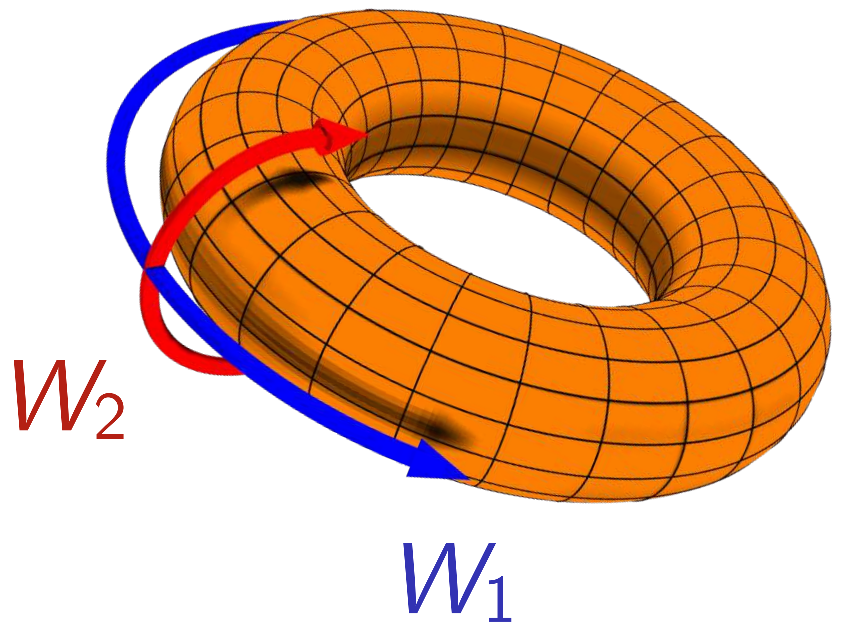
Ising
$h = h_c$



missing in Ising*

Ising*
$h = h_c$

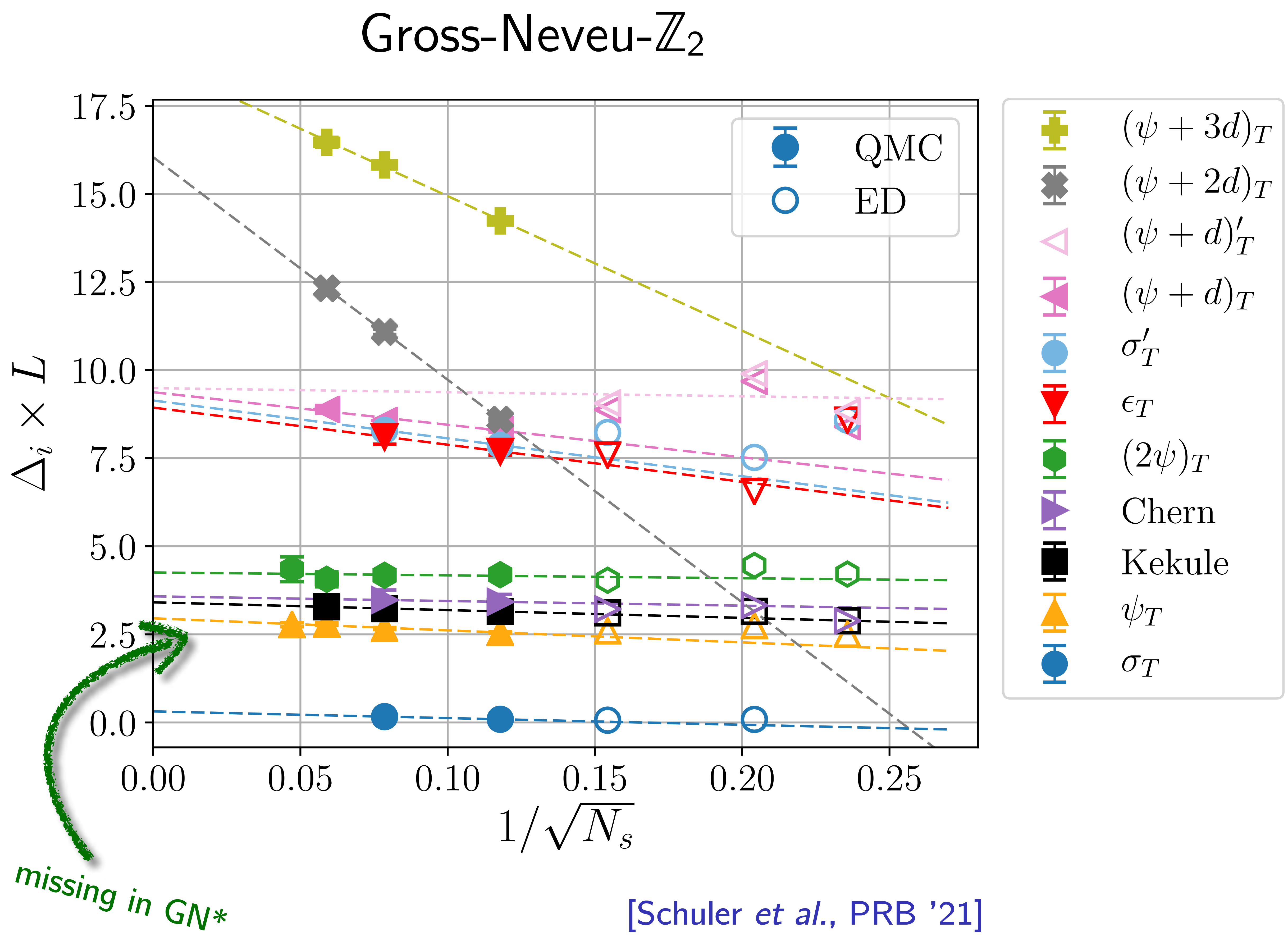




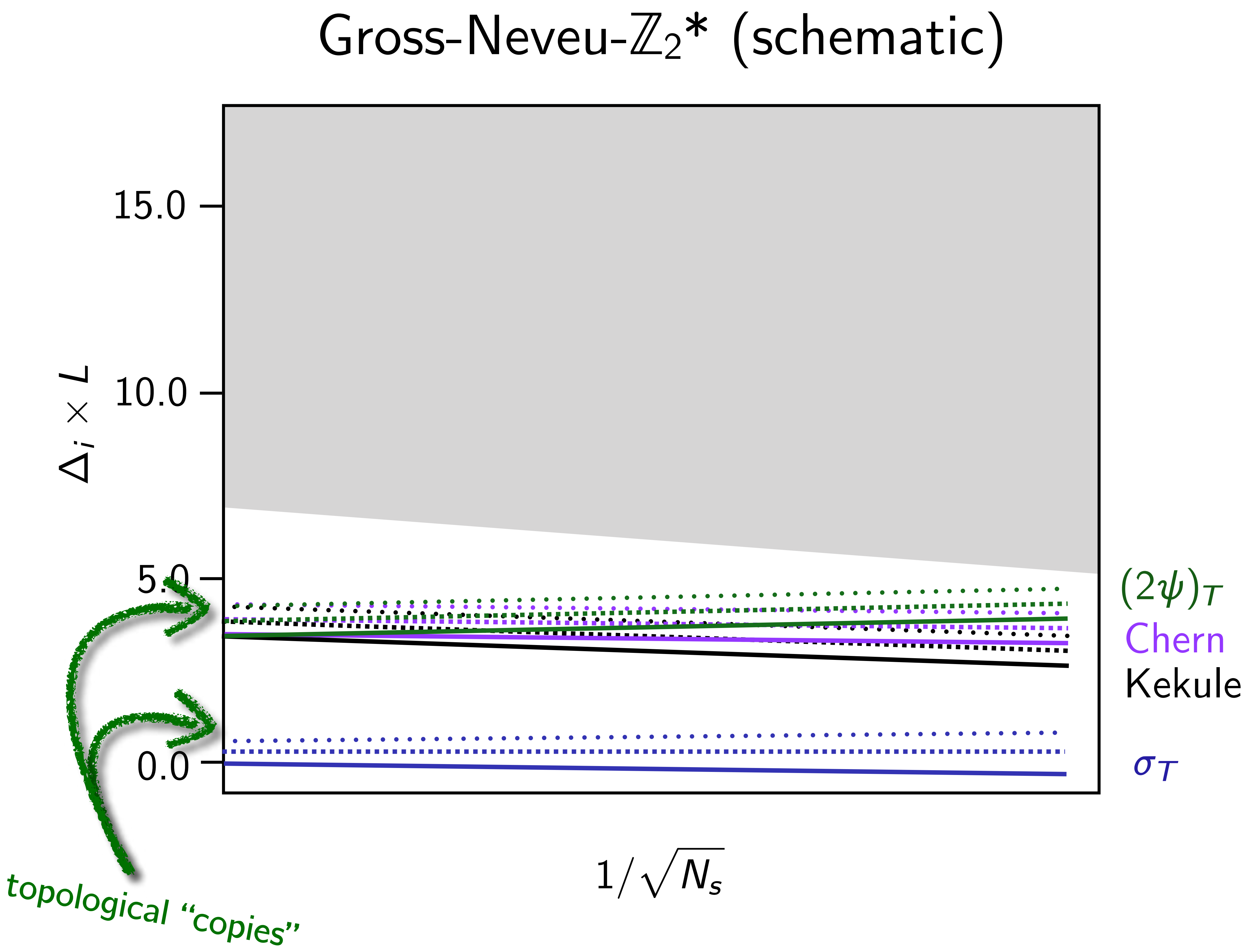
topological “copies”

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

Gross-Neveu vs Gross-Neveu*



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



... testable in future simulations

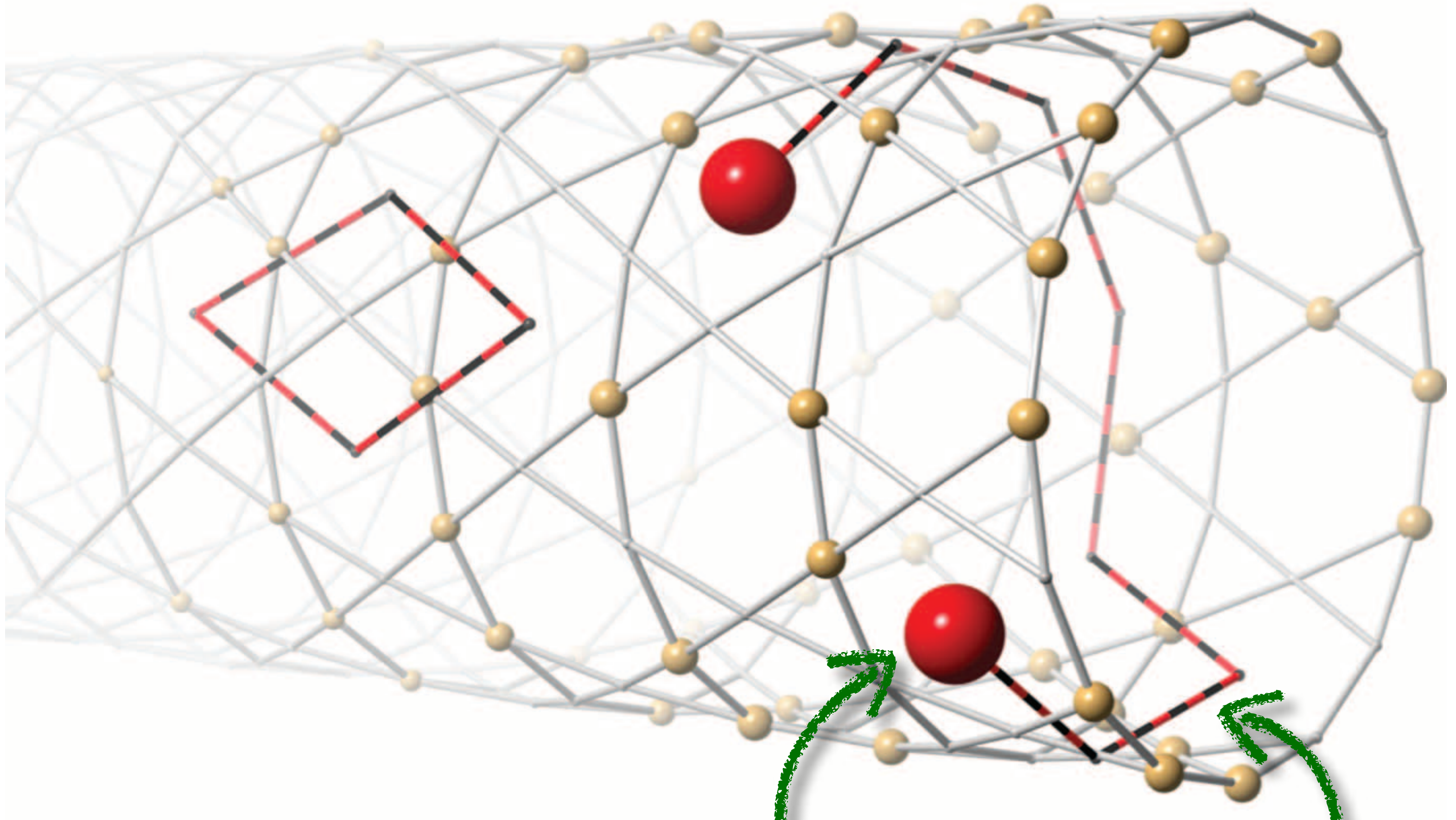
Fractionalized quantum criticality: XY*

Bose-Hubbard-like model (kagome lattice):

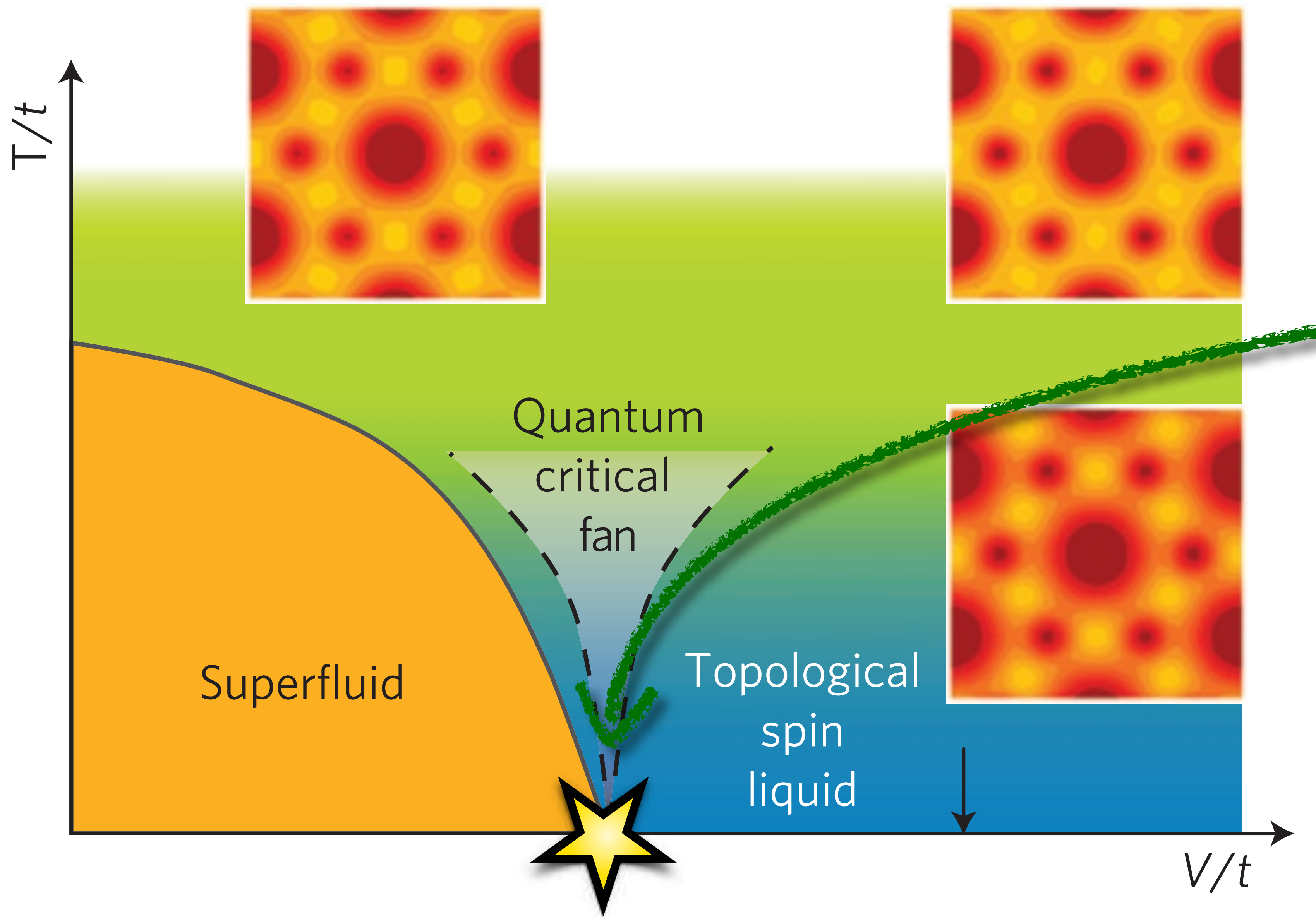
$$\mathcal{H} = -t \sum_{\langle ij \rangle} \left[b_i^\dagger b_j + b_i b_j^\dagger \right] + V \sum_{\hexagon} (n_{\hexagon})^2$$

Hopping bosons

Boson density in plaquette

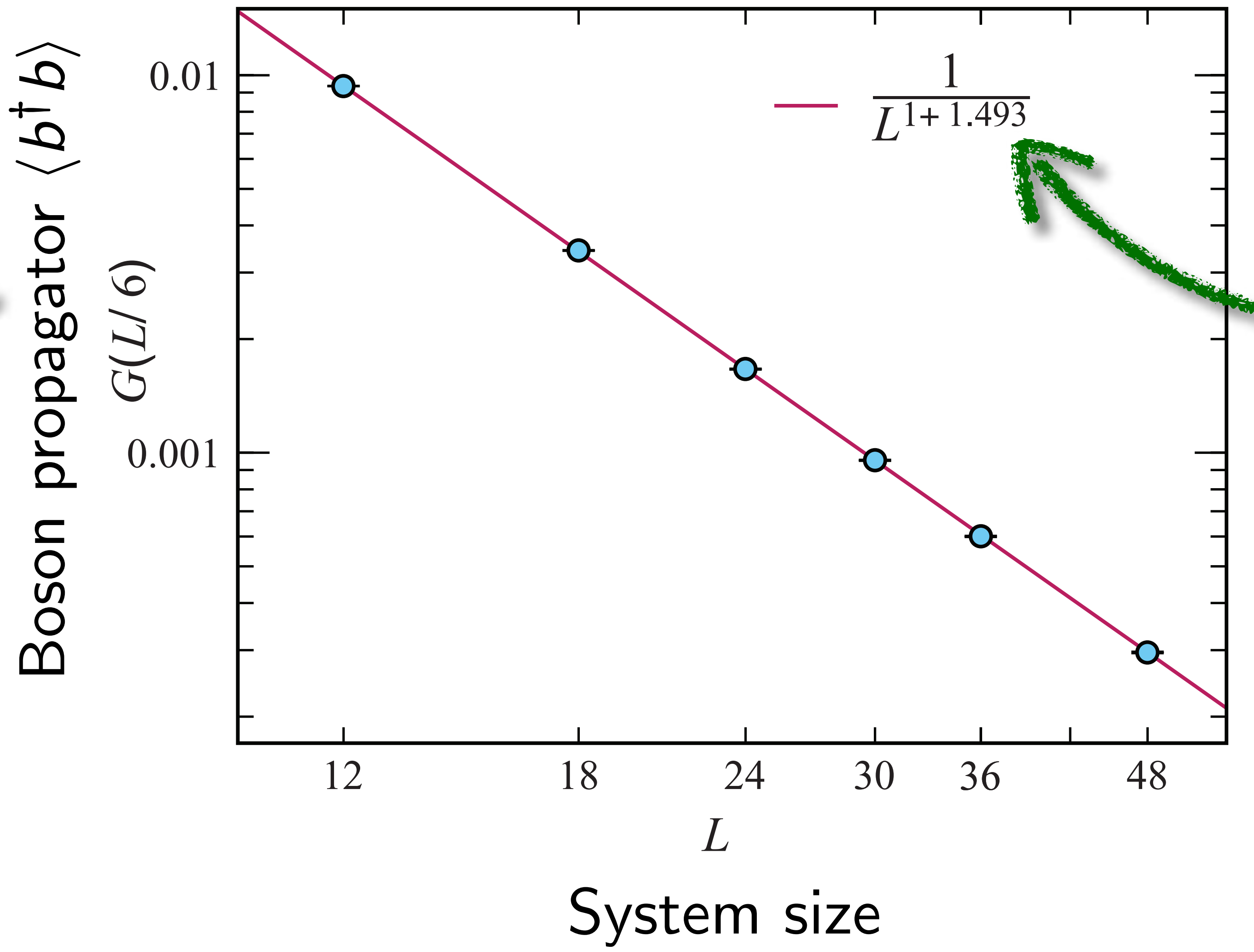


Phase diagram:



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

$V/t = (V/t)_c$



$\eta \approx 1.493$ (!)

... anomalous dimension of composite field

but $\nu \approx 0.67$

... as in conventional XY

[Isakov, Melko, Hastings, Science '12]

[Chubukov, Senthil, Sachdev, PRL '94]