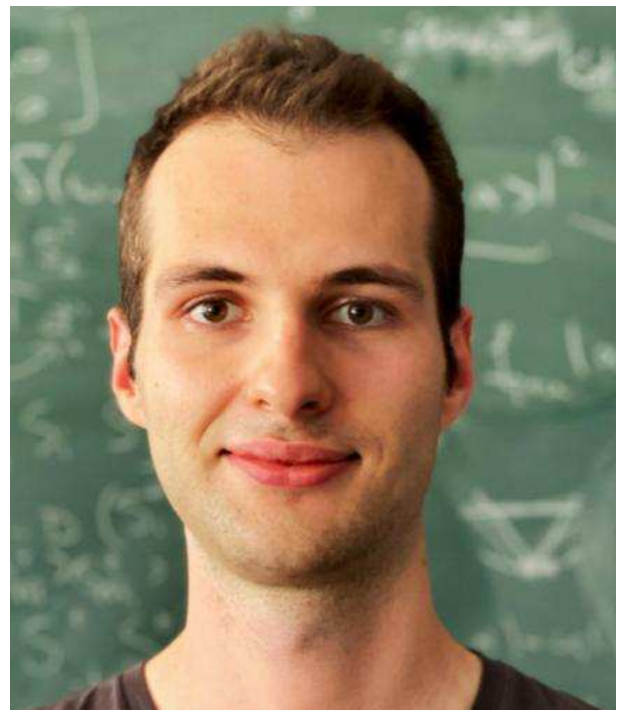
Fractionalized fermionic quantum criticality

Lukas Janssen
TU Dresden



Urban Seifert, Santa Barbara

Zihong Liu, Würzburg

Fakher Assaad, Würzburg
Sreejith Chulliparambil, Dresden
Xiao-Yu Dong, Ghent
Hong-Hao Tu, Dresden
Matthias Vojta, Dresden

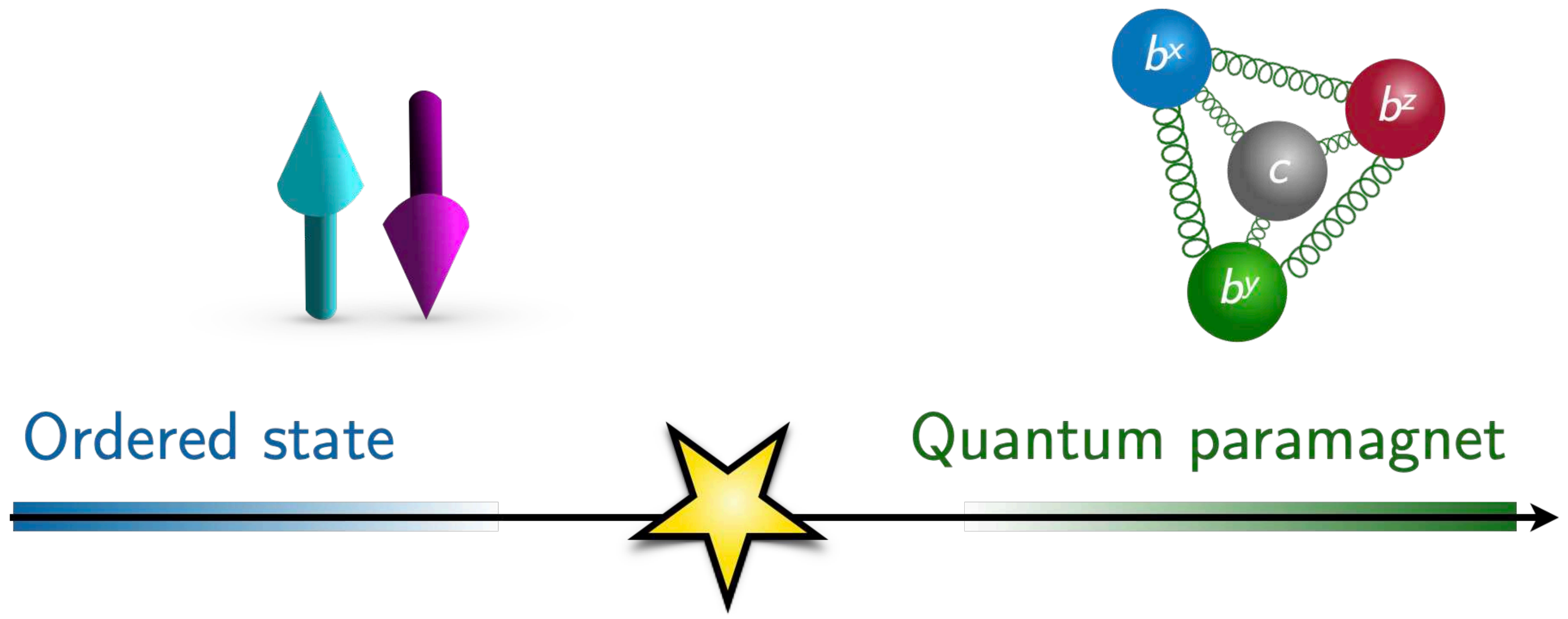
Emmy Noether-Programm
JA 2306/4-1
DFG Deutsche Forschungsgemeinschaft

ct.qmat
Complexity and Topology in Quantum Matter
Würzburg-Dresden Cluster of Excellence

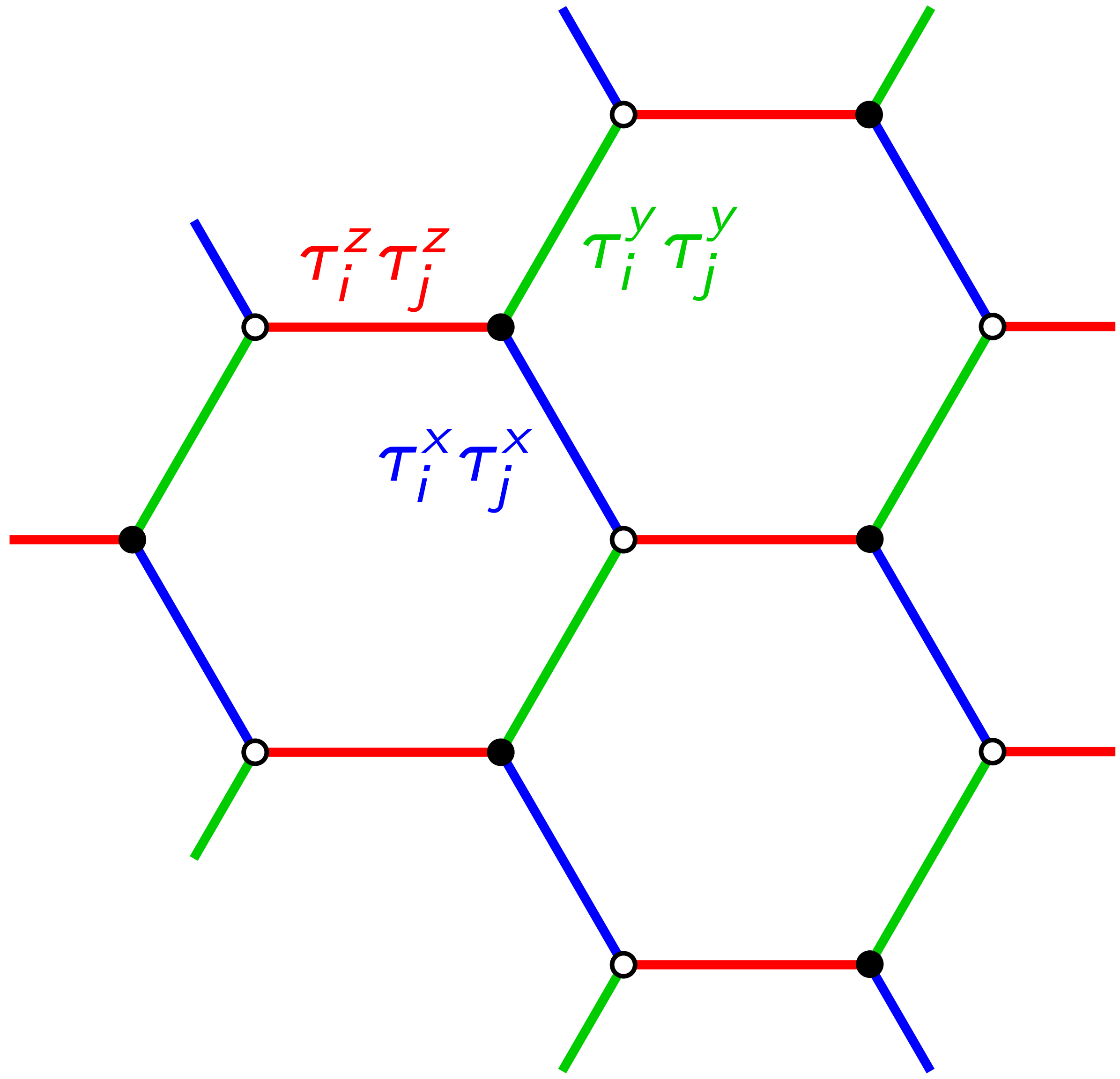
SFB 1143

Outline

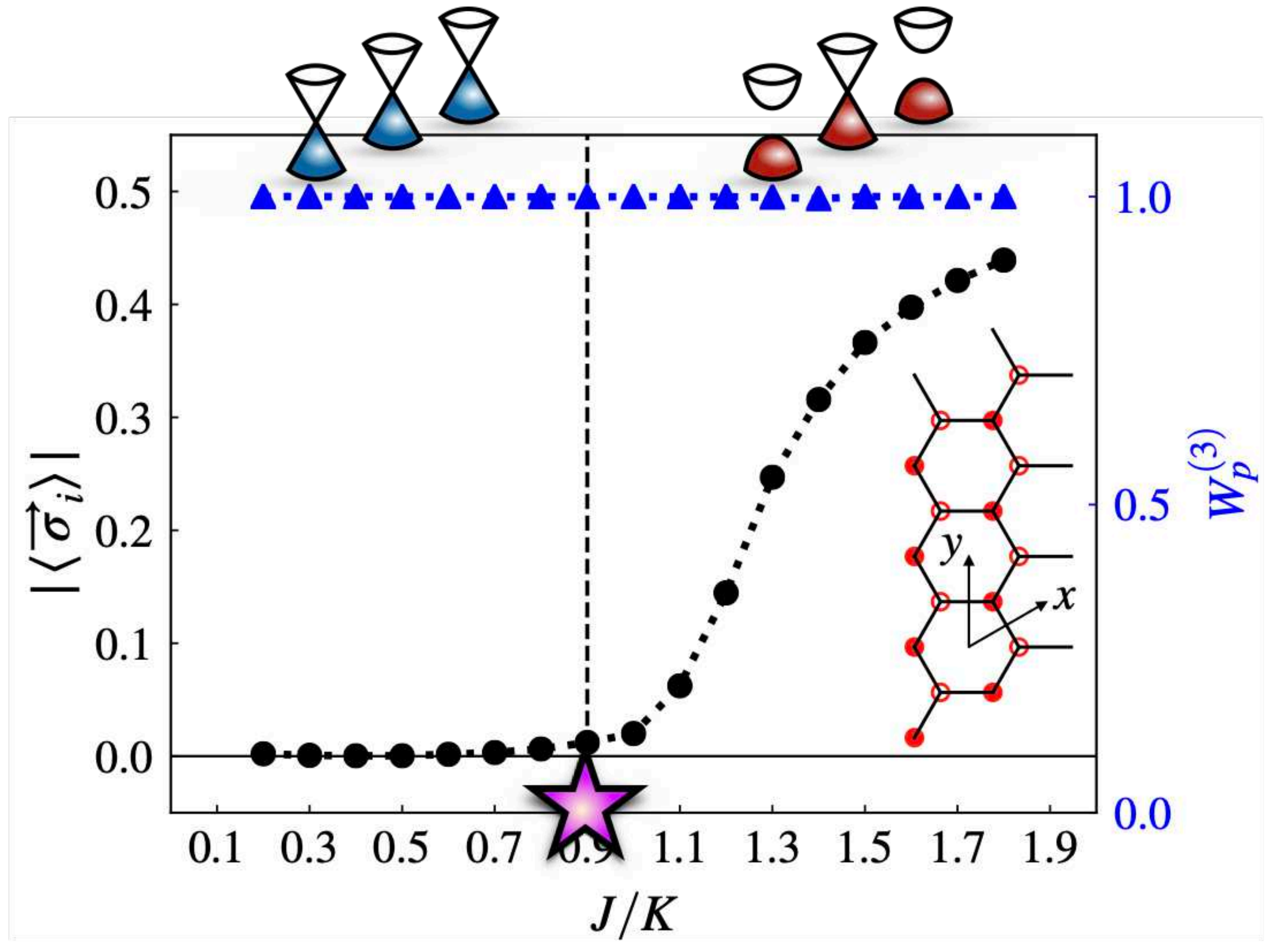
(1) Fractionalized quantum criticality



(2) From Kitaev to Kitaev-Kugel-Khomskii



(3) Kitaev-Heisenberg spin-orbital models



(4) Conclusions

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

Outline

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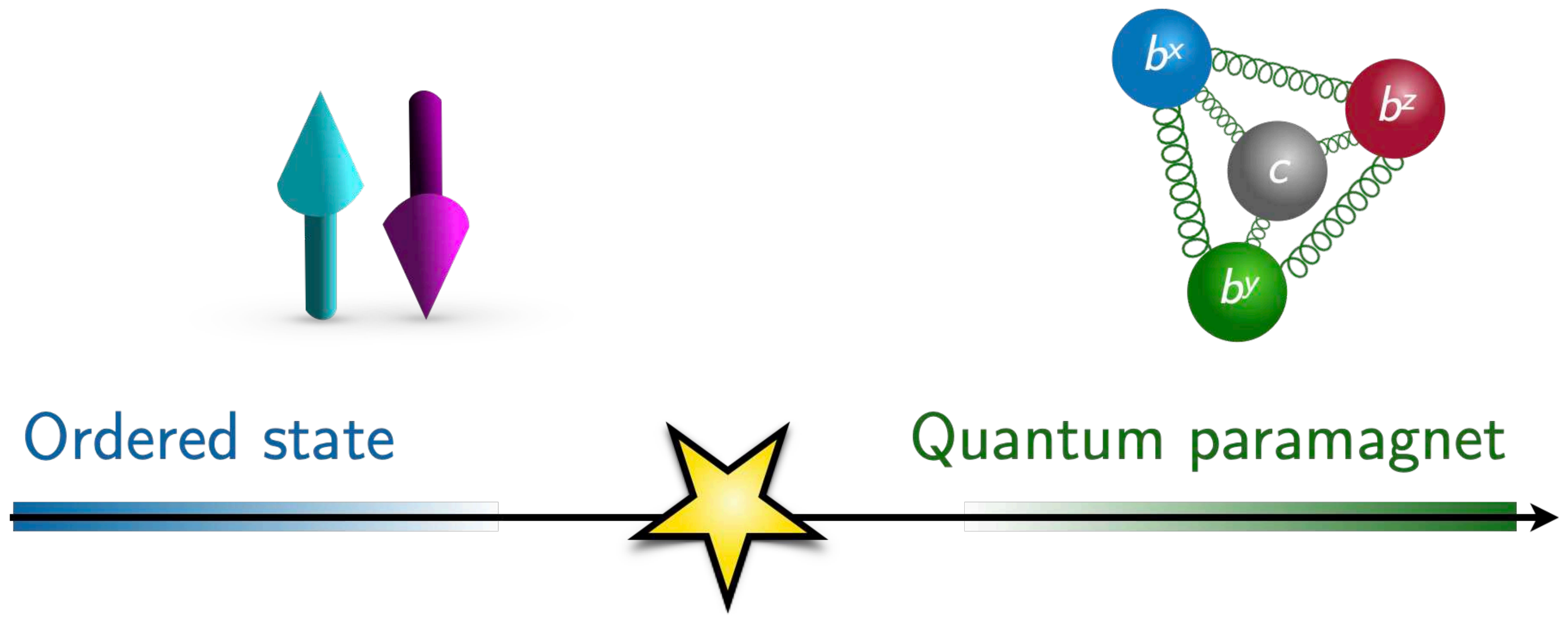

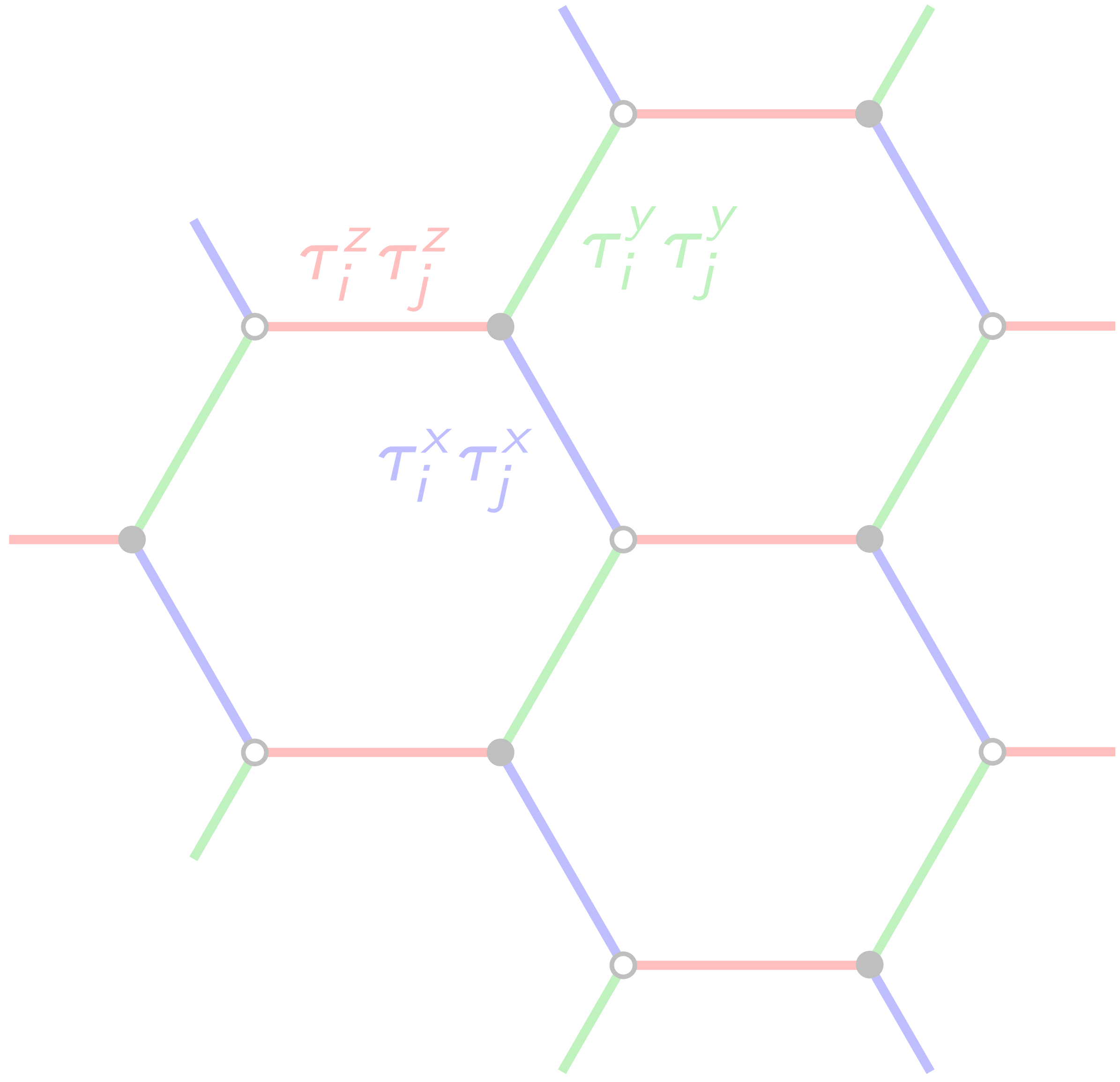

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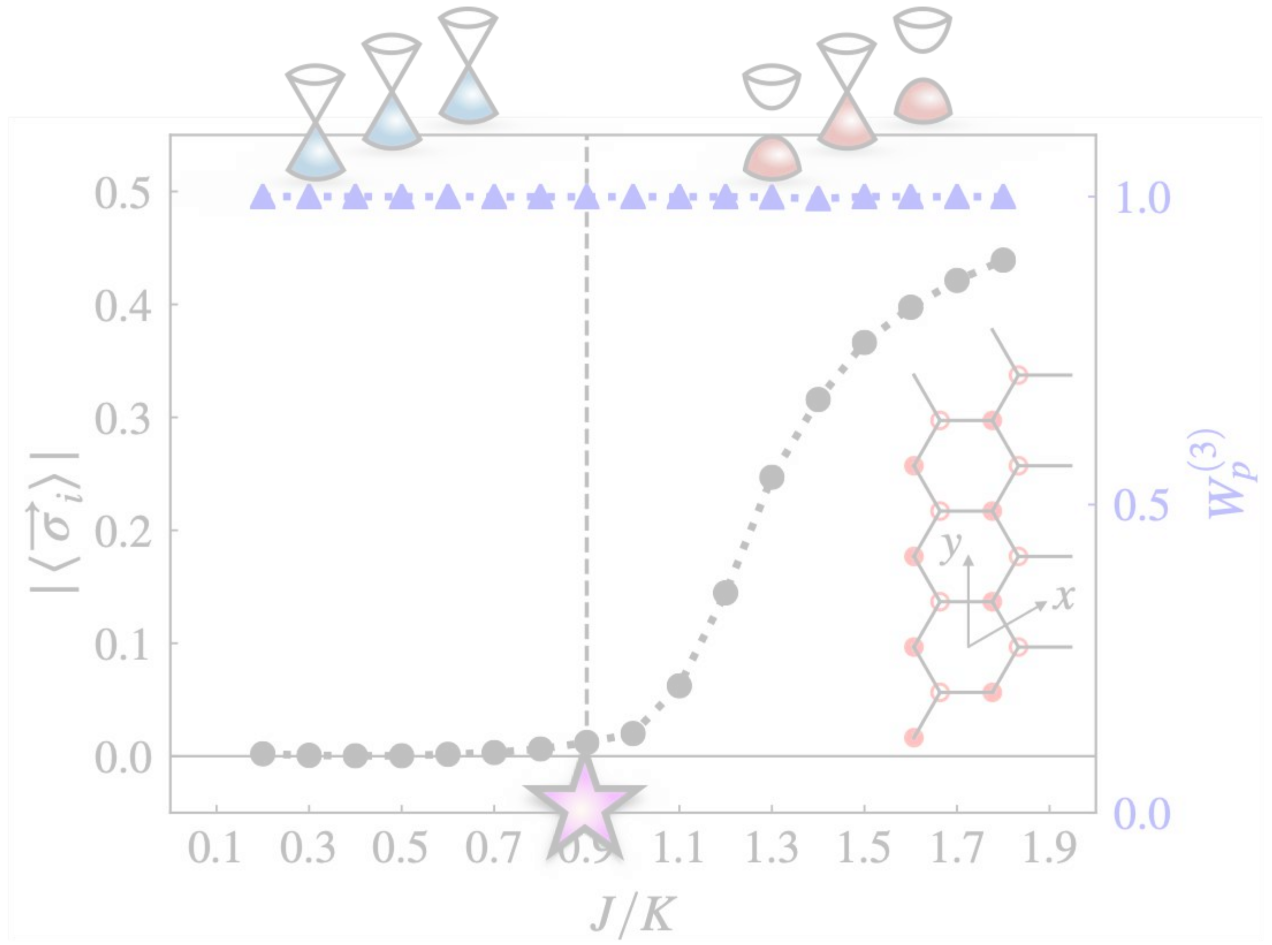
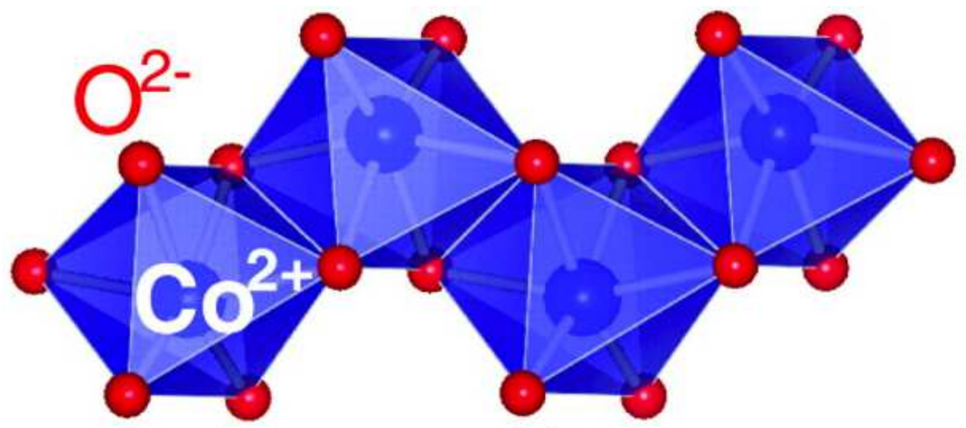


(4) Conclusions

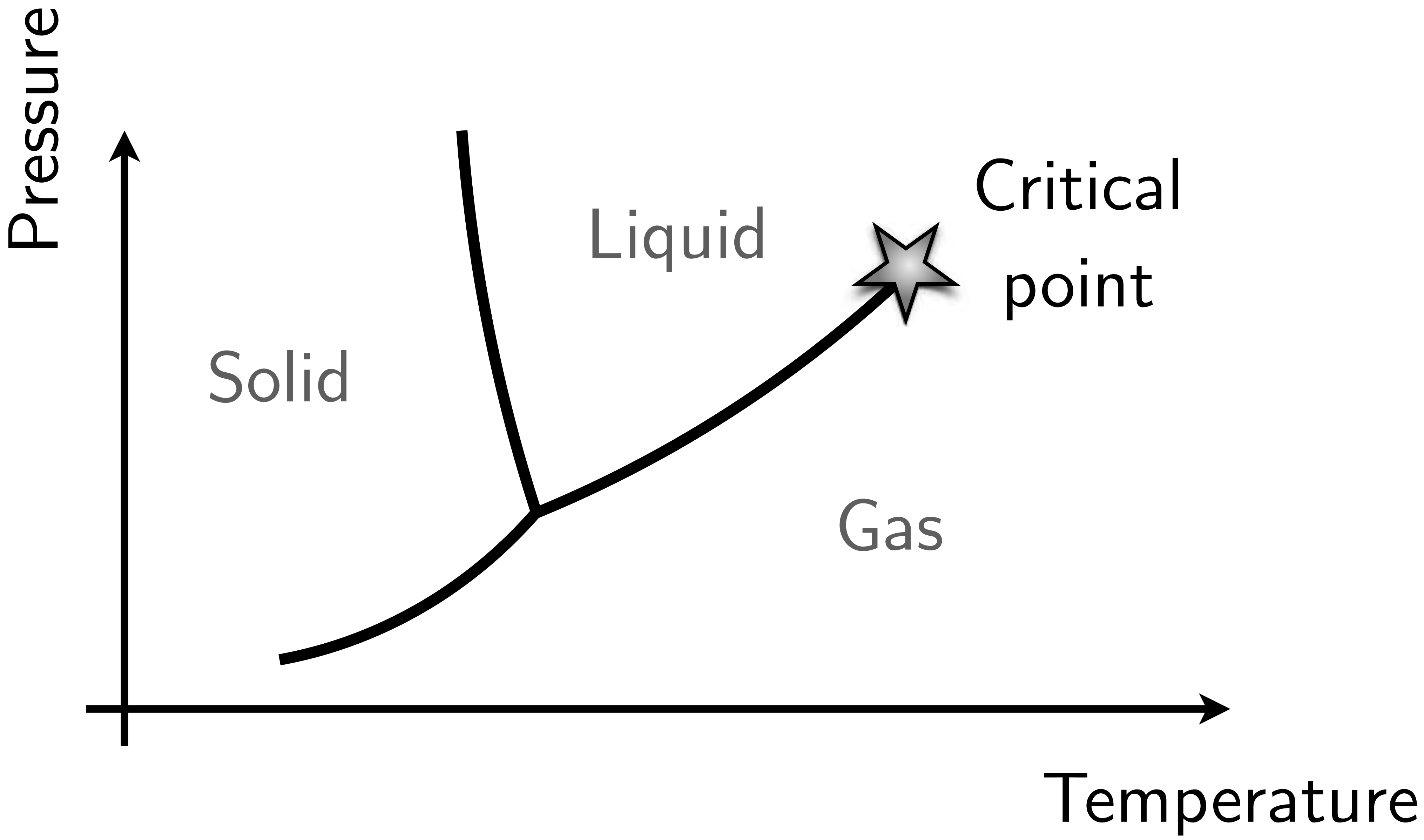
Slides available on https://tu-dresden.de/physik/qcm/vortraege

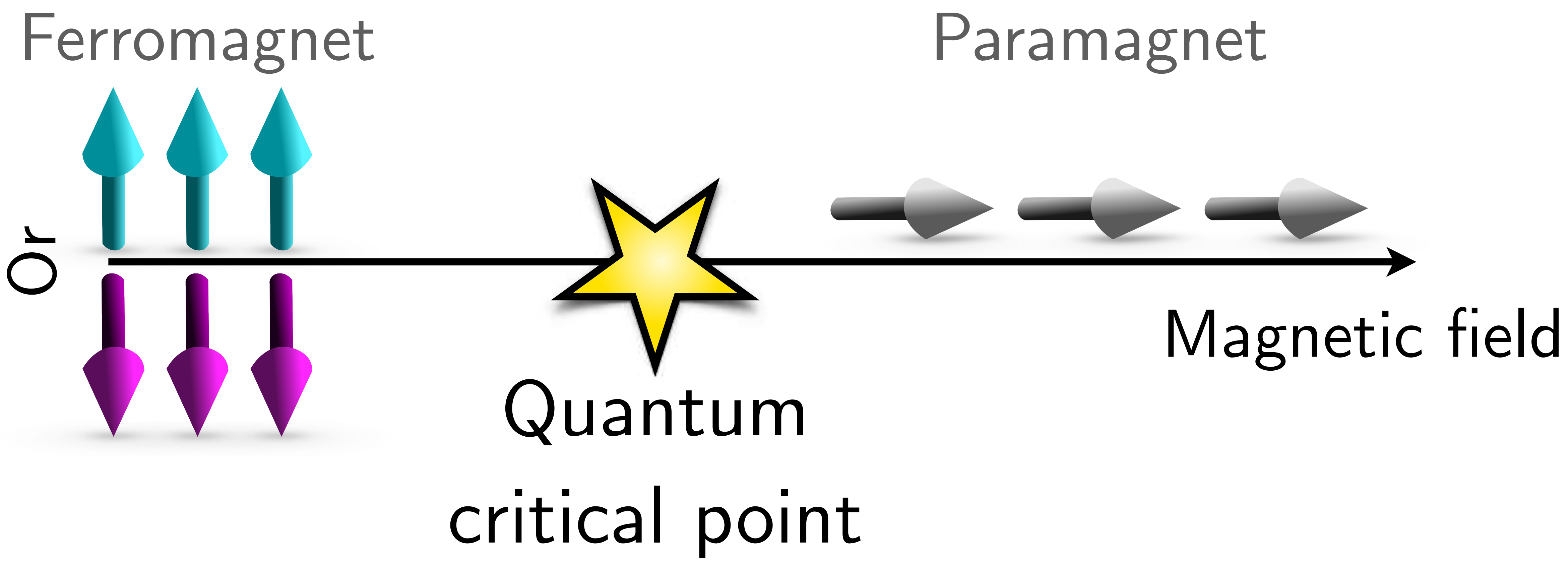
Classical vs quantum criticality



H_2O $\boldsymbol{T > 0}$

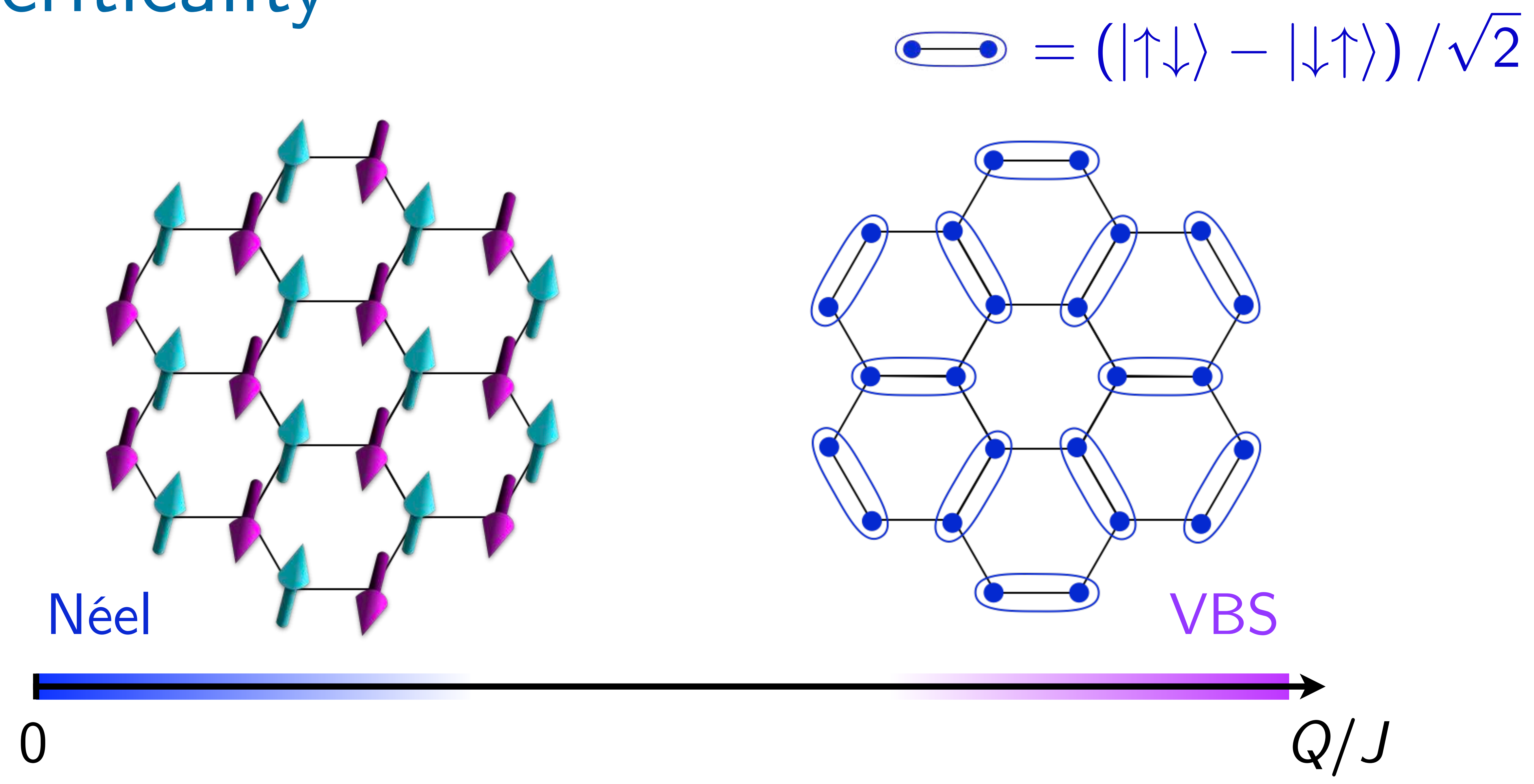
$CoNb_2O_6$ $\boldsymbol{T \to 0}$





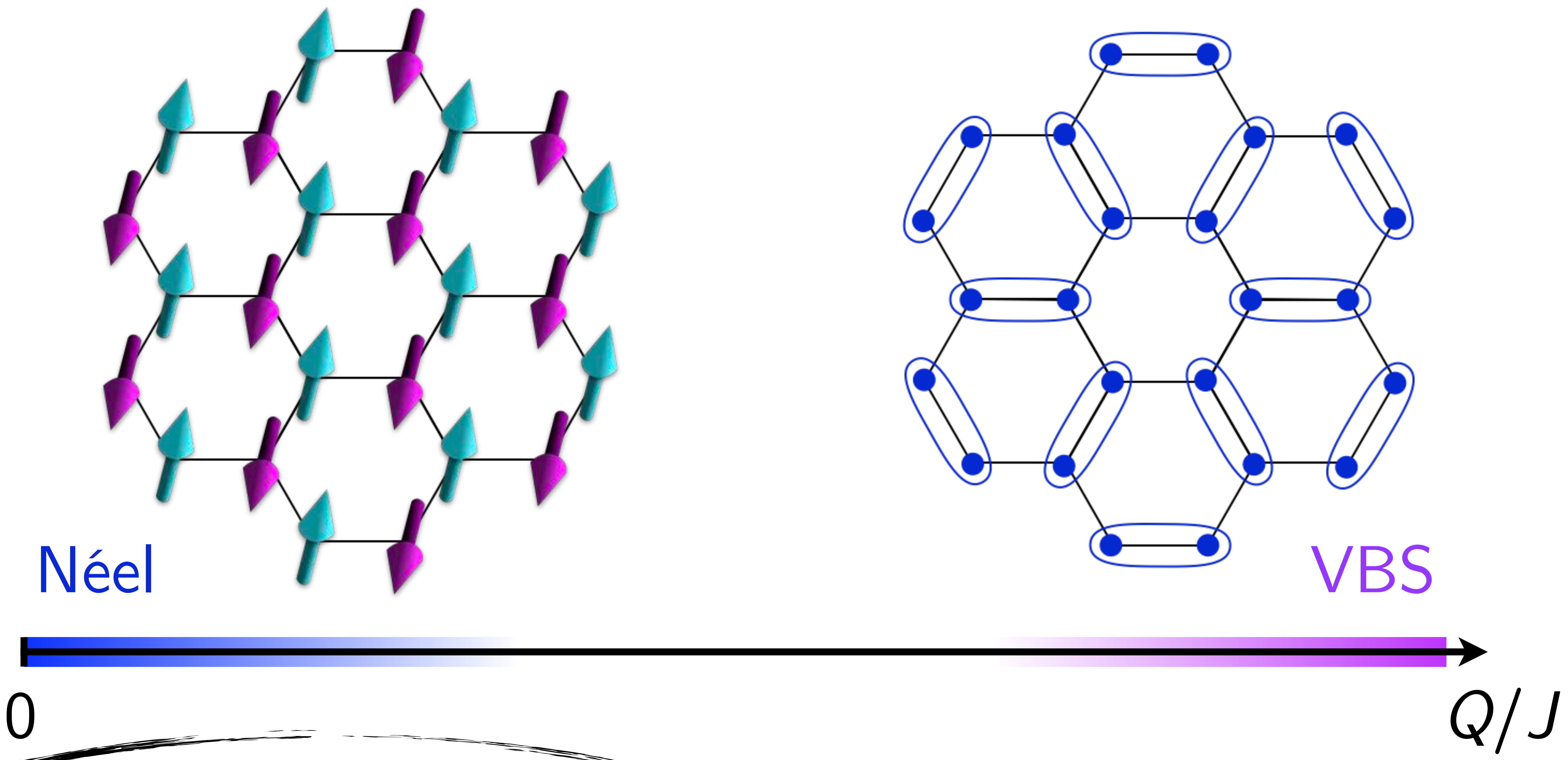
[Coldea *et al.*, Science '10]
[Kinross *et al.*, PRX '14]
[Morris *et al.*, Kaul, Armitage, Nat. Phys. '21]
...

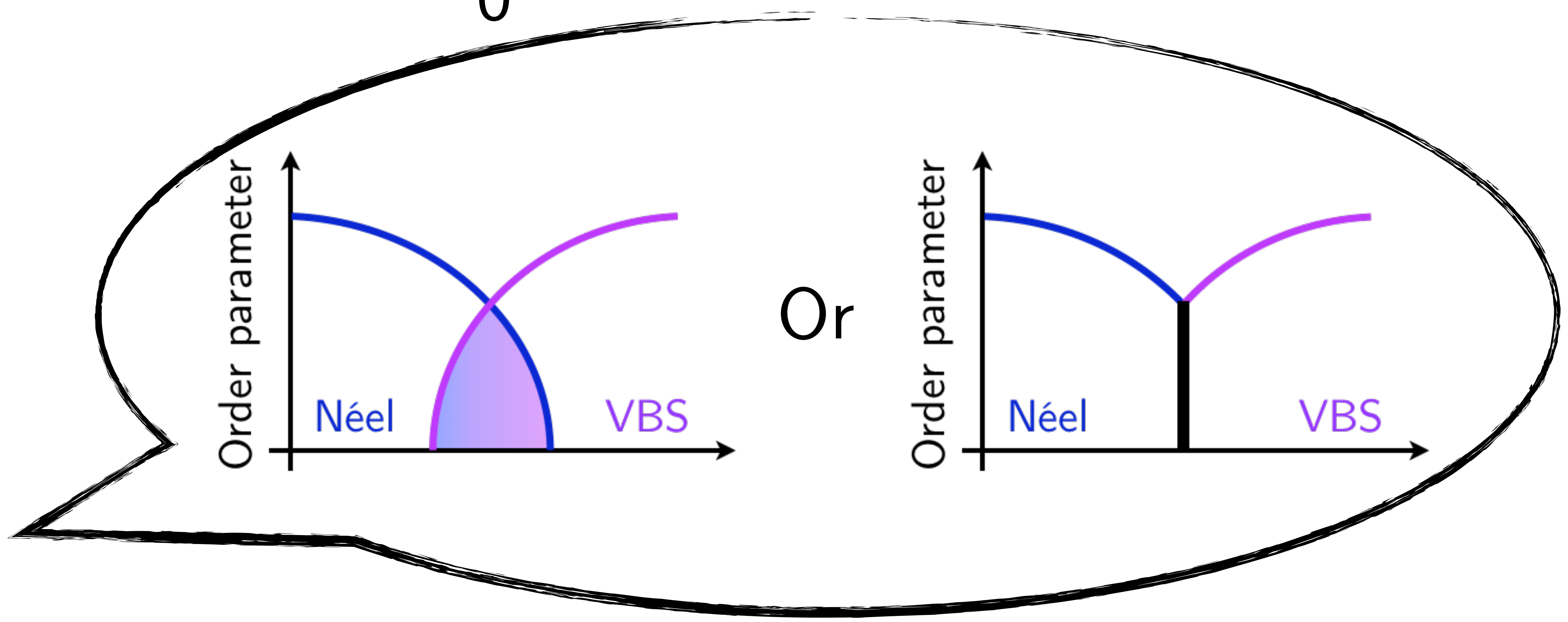
Deconfined quantum criticality

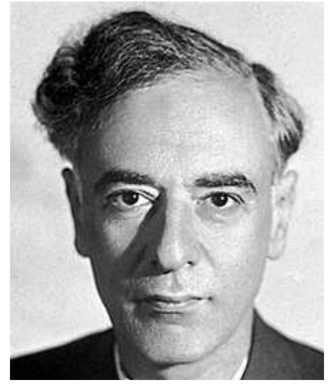


Deconfined quantum criticality

$\bullet\!\!-\!\!\bullet = \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)/\sqrt{2}$



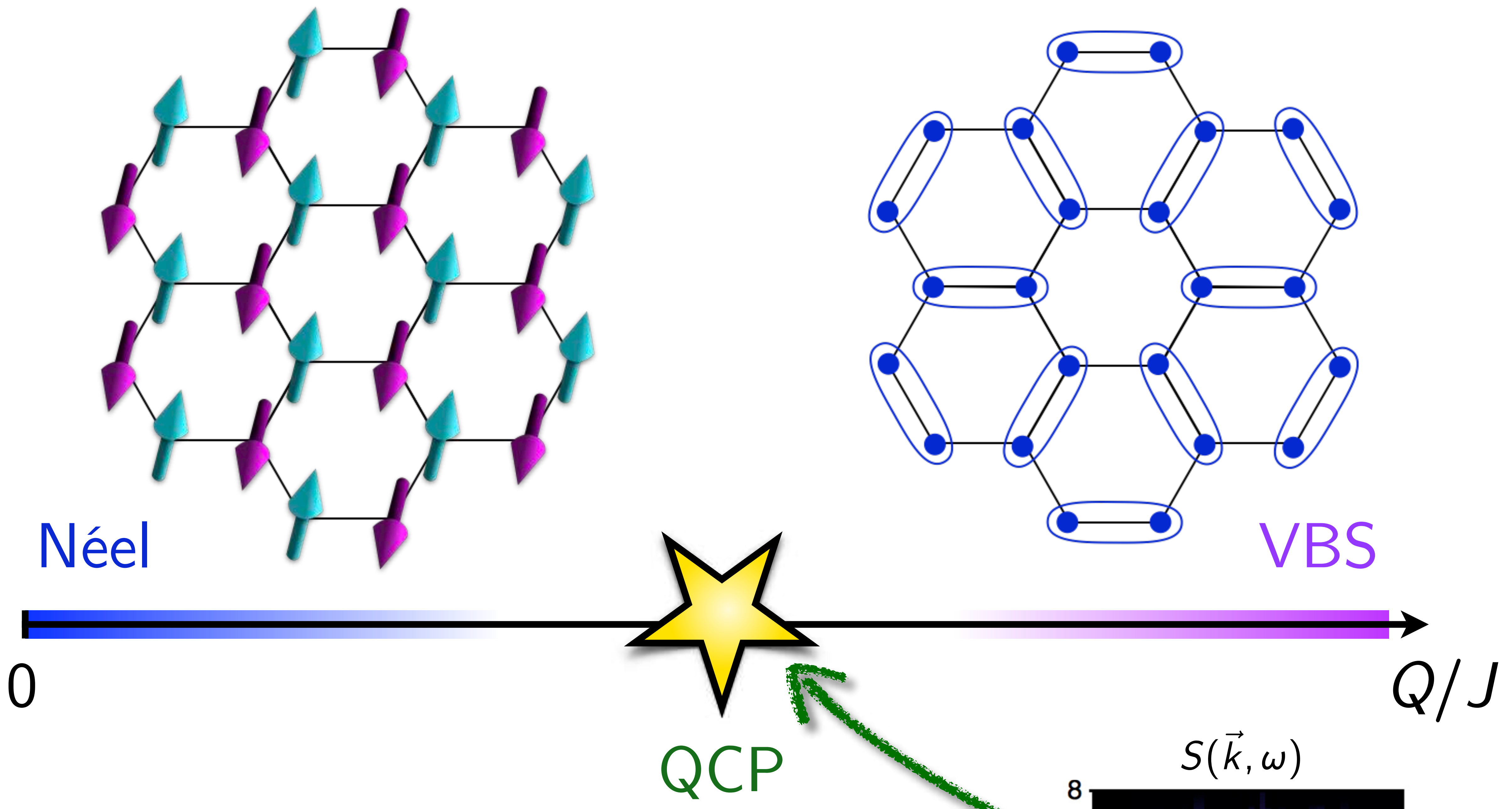


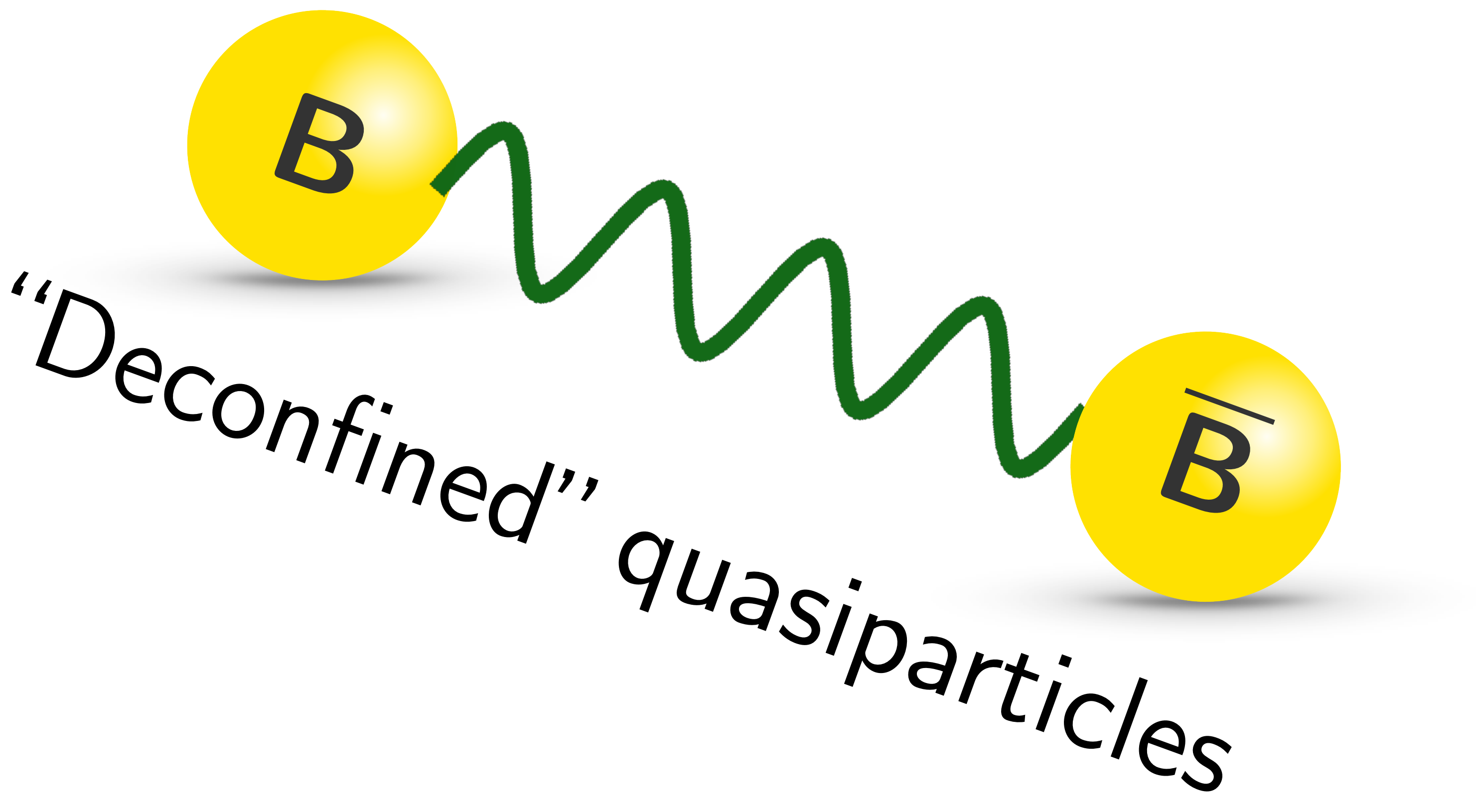


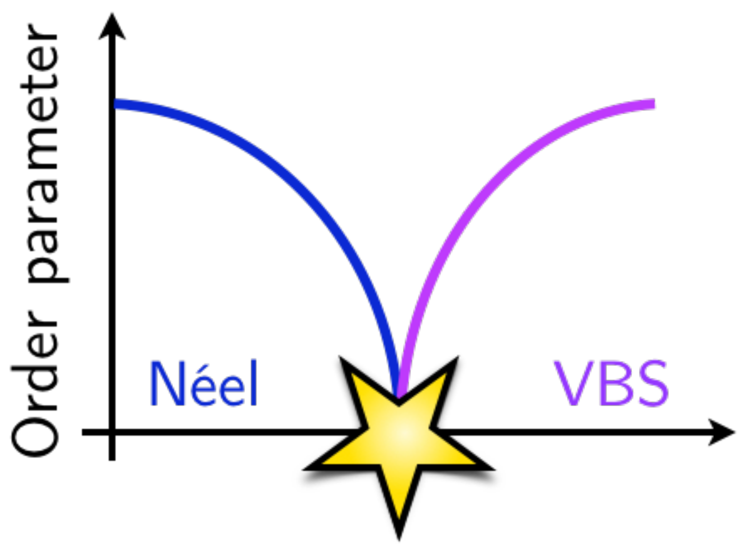
Landau

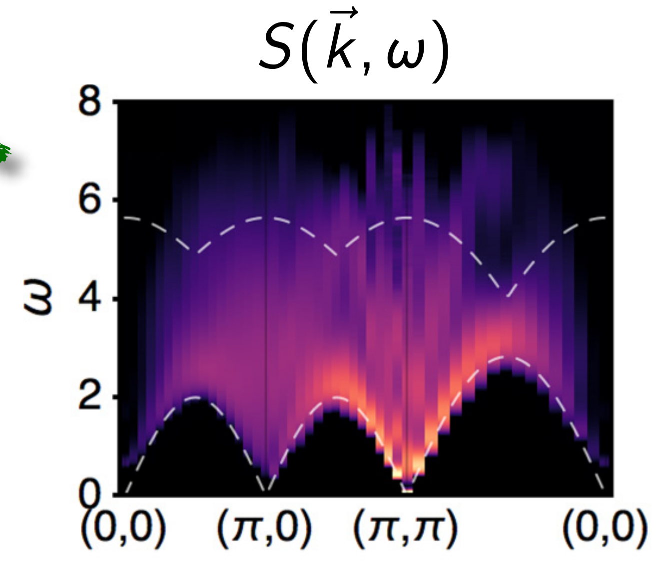
Deconfined quantum criticality

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





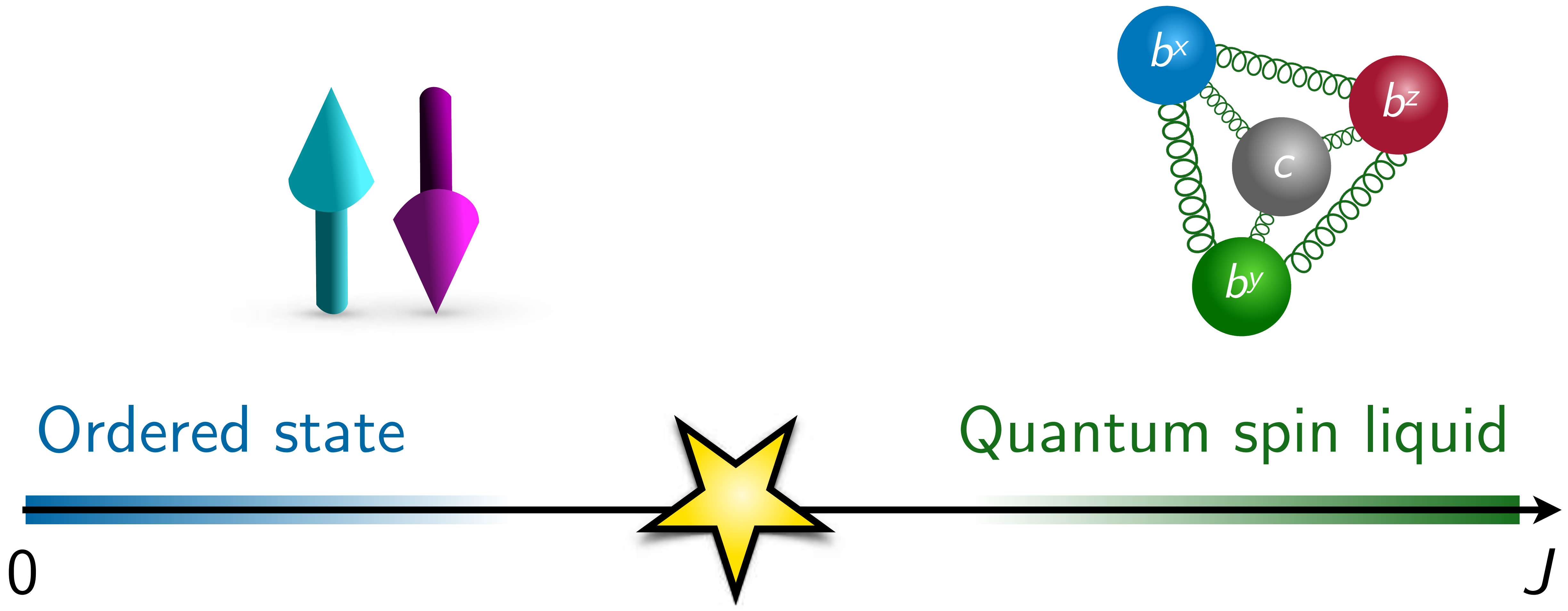




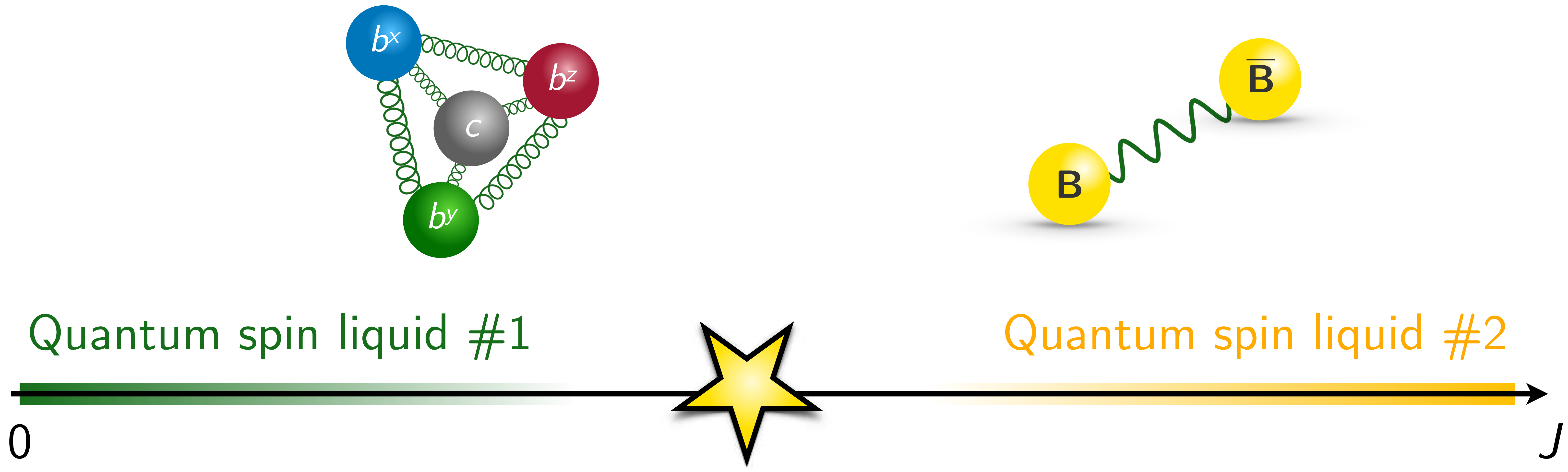
[Ma *et al.*, PRB '18]

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

Fractionalized quantum criticality



[Isakov, Melko, Hastings, Science '12]
[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]
...

Fractionalized quantum criticality

[Isakov, Melko, Hastings, Science '12]
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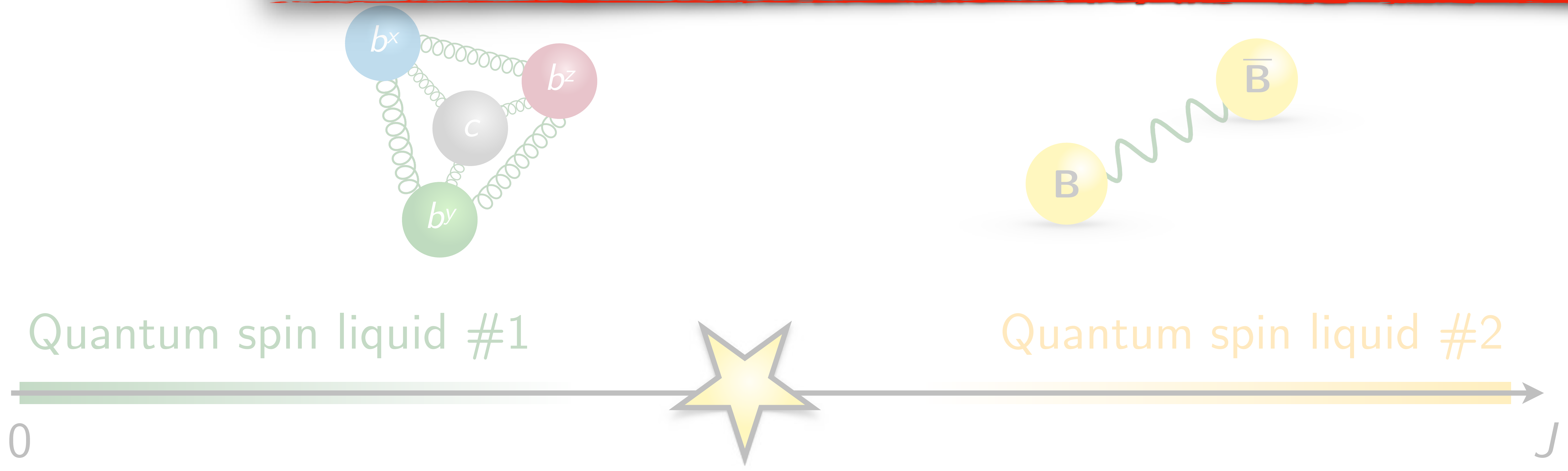
...

Goal: Fractionalized transition in microscopic model



[Metlitski, Mross, Sachdev, Senthil, PRB '15]
[LJ & He, PRB '17]
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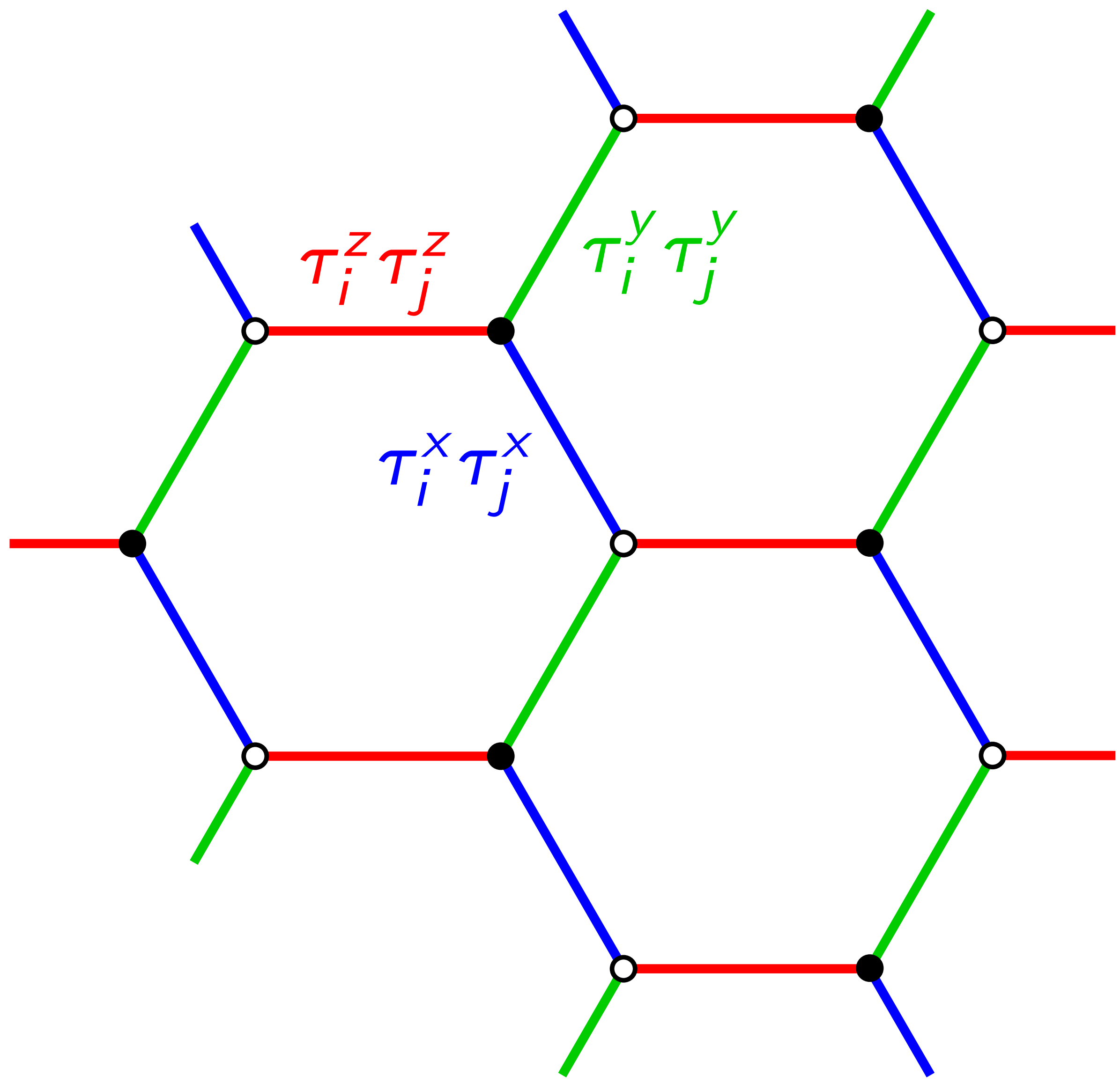
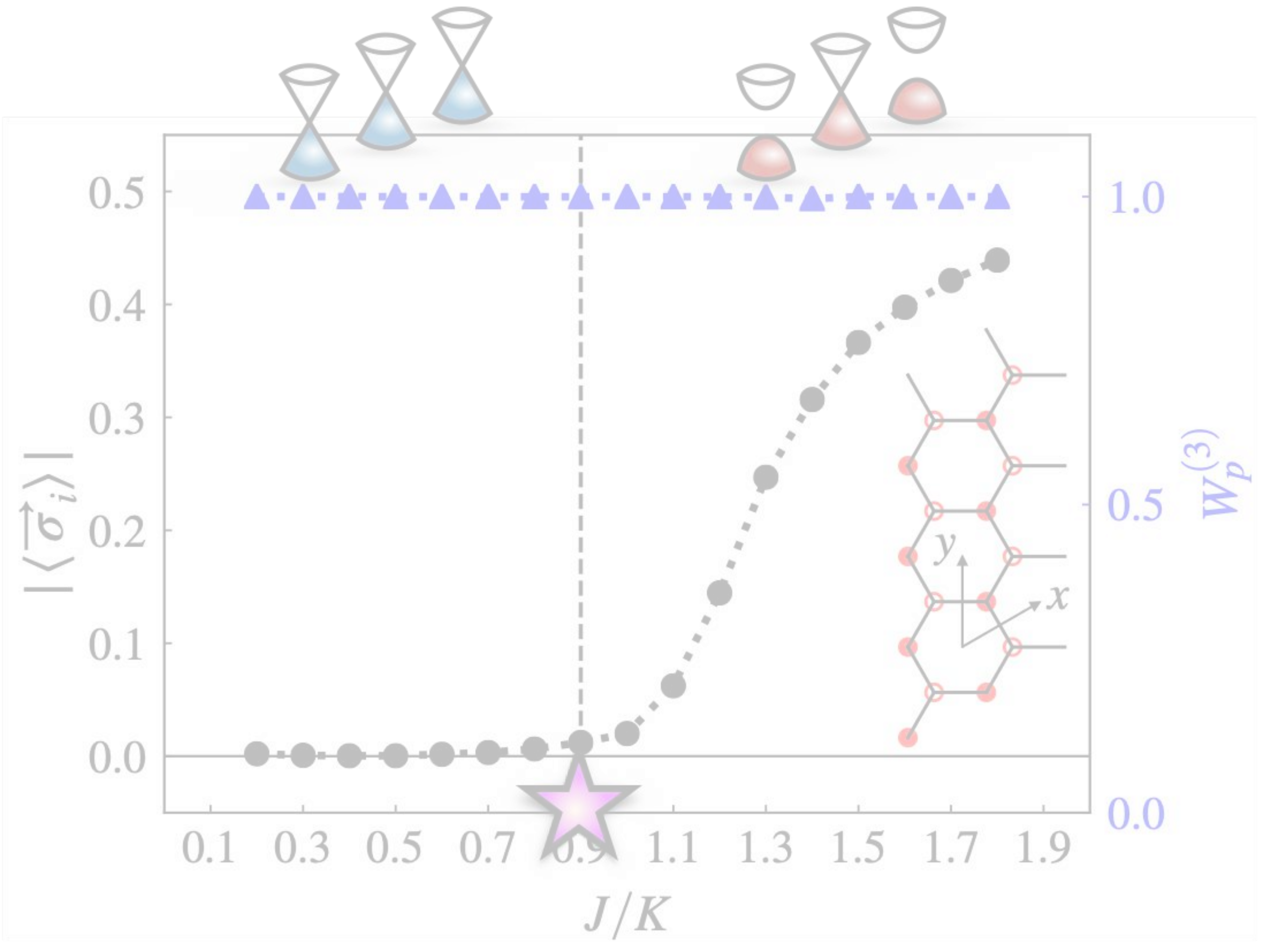


(3) Kitaev-Heisenberg spin-orbital models

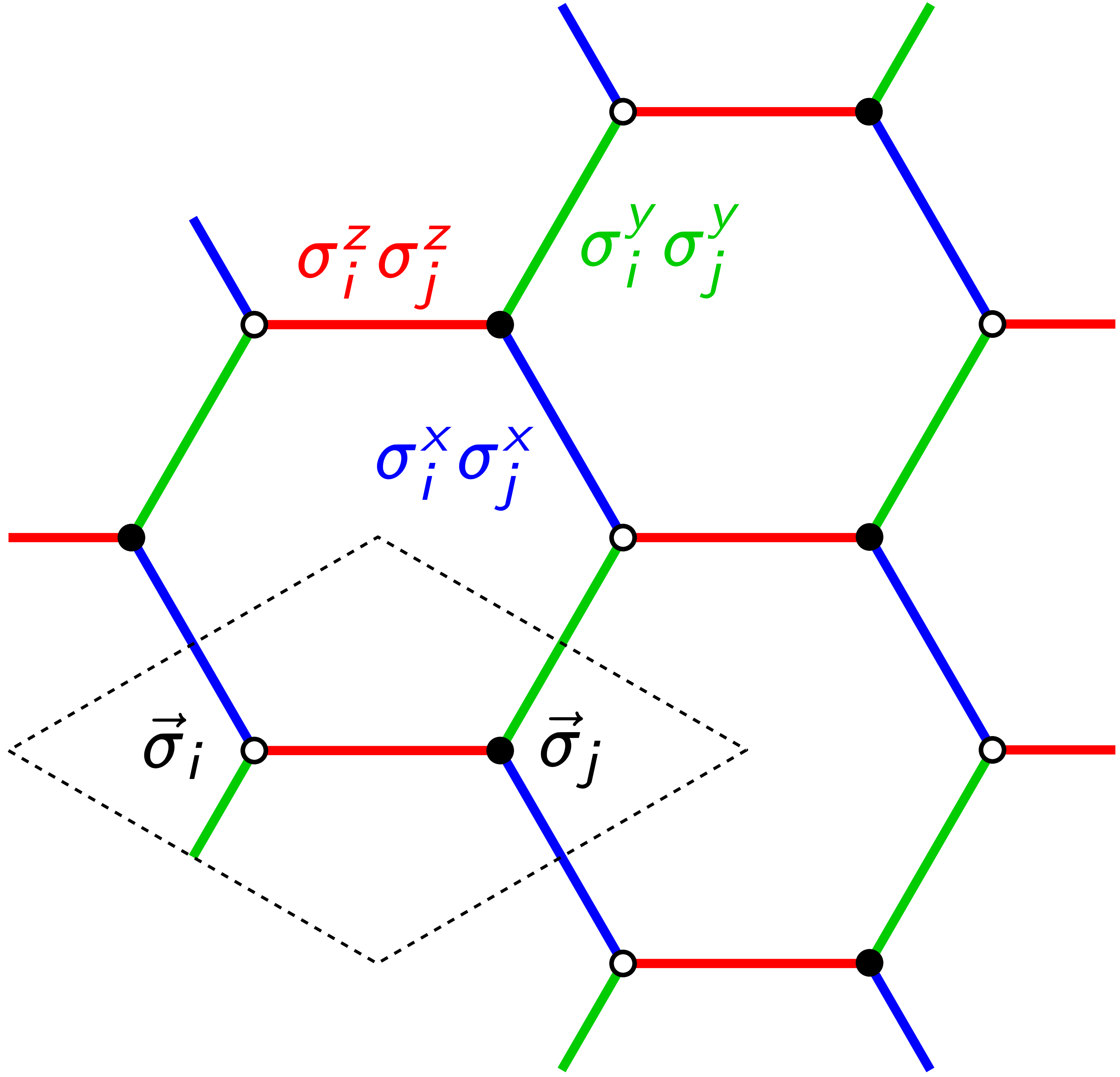


(4) Conclusions

Kitaev spin-1/2 model

Hamiltonian:

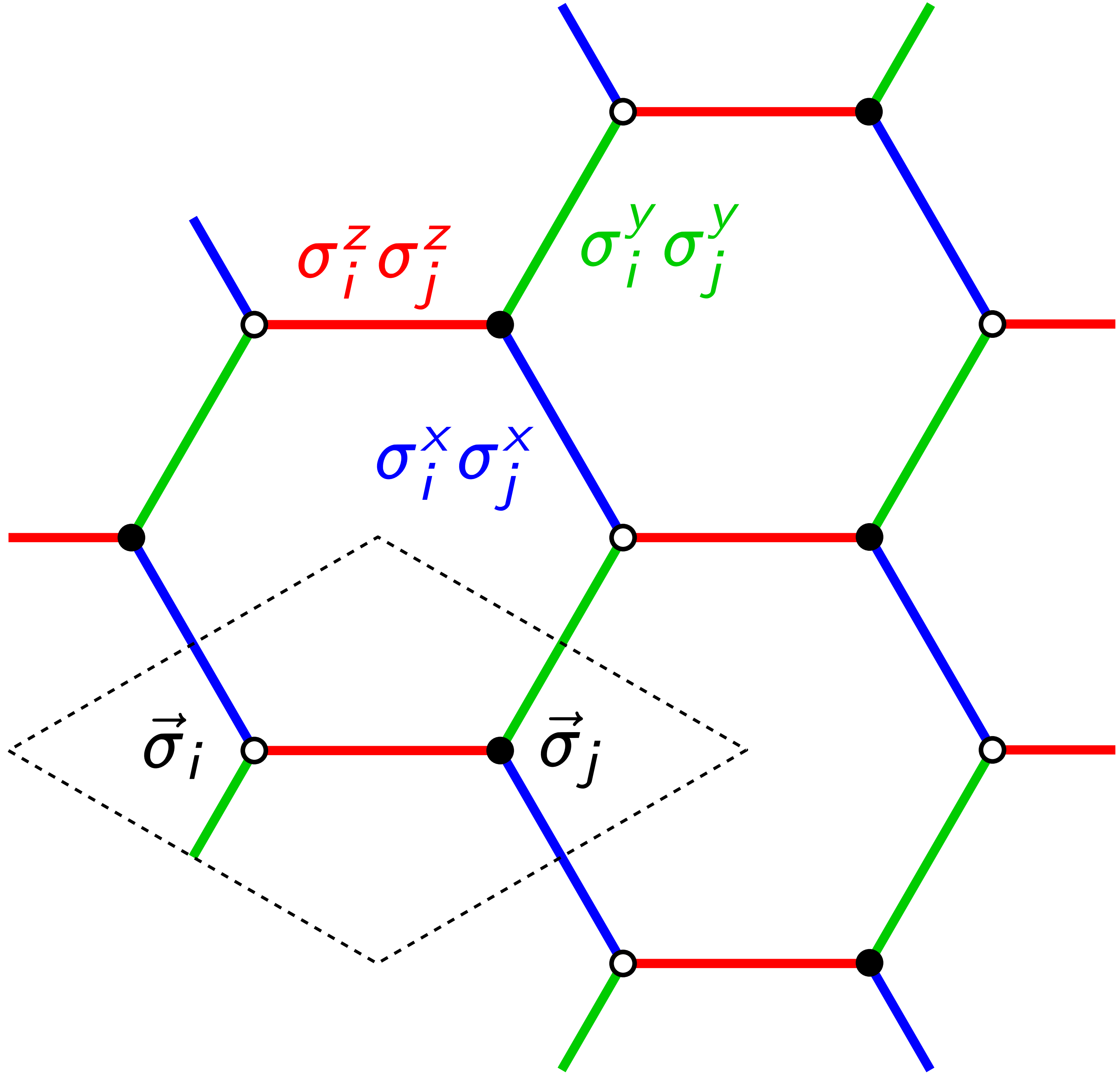
$$\mathcal{H} = K \sum_{\text{blue links}} \sigma_i^x \sigma_j^x + K \sum_{\text{green links}} \sigma_i^y \sigma_j^y + K \sum_{\text{red links}} \sigma_i^z \sigma_j^z$$



→ **talks by N. Perkins, Y. Matsuda, R. Valentí, ...**

[Kitaev, Ann. Phys. '06]

Kitaev spin-1/2 model



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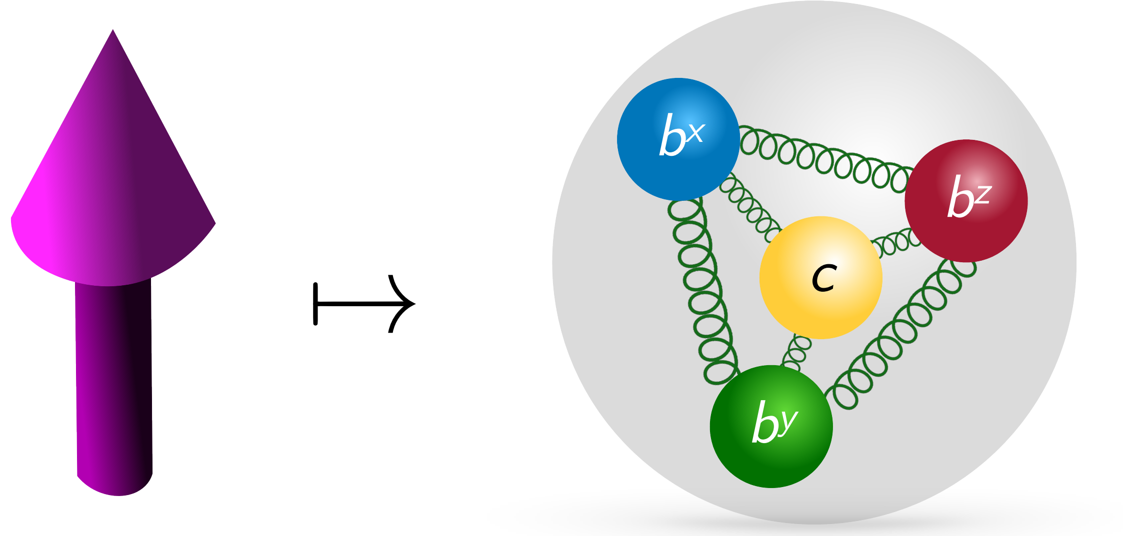
Majorana representation:

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

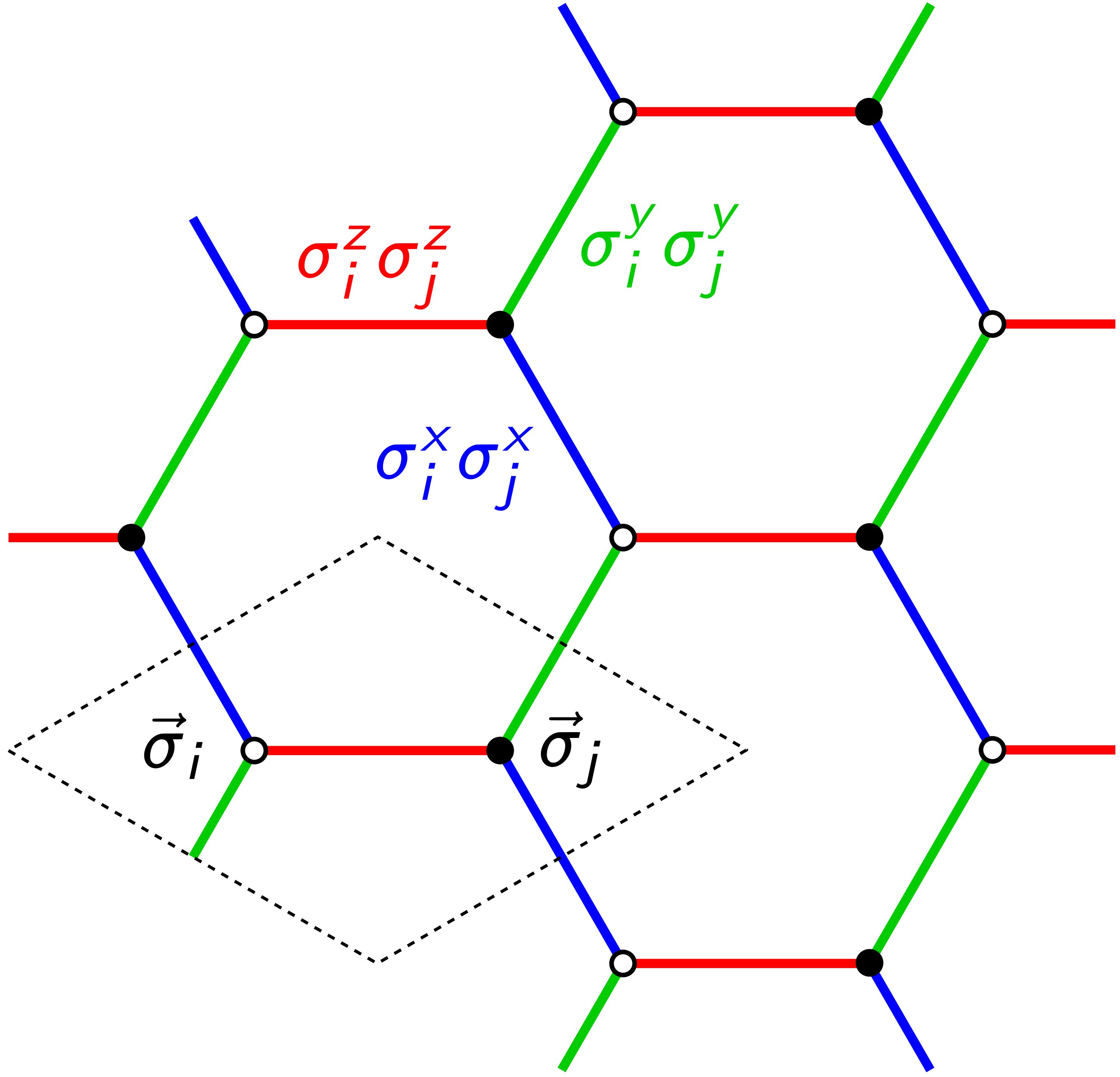


1 spin $\mapsto$ 4 Majoranas with gauge constraint

→ **talks by N. Perkins, Y. Matsuda, R. Valentí, ...**

[Kitaev, Ann. Phys. '06]

Kitaev spin-1/2 model



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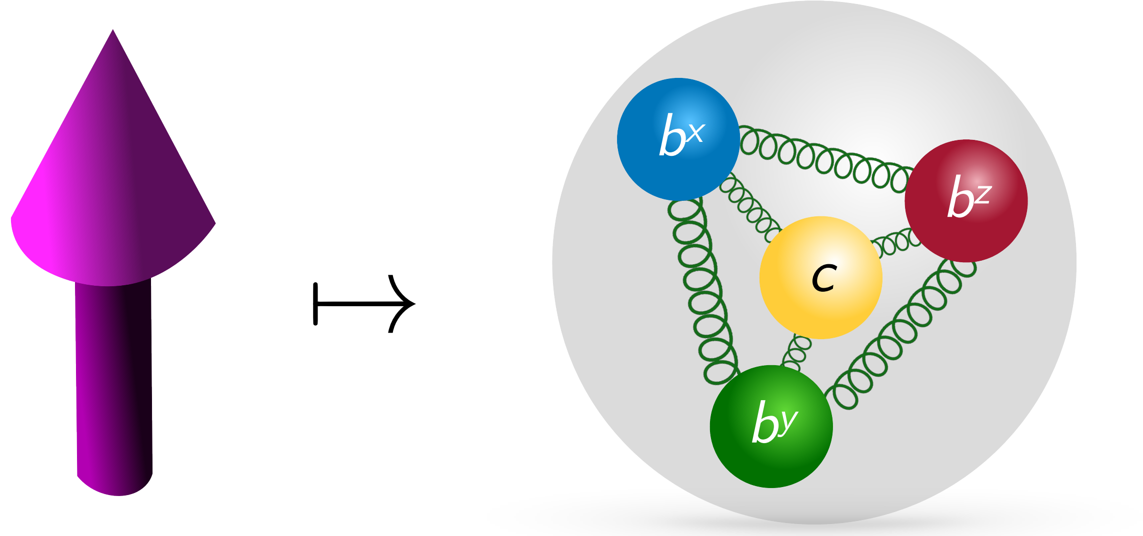
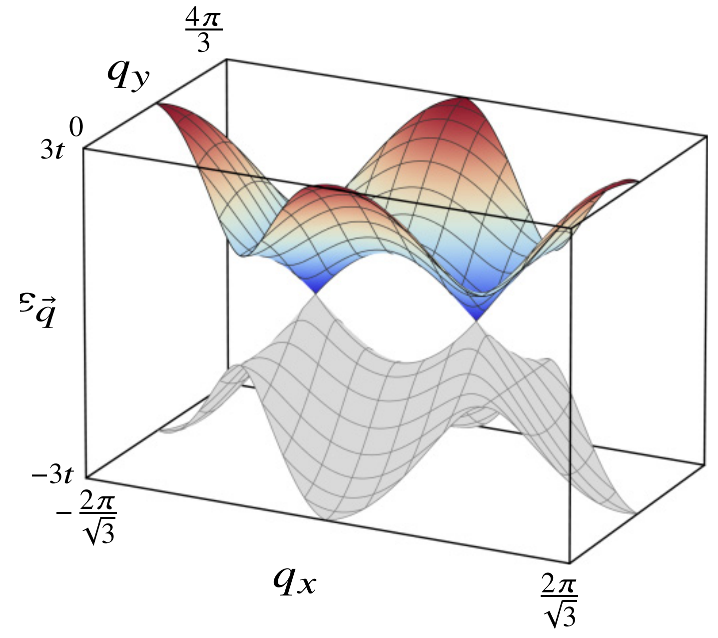


1 spin

4 Majoranas
with gauge constraint

Fractionalization:

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



with $\left[\hat{u}_{ij}, \tilde{\mathcal{H}}\right] = 0 \quad \Rightarrow \quad$ static $\mathbb{Z}_2$ gauge field!

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

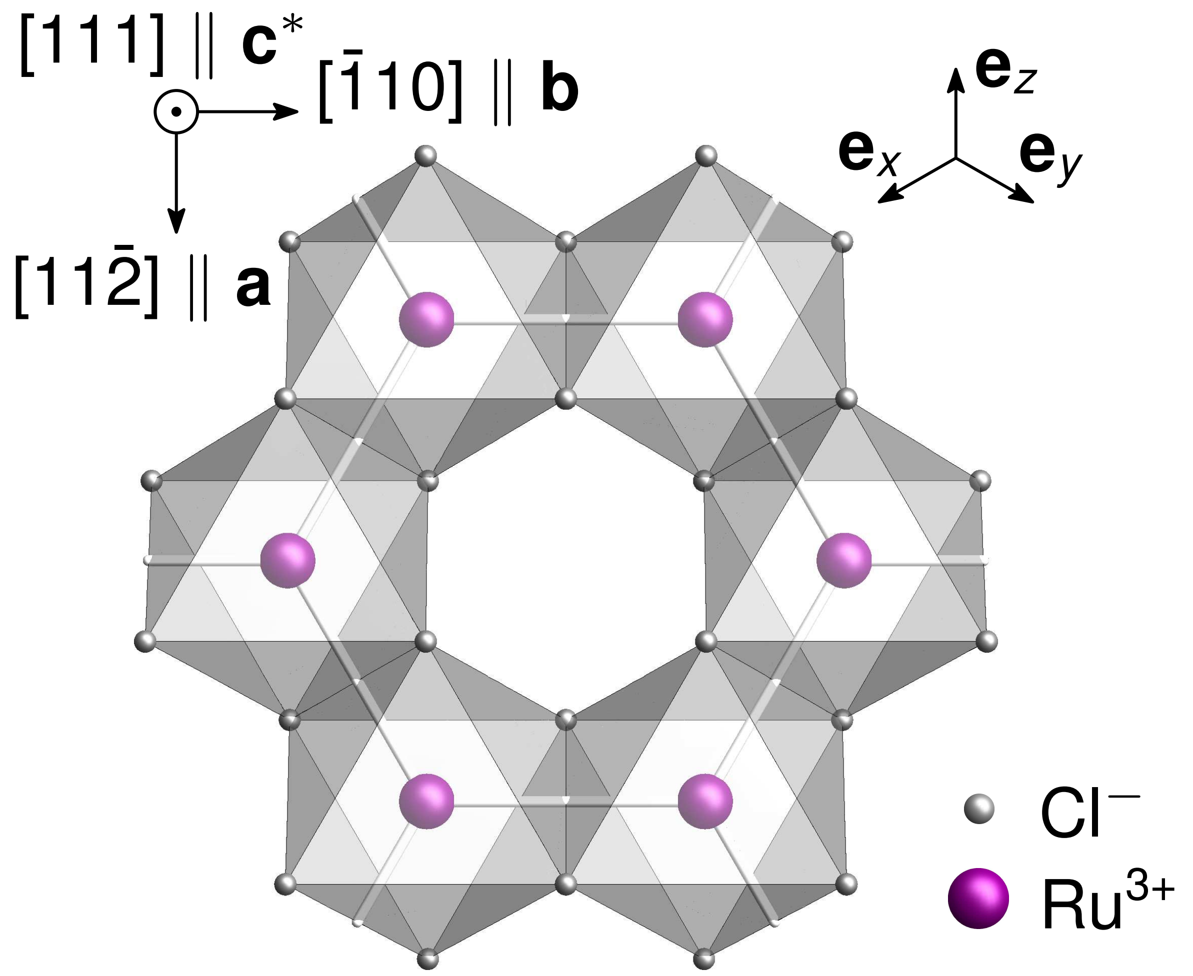
→ **talks by N. Perkins, Y. Matsuda, R. Valentí, ...**

[Kitaev, Ann. Phys. '06]

Kitaev-Heisenberg spin-1/2 model

Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\gamma} \sigma_i^\gamma \sigma_j^\gamma + J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$$



... possible relevance to α-$RuCl_3$, Na_2IrO_3, $Na_2Co_2TeO_6$, ...

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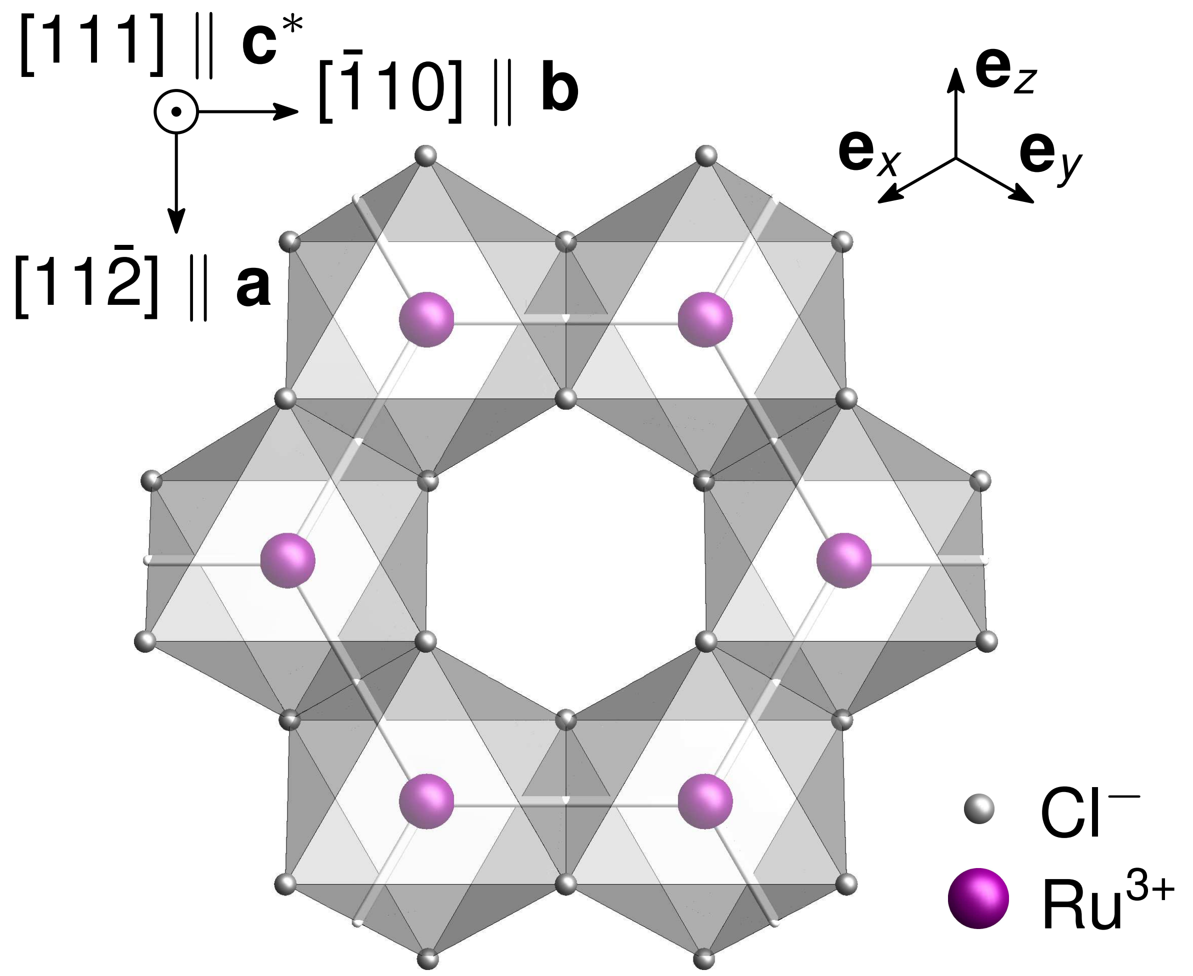

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Phase diagram:

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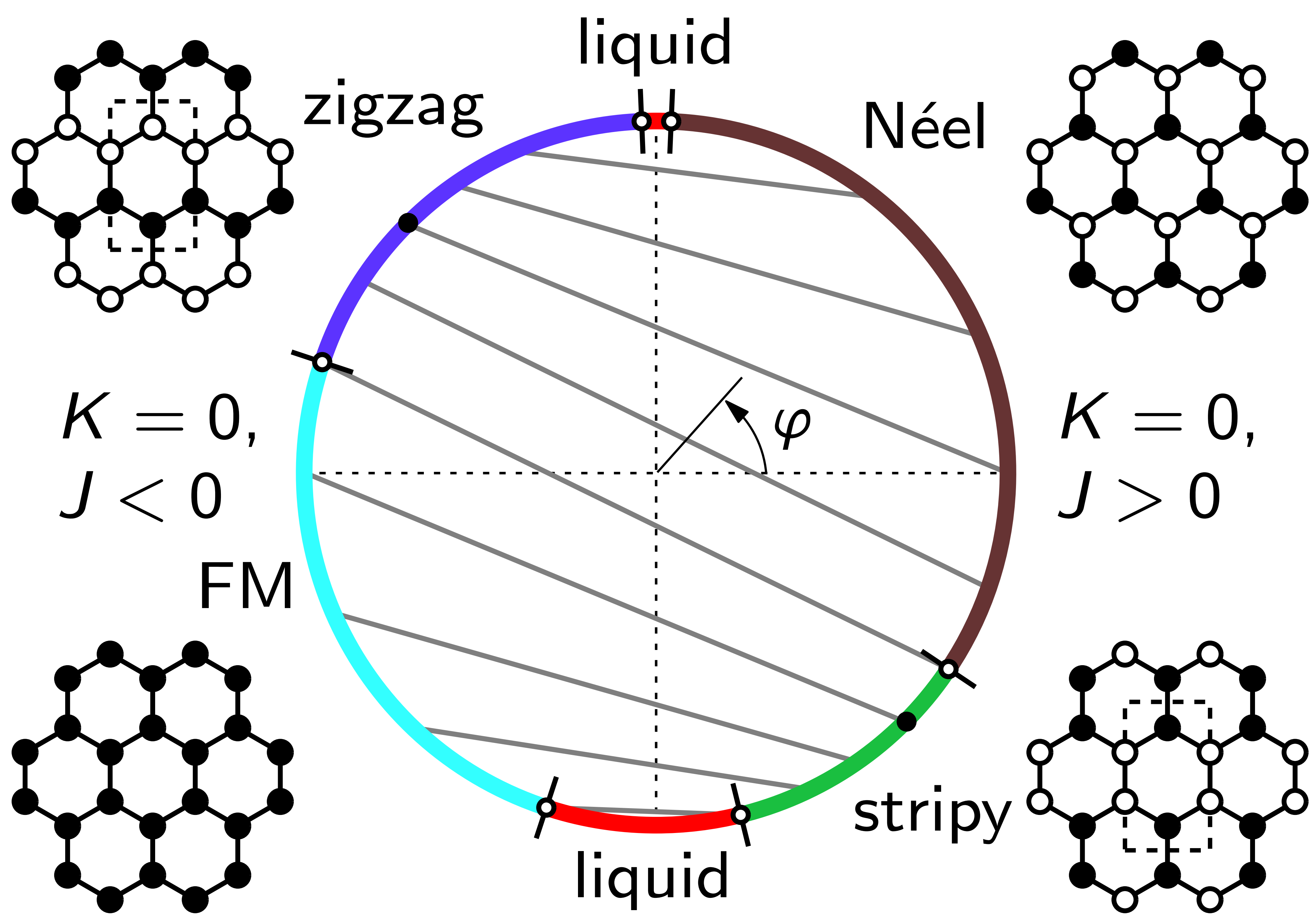
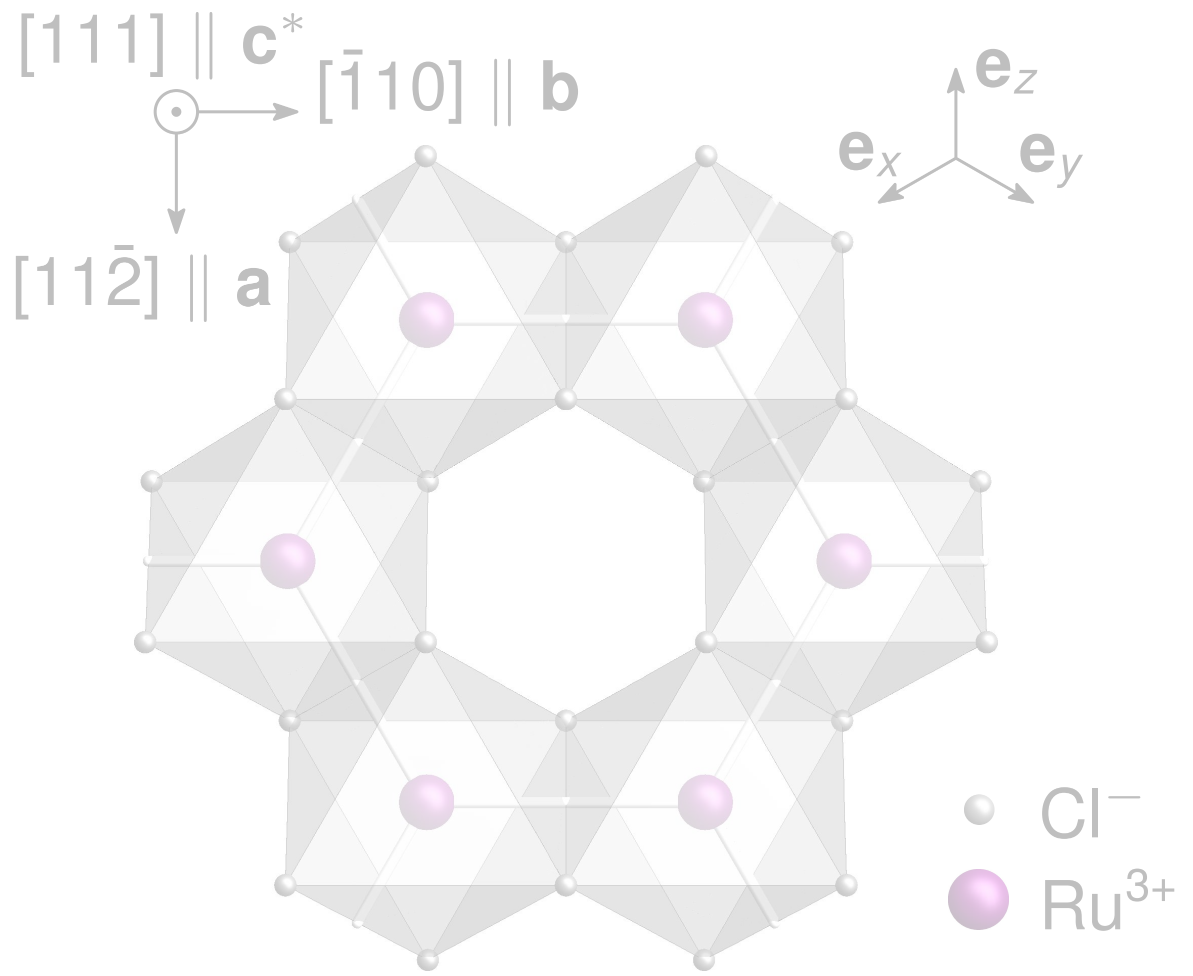


$$J = A \cos \varphi$$

$$K = 2A \sin \varphi$$

... from 24-site ED: [Chaloupka, Jackeli, Khaliullin, PRL '13]

Kitaev-Heisenberg spin-1/2 model



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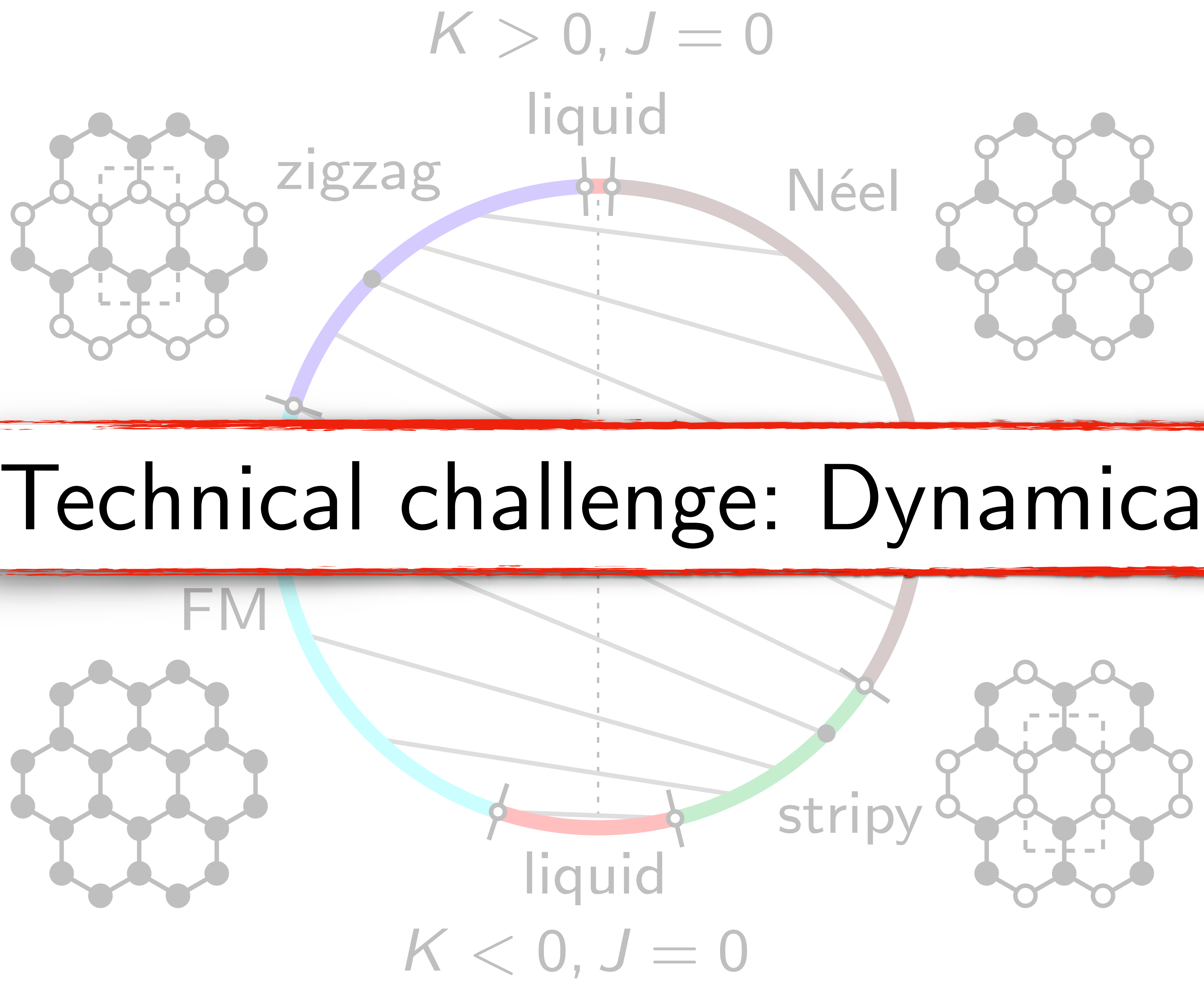
Phase diagram:



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

... no sign-problem-free QMC available: [Sato & Assaad, PRB '21]

→ talk by F. Assaad

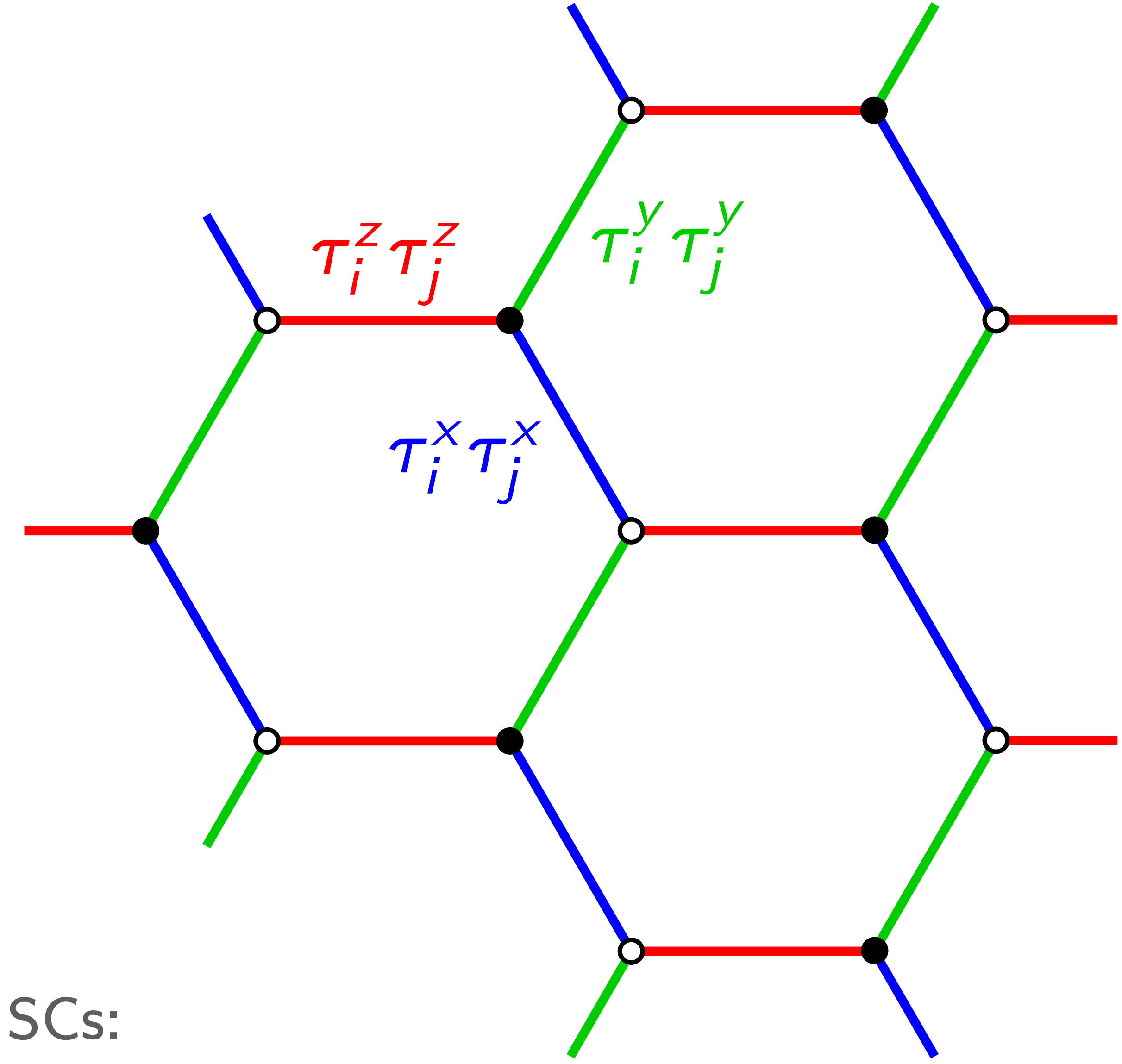
... from 24-site ED: [Chaloupka, Jackeli, Khaliullin, PRL '13]

Kitaev spin-orbital models

Spin-orbital generalization:

$\sigma^\alpha \quad 2 \times 2$

$\sigma^\alpha \otimes \tau^\beta = \gamma^i \quad 4 \times 4$



... can realize all 16 topological SCs:

[Chulliparambil, *et int.*, LJ, Tu, PRB '20]

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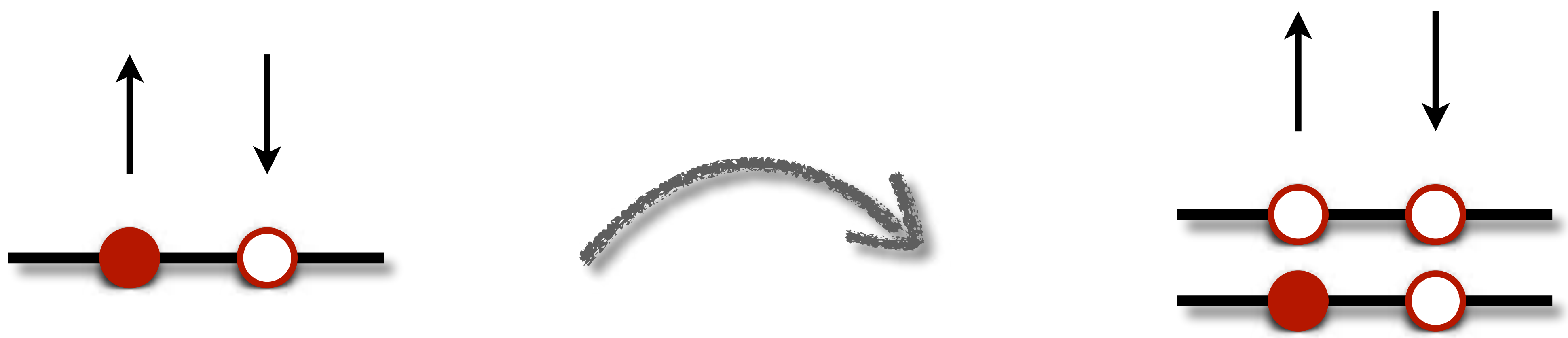

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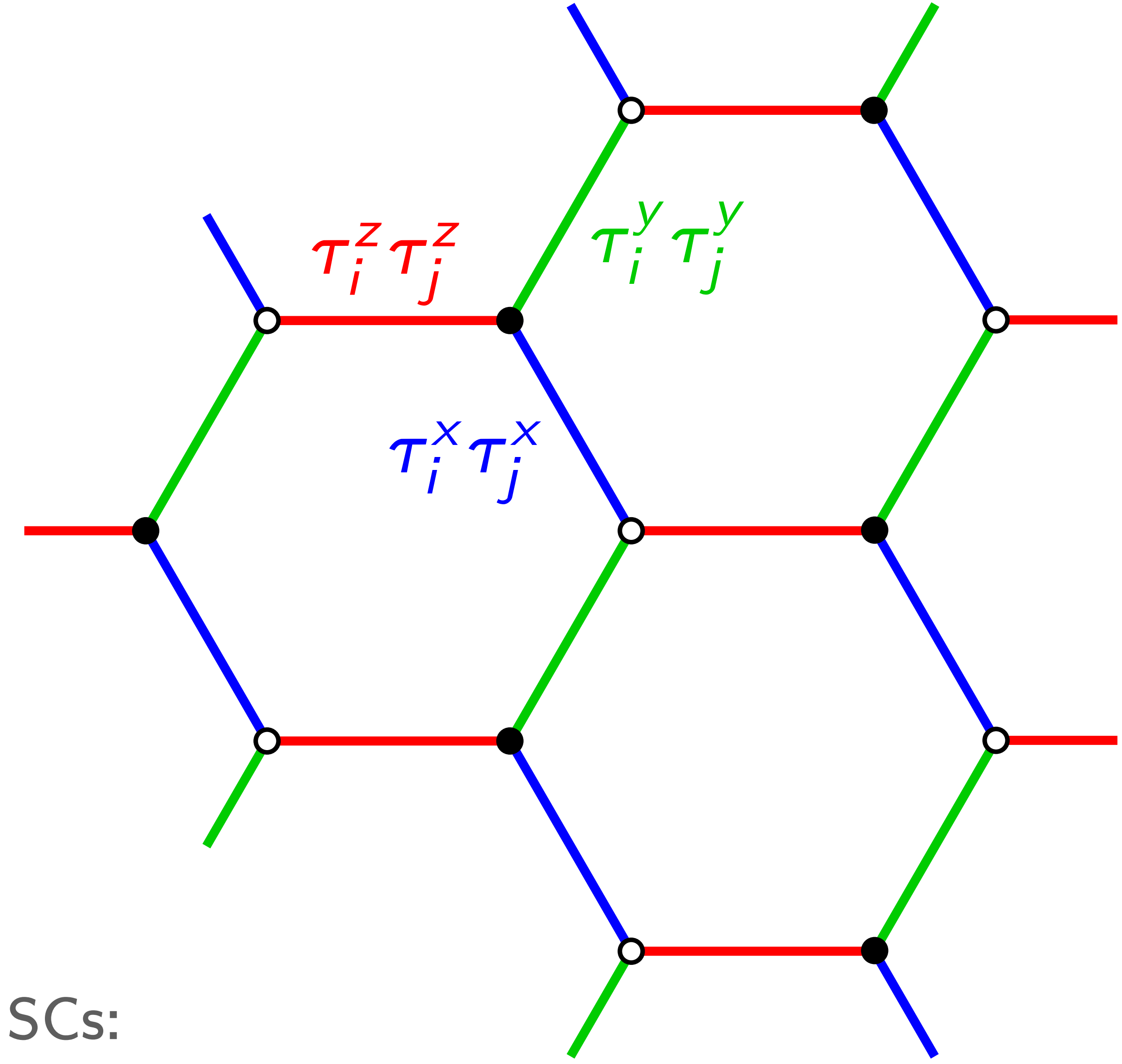

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Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\gamma} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma$$

Heisenberg spin

Kitaev orbital

Kitaev spin-orbital models

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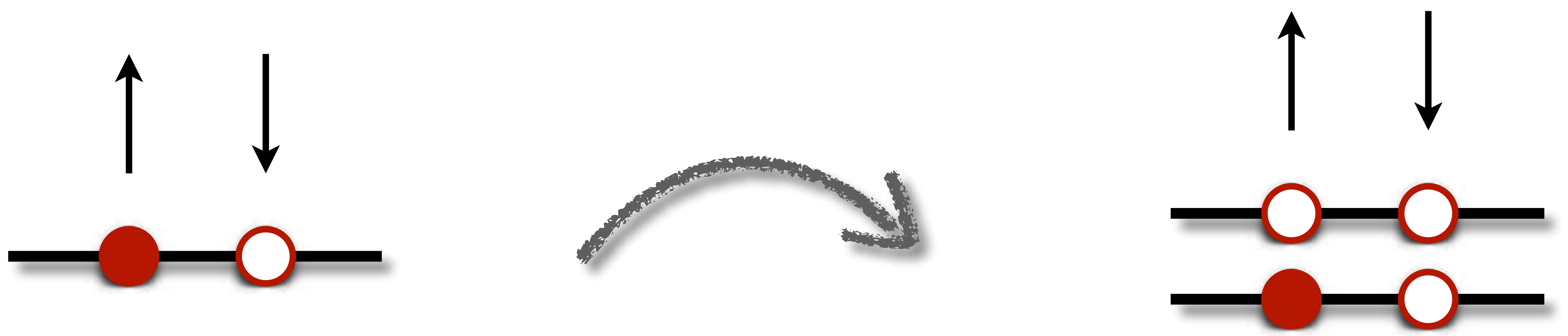

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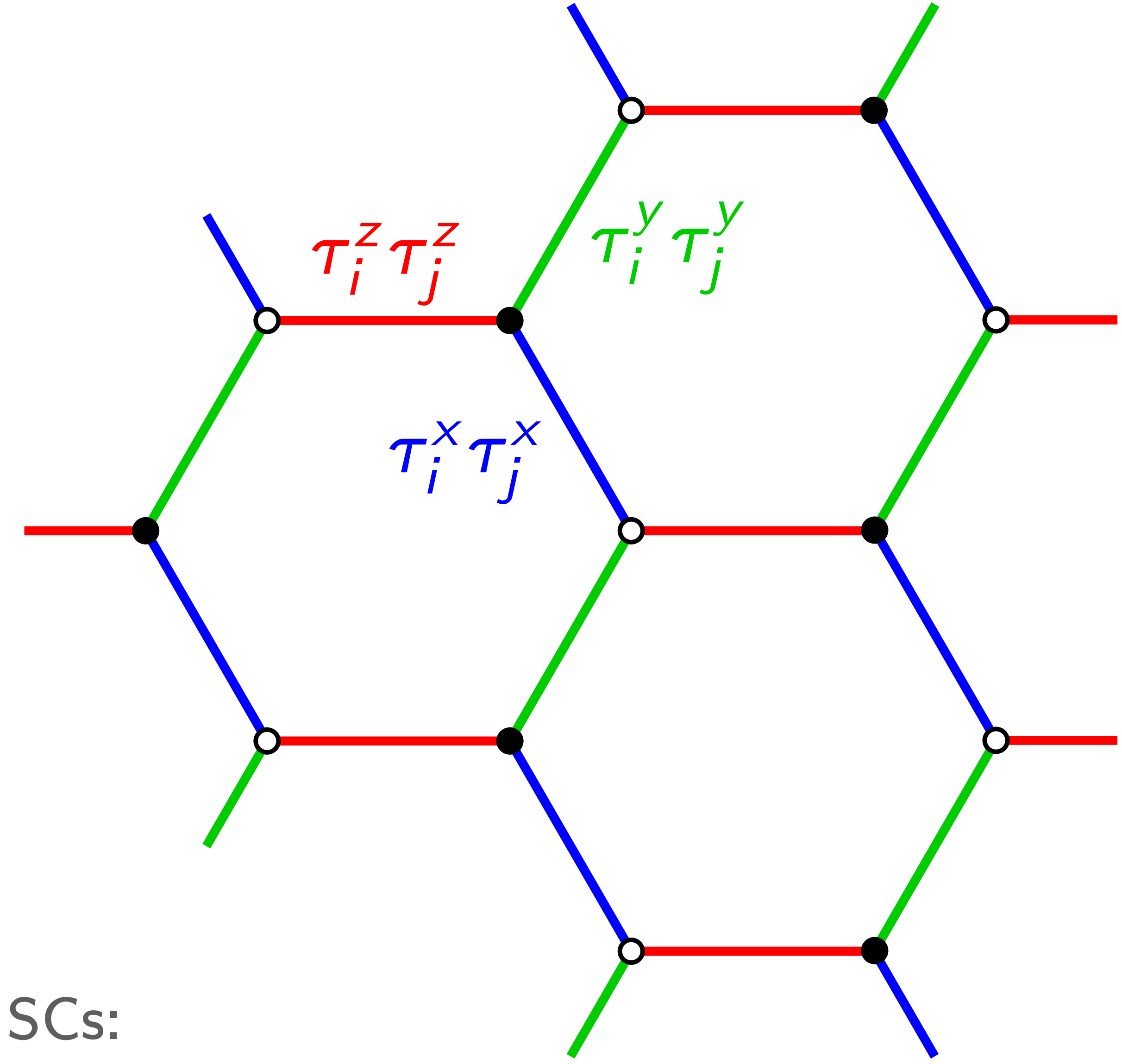

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Kitaev orbital

Majorana representation:

$$\sigma^y \otimes \tau^x = i b^1 c^x$$
$$\sigma^y \otimes \tau^y = i b^2 c^x$$
$$\sigma^y \otimes \tau^z = i b^3 c^x$$
$$\sigma^x \otimes \mathbb{1} = i c^y c^x$$
$$\sigma^z \otimes \mathbb{1} = i c^z c^x$$

Fractionalization:

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

$$\mathcal{H} \mapsto \tilde{\mathcal{H}} = iK \sum_{\langle ij \rangle_\gamma} \hat{u}_{ij} c_i^\top c_j$$

with $\left[\hat{u}_{ij}, \tilde{\mathcal{H}}\right] = 0$

... cf. also [Yao & Lee, PRL '11]

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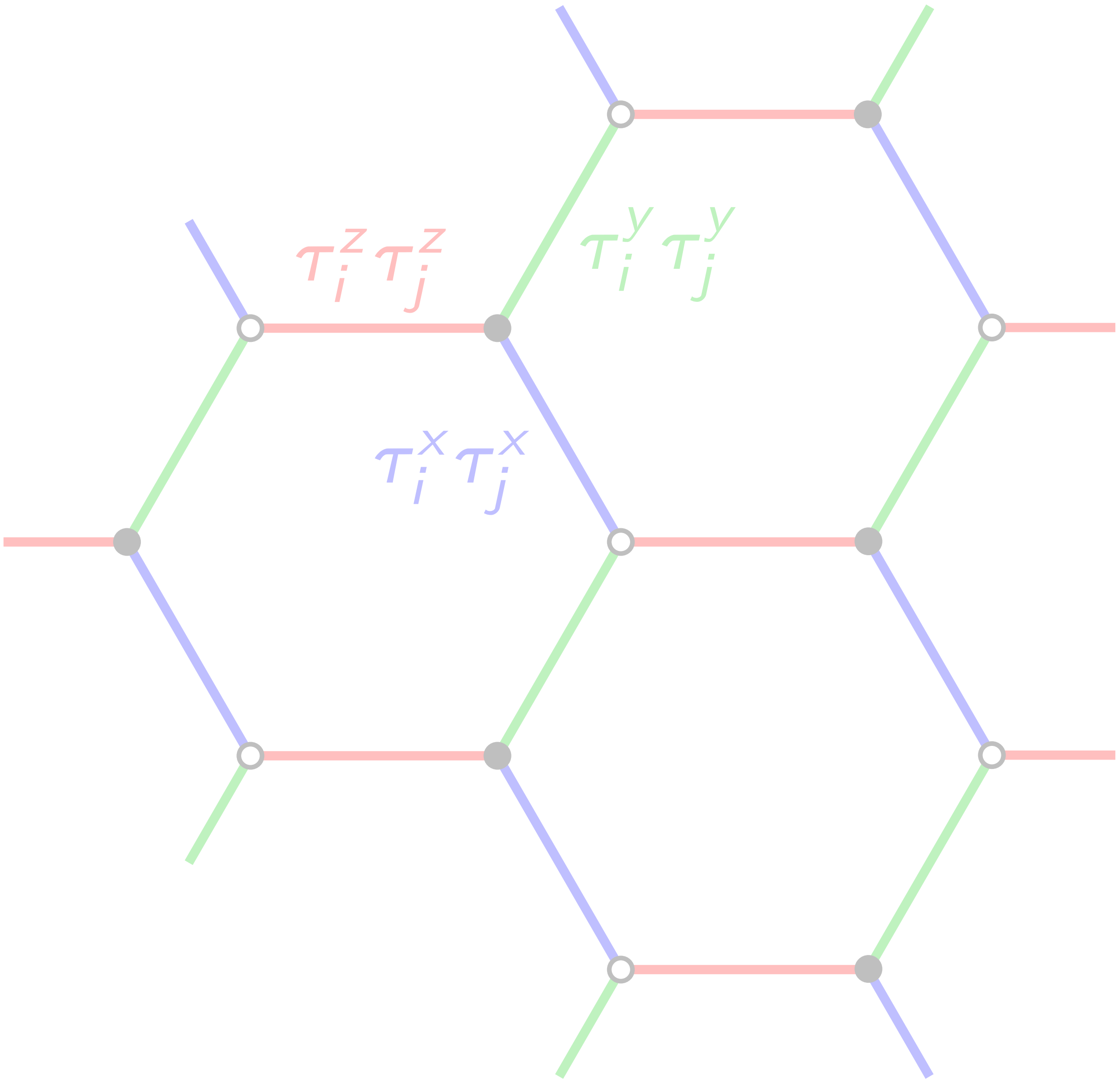
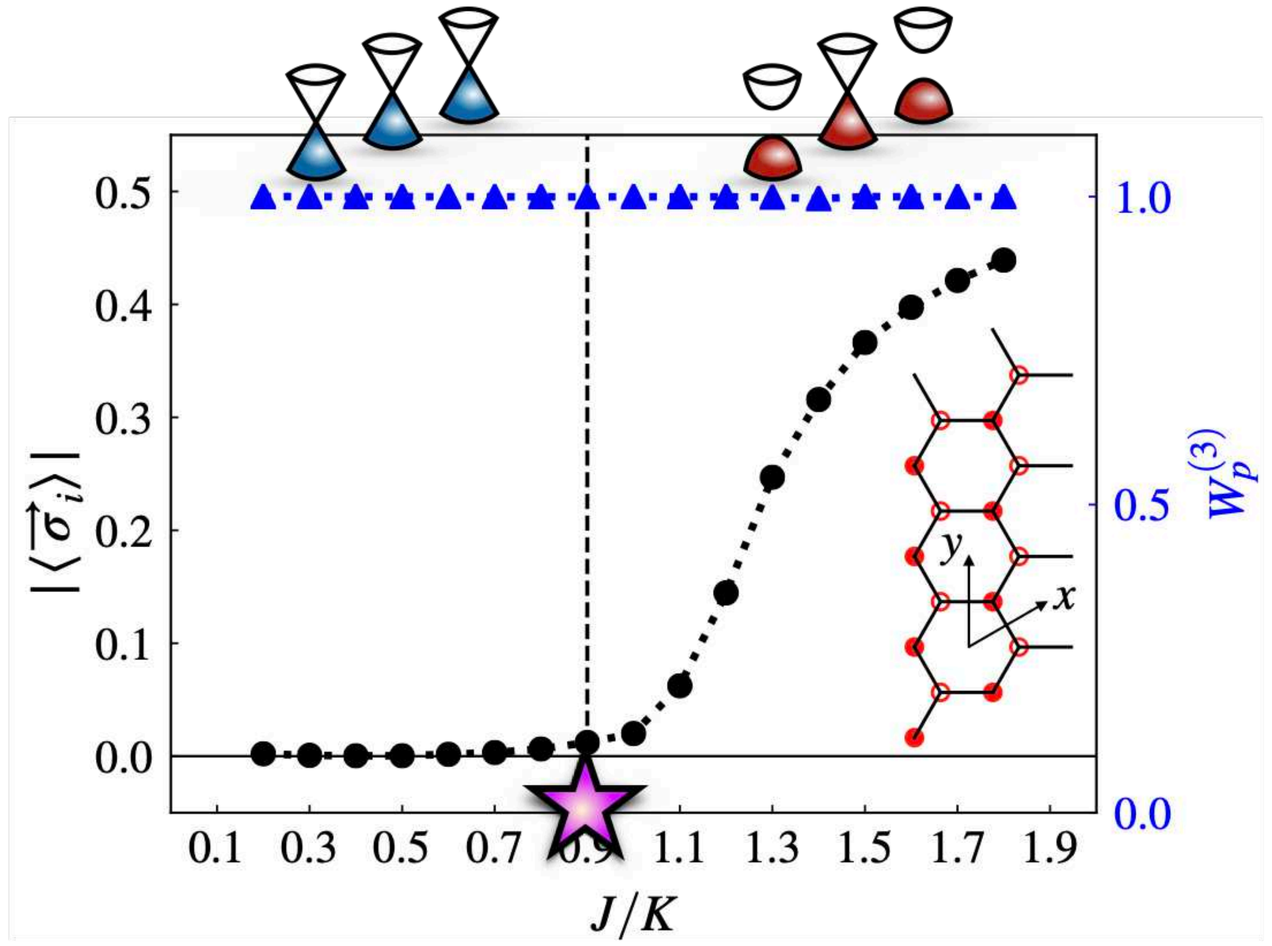


(3) Kitaev-Heisenberg spin-orbital models



(4) Conclusions

Kitaev-Heisenberg spin-orbital model

Hamiltonian:

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

spin-1 matrices

$$\mapsto \ \tfrac{1}{4}(c_i^\top \vec{L} c_i) \cdot (c_j \vec{L} c_j)$$

with $[\hat{u}_{ij}, \mathcal{H}] = 0$ still static!

Kitaev-Heisenberg spin-orbital model

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$$\mapsto \quad \tfrac{1}{4}(c_i^\top \vec{L} c_i) \cdot (c_j \vec{L} c_j)$$

with $[\hat{u}_{ij}, \mathcal{H}] = 0$ still static!

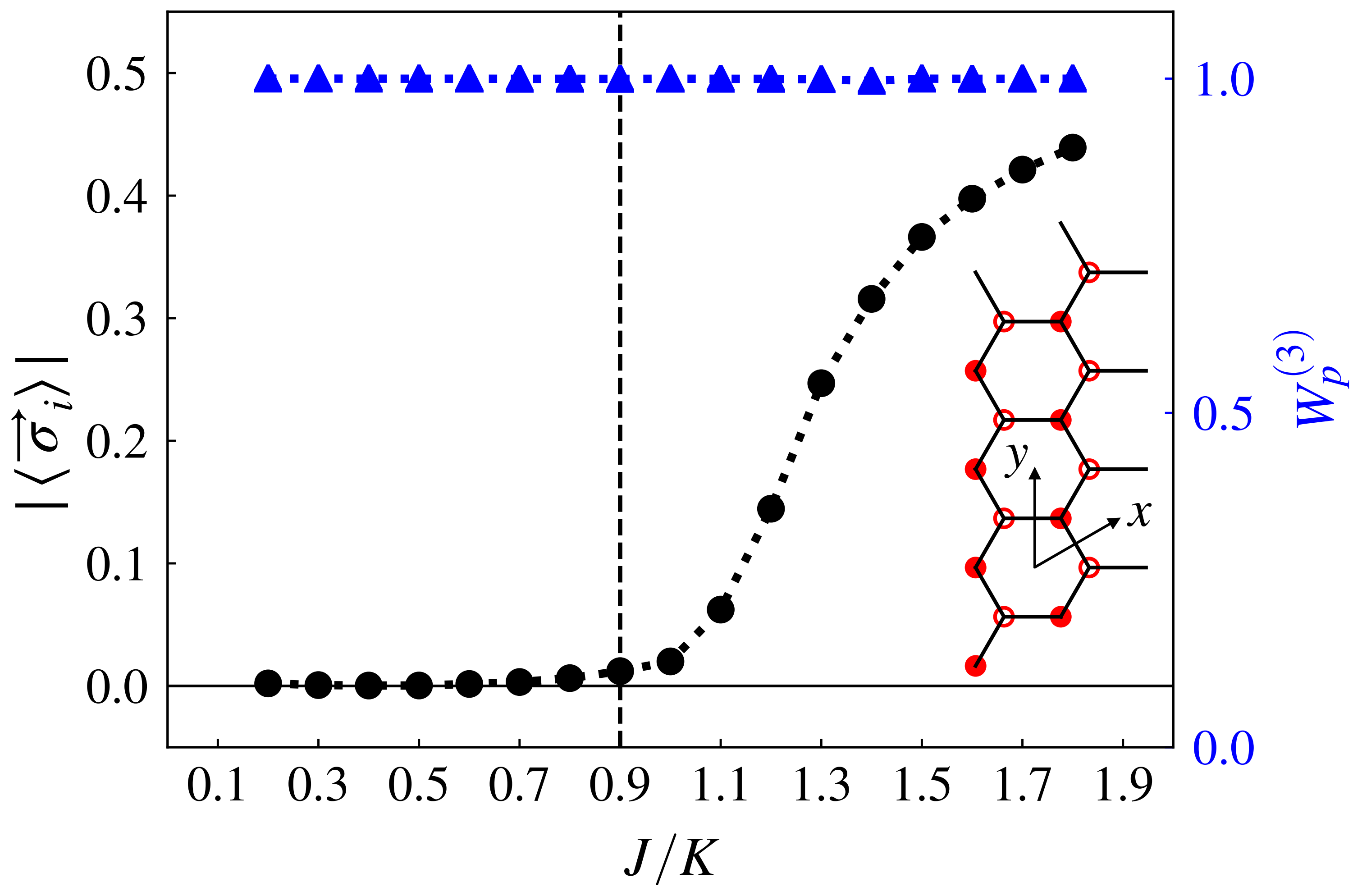
Phase diagram:

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

“spin density wave”

Gross-Neveu-SO(3)* transition

iDMRG:



... on cylinder with $L_y = 4$ unit cells

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

Gross-Neveu-SO(3)* transition

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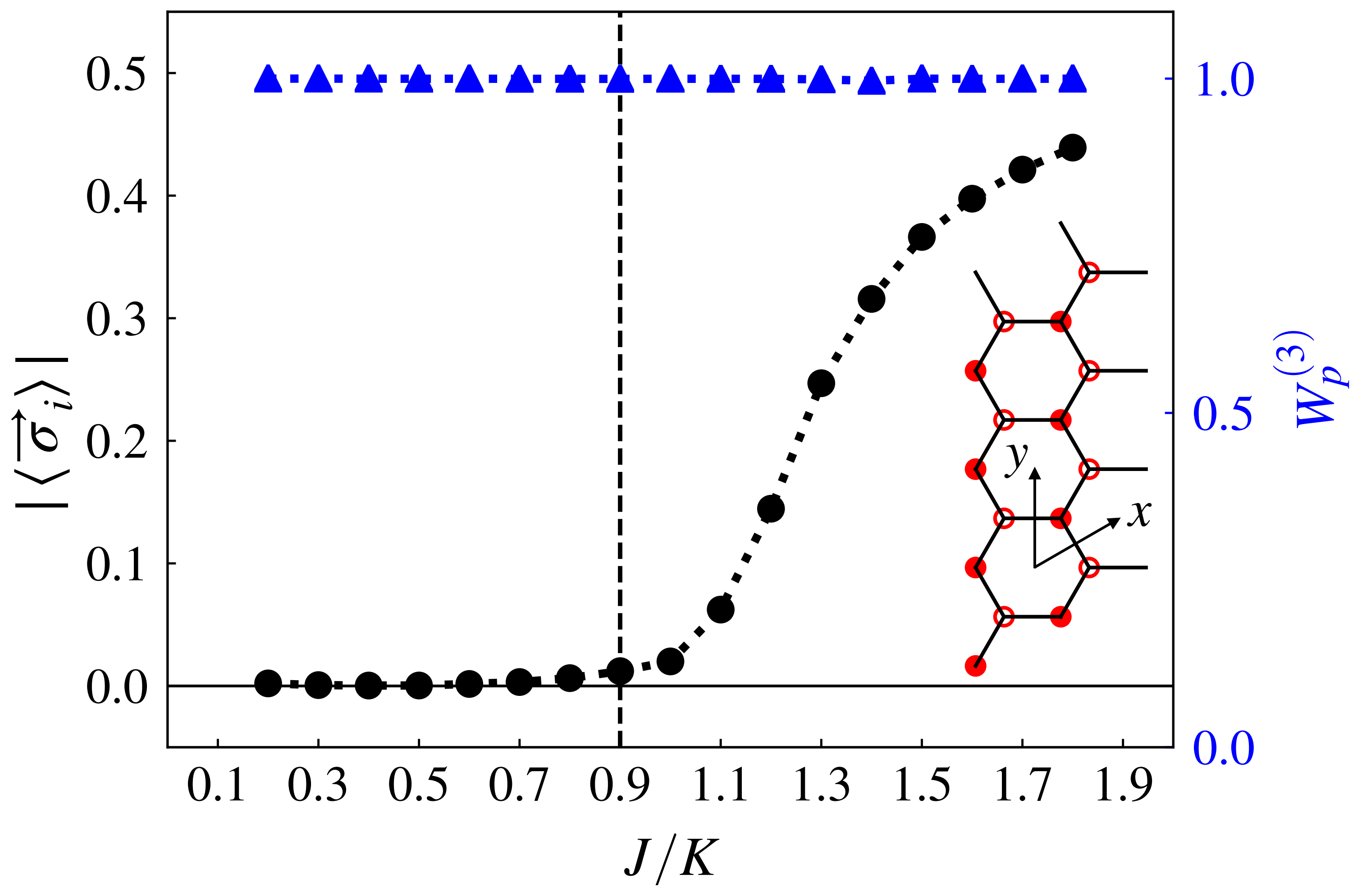

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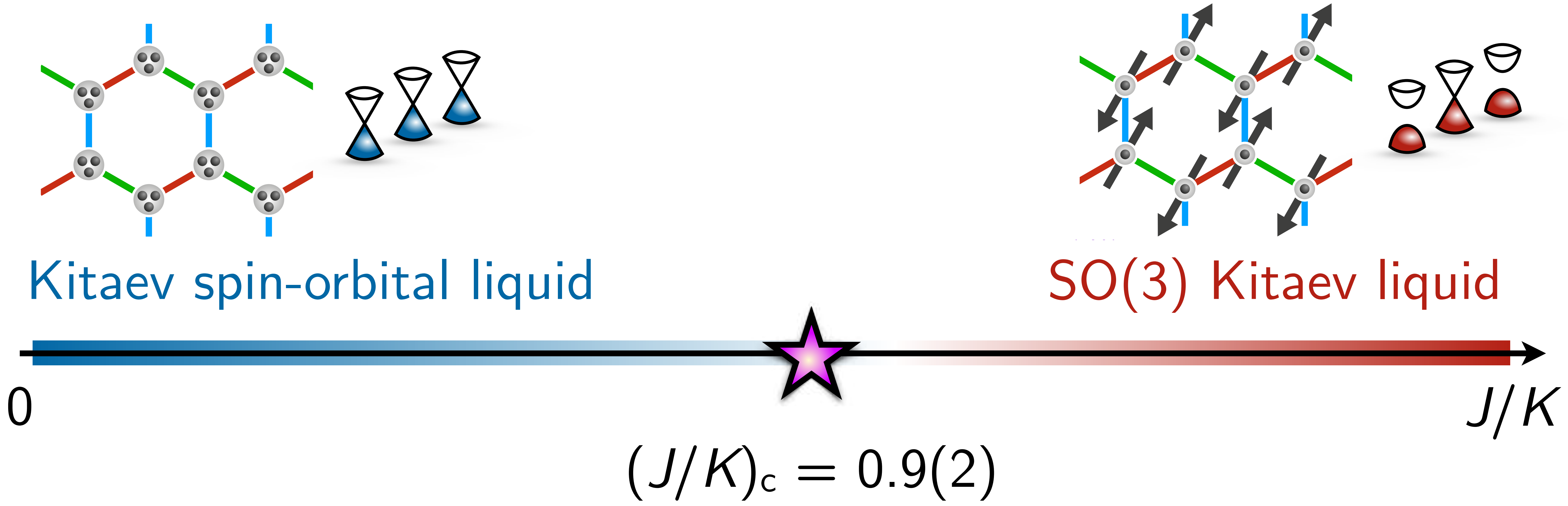

[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]

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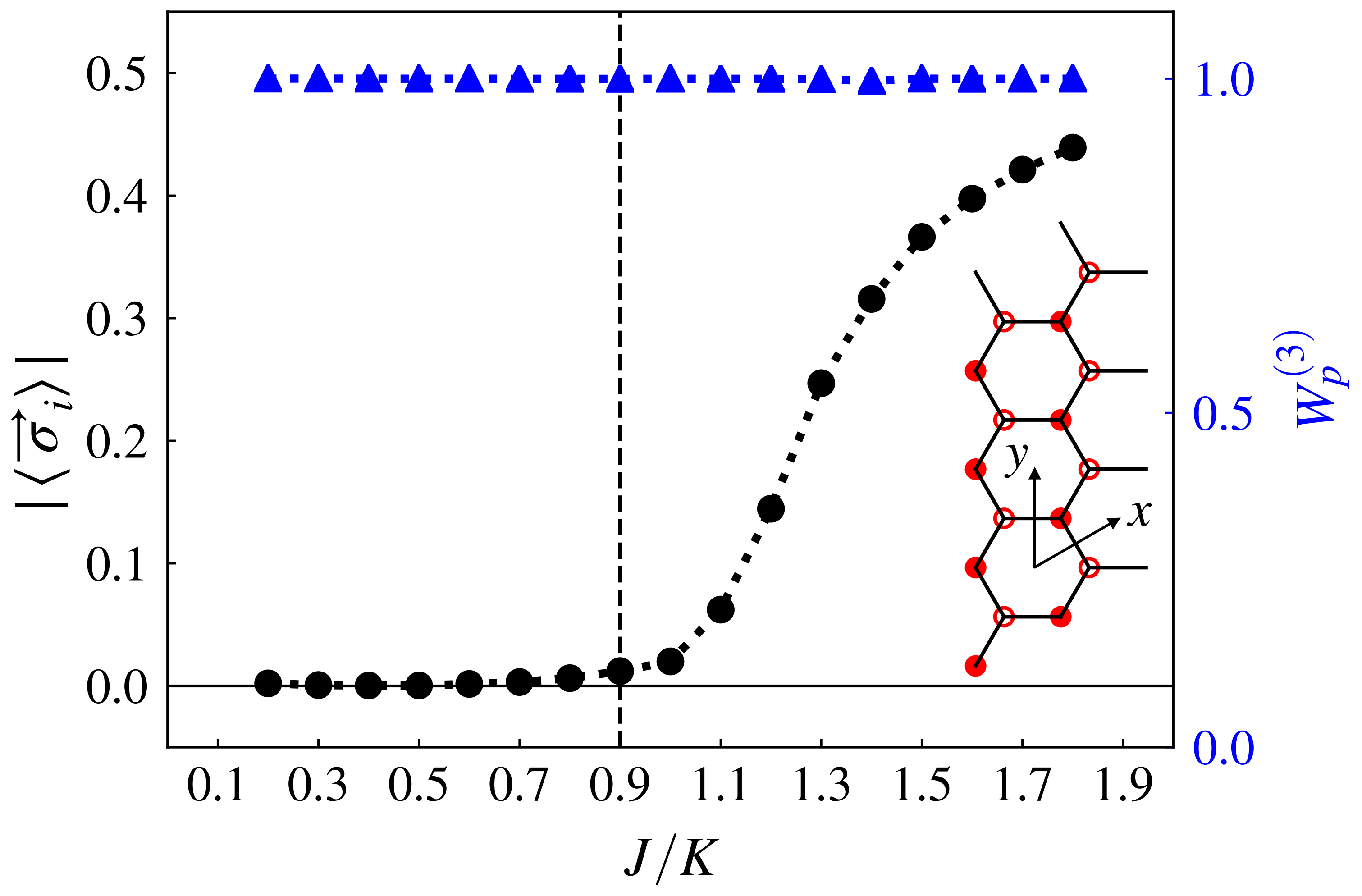


... on cylinder with $L_y = 4$ unit cells

Phase diagram:

[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)"*

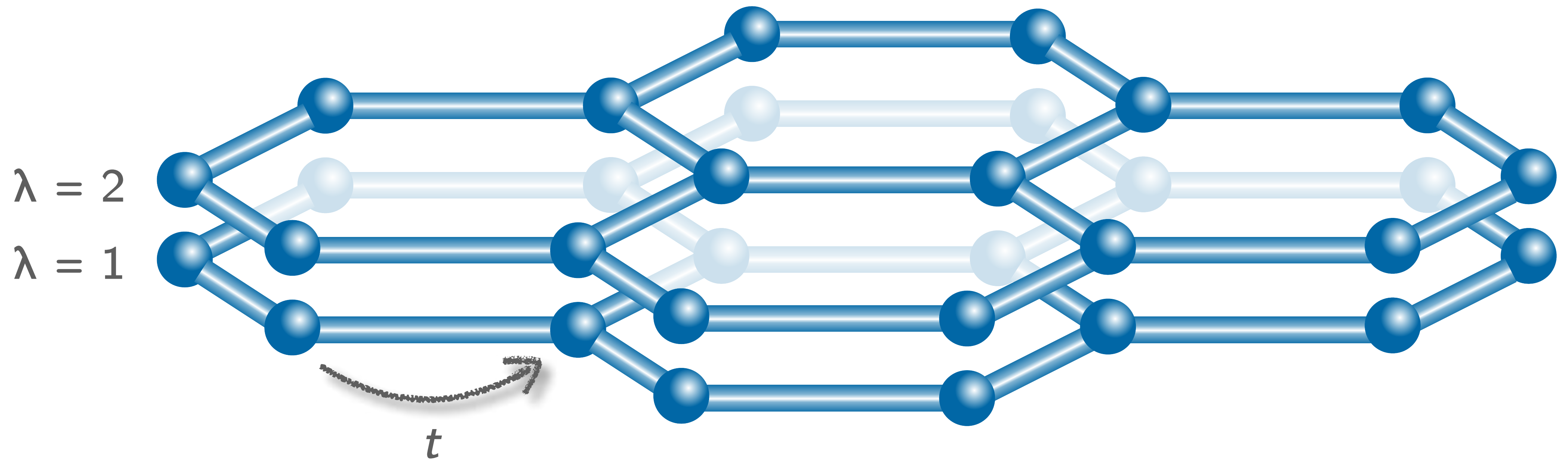
[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

Sign-problem-free bilayer model

Hamiltonian:

spin-1 matrices

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c^\dagger_{i\lambda} c_{j\lambda} - J \sum_i \left(c^\dagger_{i\lambda} \vec{L} \tau^z_{\lambda\lambda'} c_{i\lambda'} \right)^2$$



... with $SO(3) \times U_\lambda(1) \times U_c \times \mathbb{Z}_2$ symmetry

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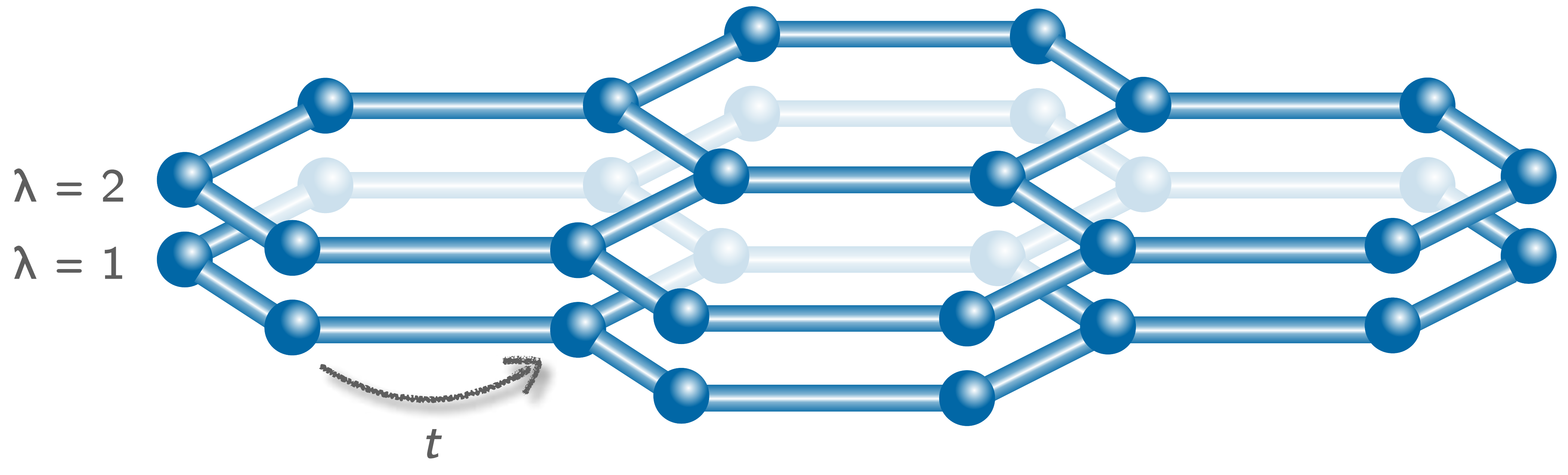

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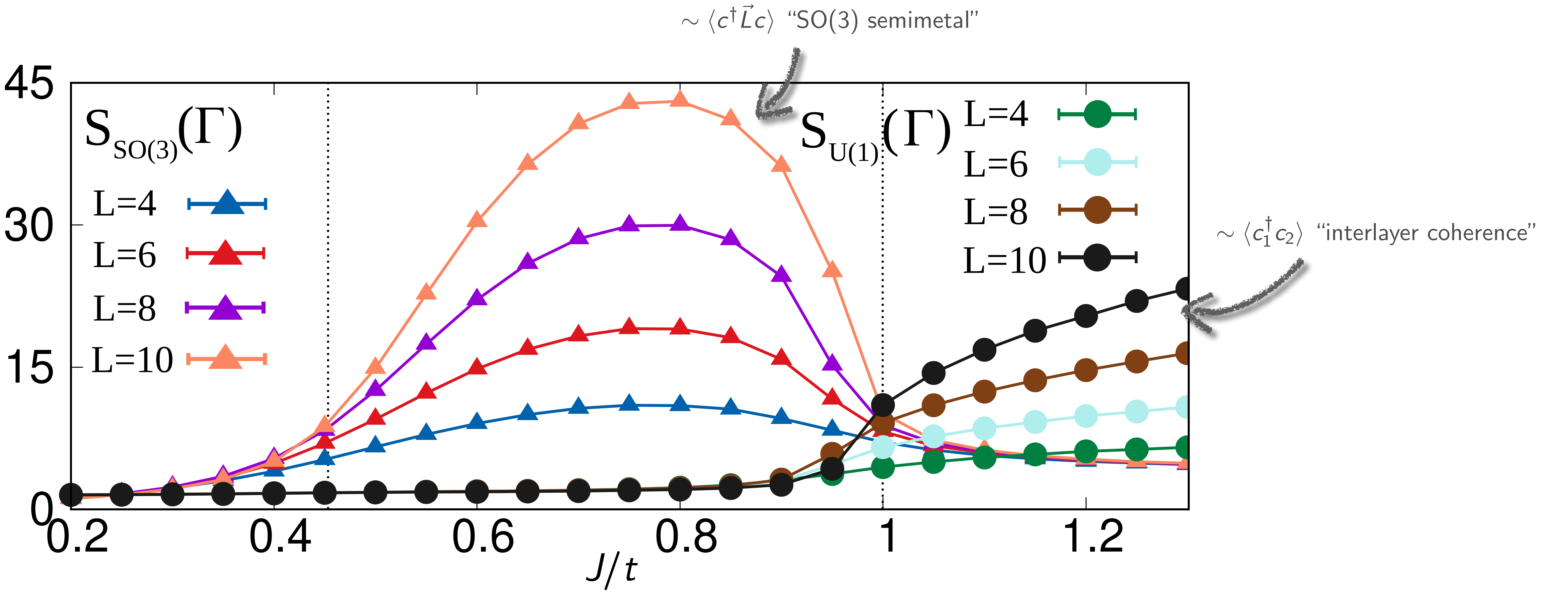
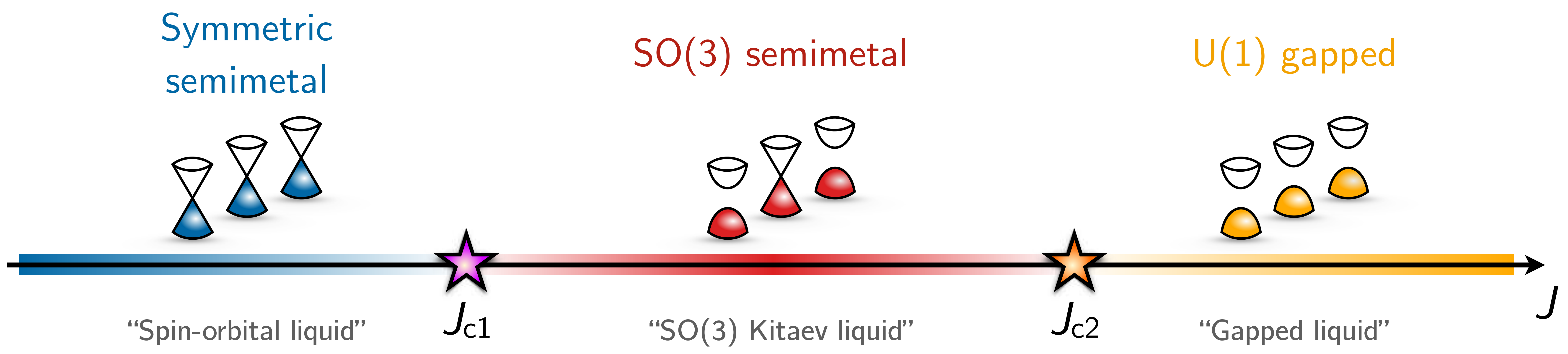
QMC structure factors:



Sign-problem-free bilayer model

Phase diagram:



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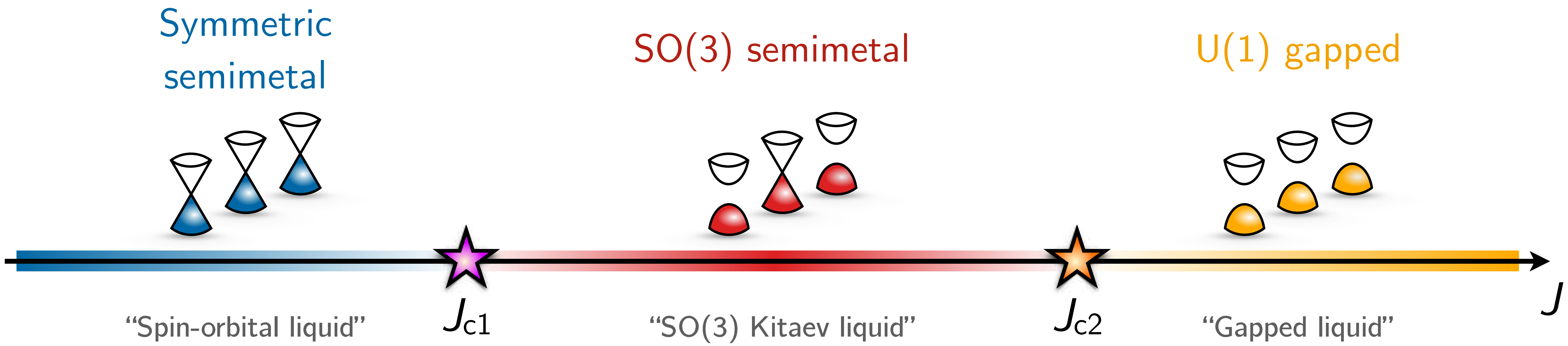
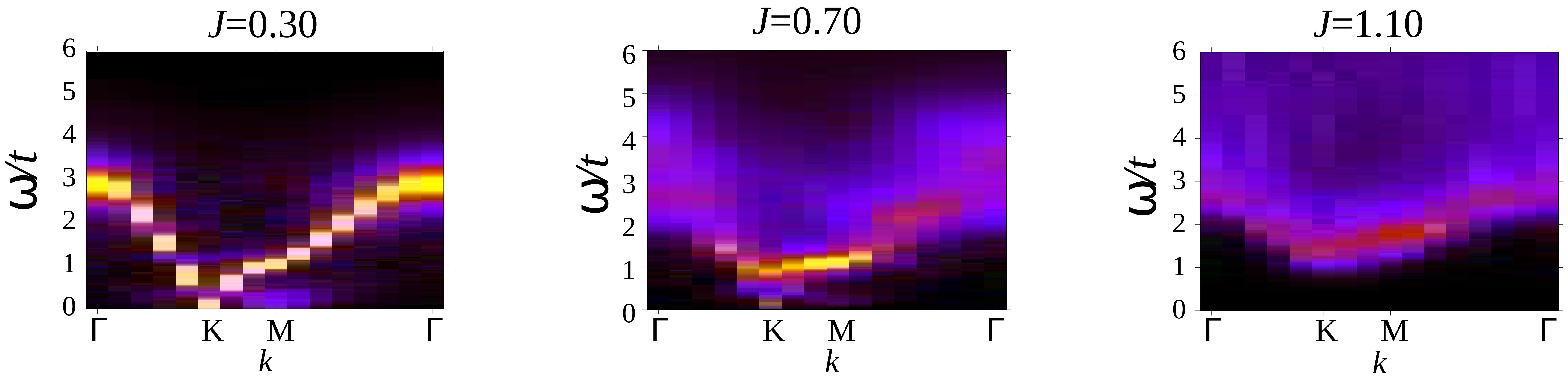


Fermion spectral function:



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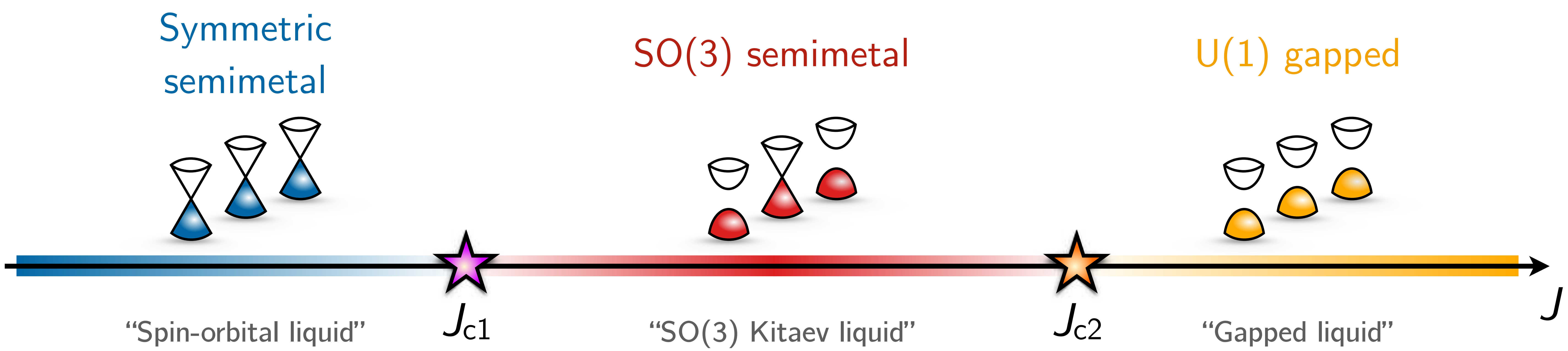

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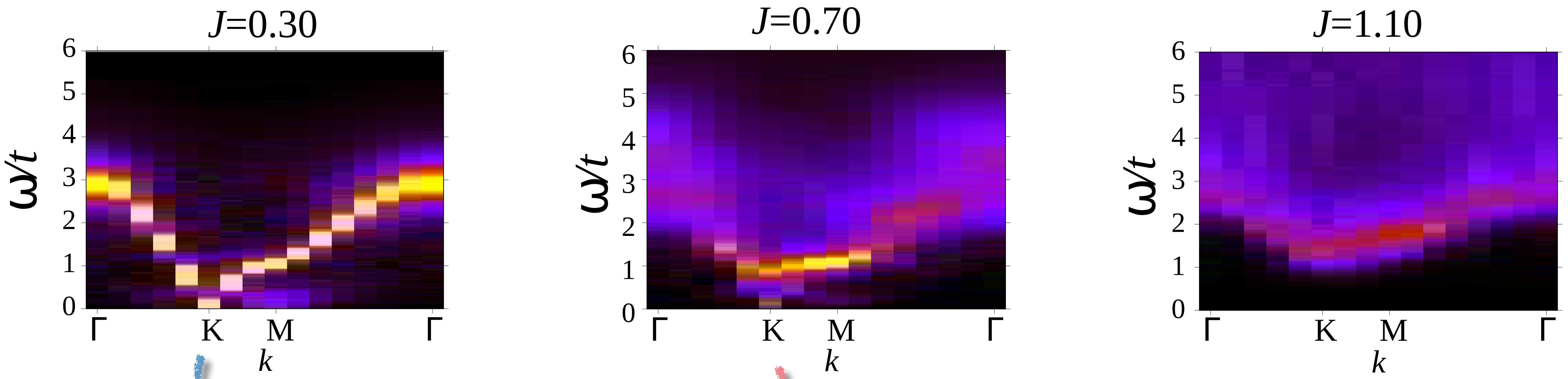
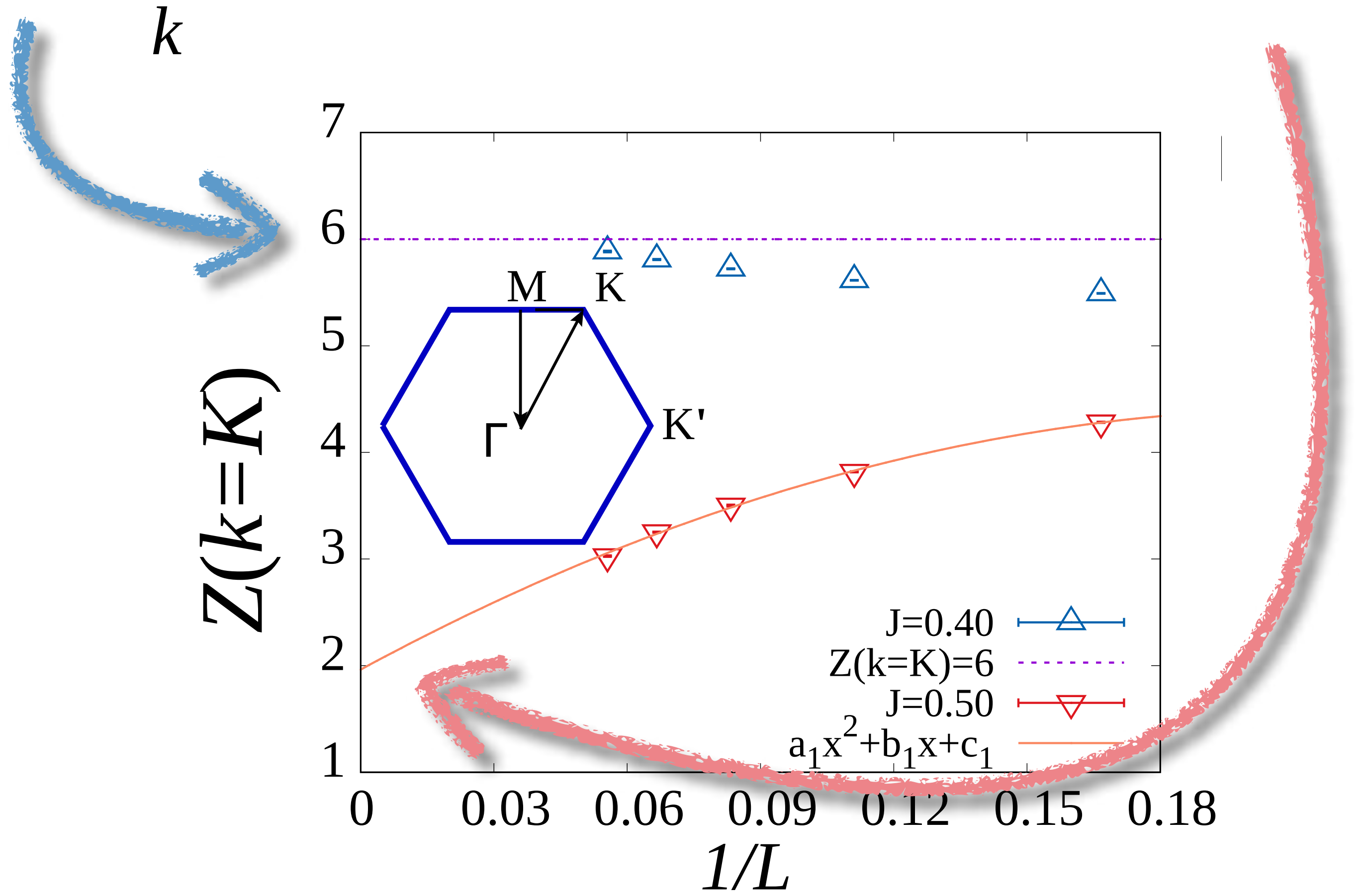
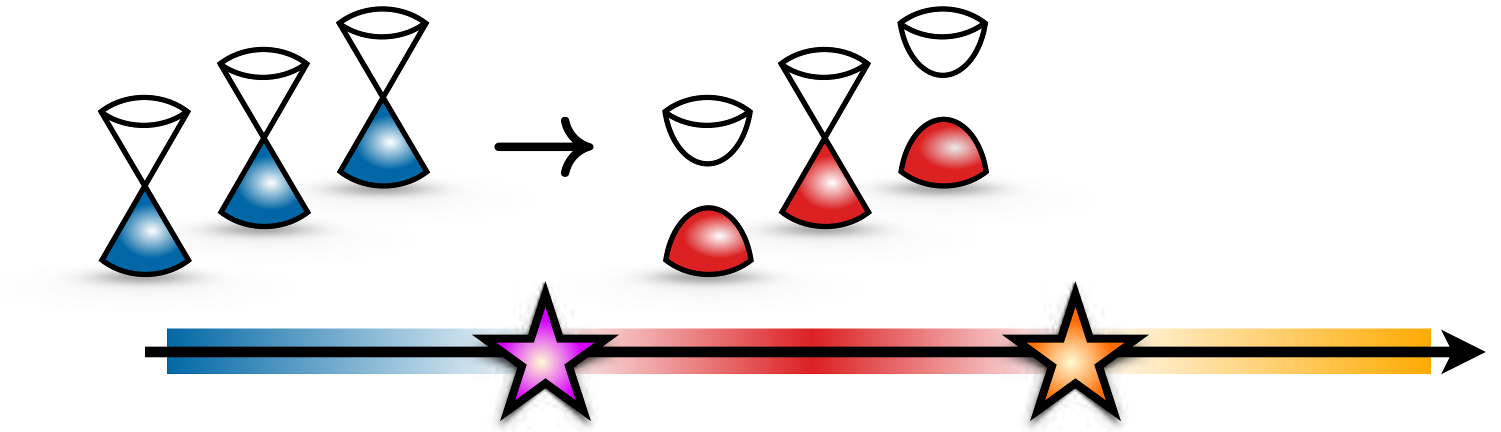


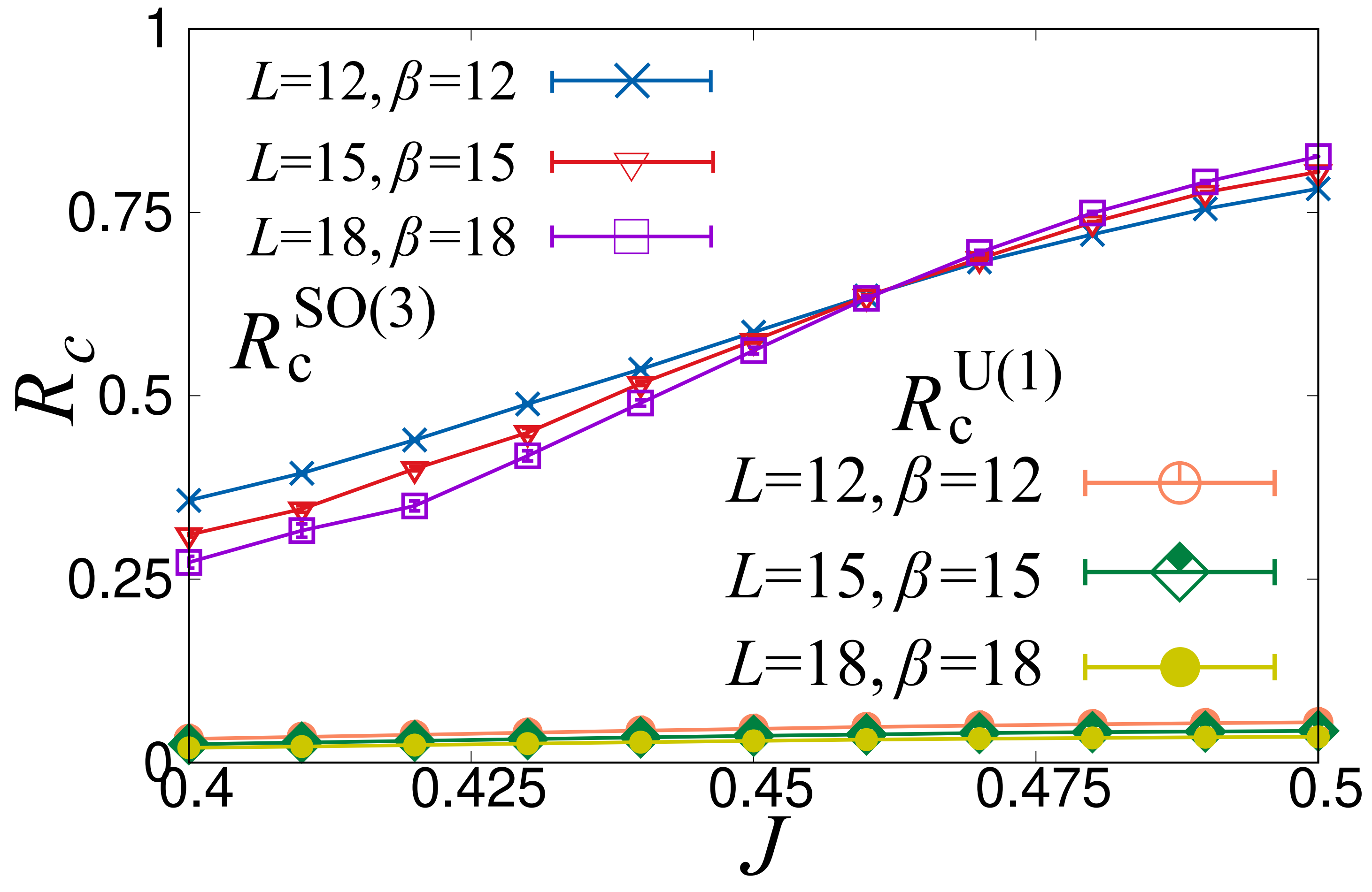
Quasiparticle weight:

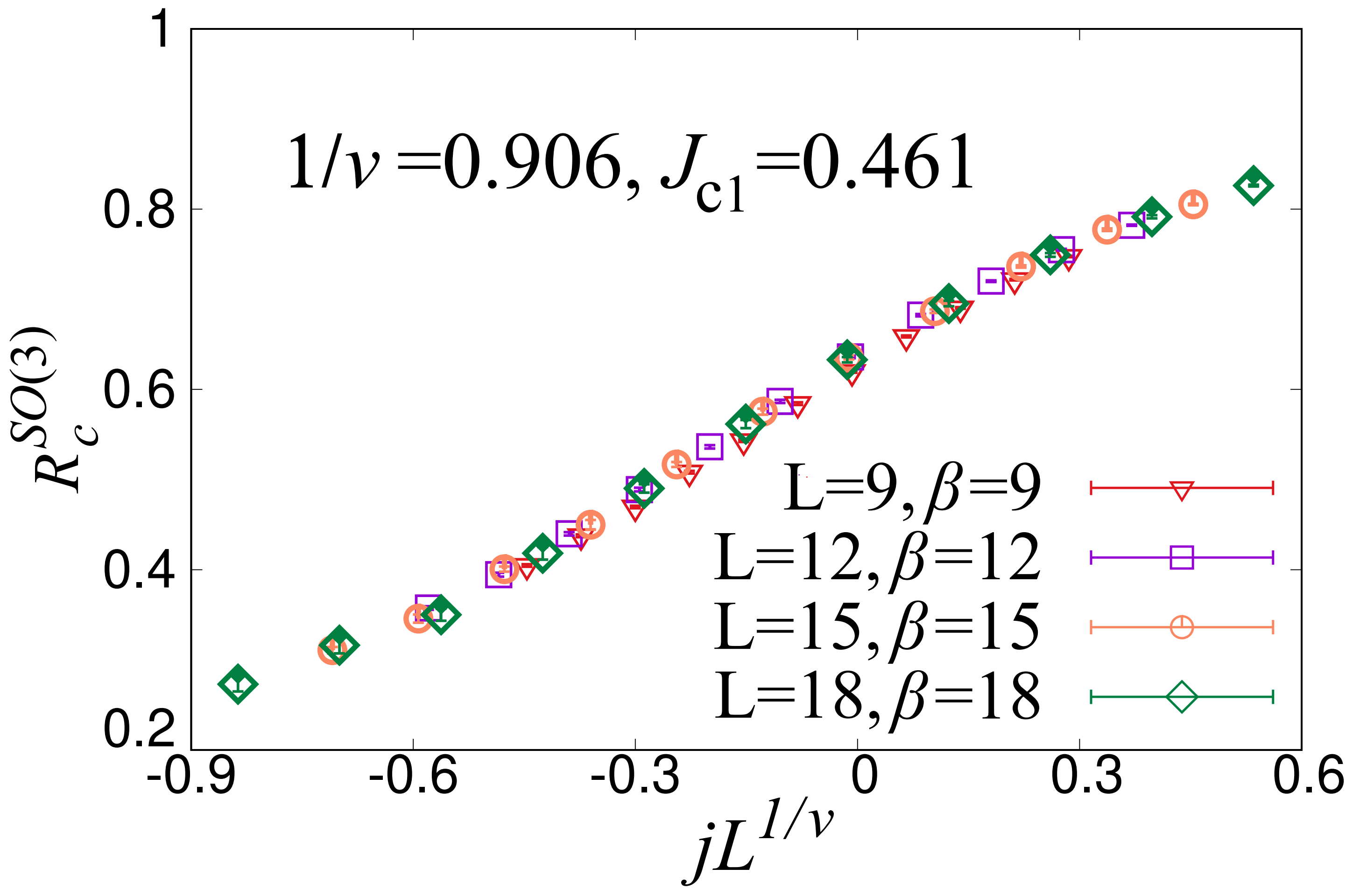


Gross-Neveu-SO(3) transition at J_{c1}



Correlation ratio: $$R_c = 1 - \frac{S(\Gamma + d\vec{k})}{S(\Gamma)}$$





$\Rightarrow \quad 1/\nu = 0.906(35)$

... cf. $1/\nu = 0.93(4)$ and $\eta_\phi = 0.83(4)$ from field theory ($N = 12$)
[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

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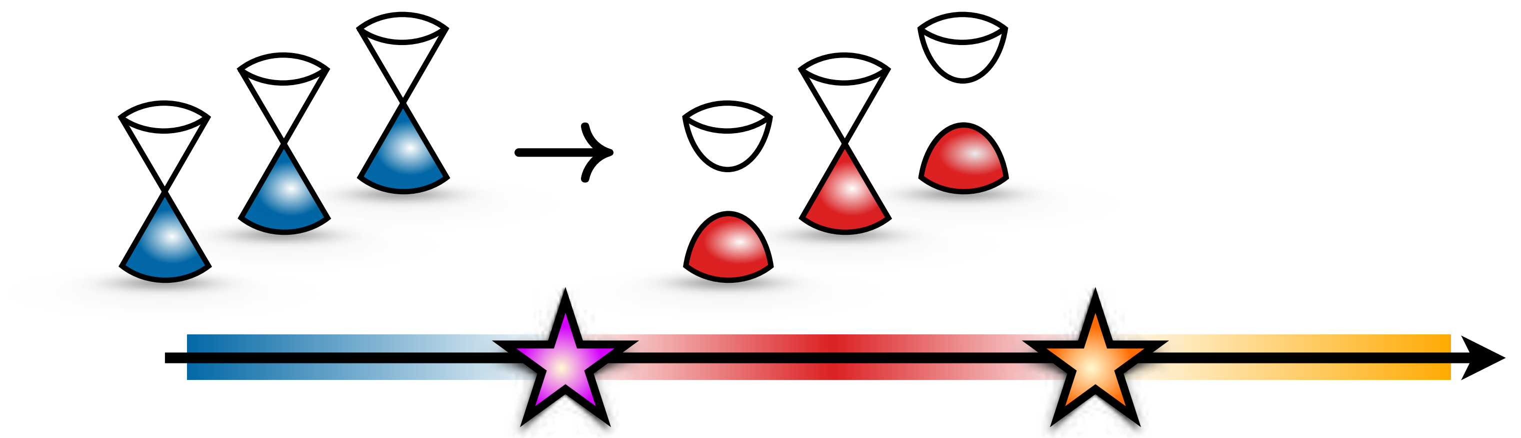

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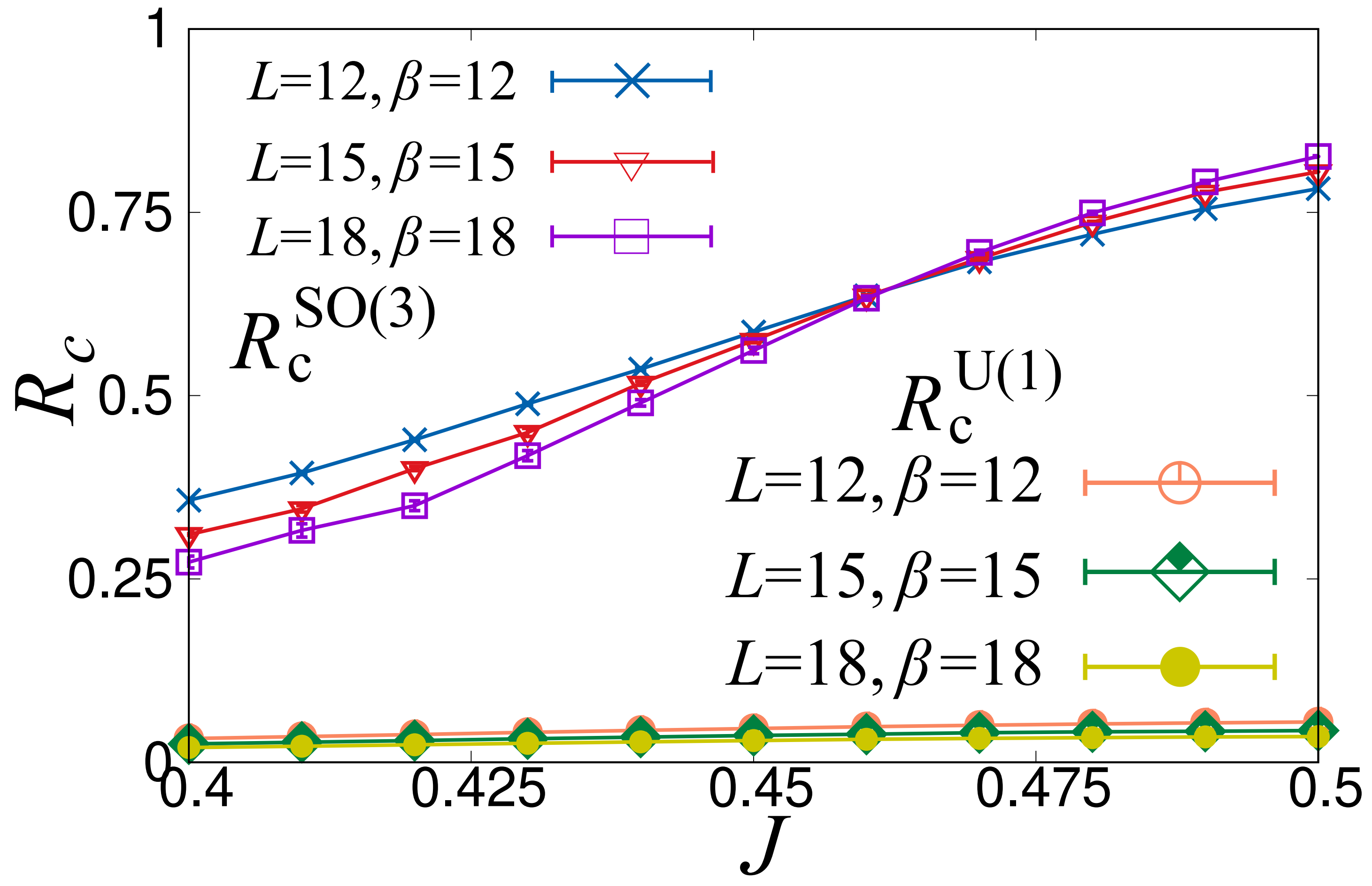
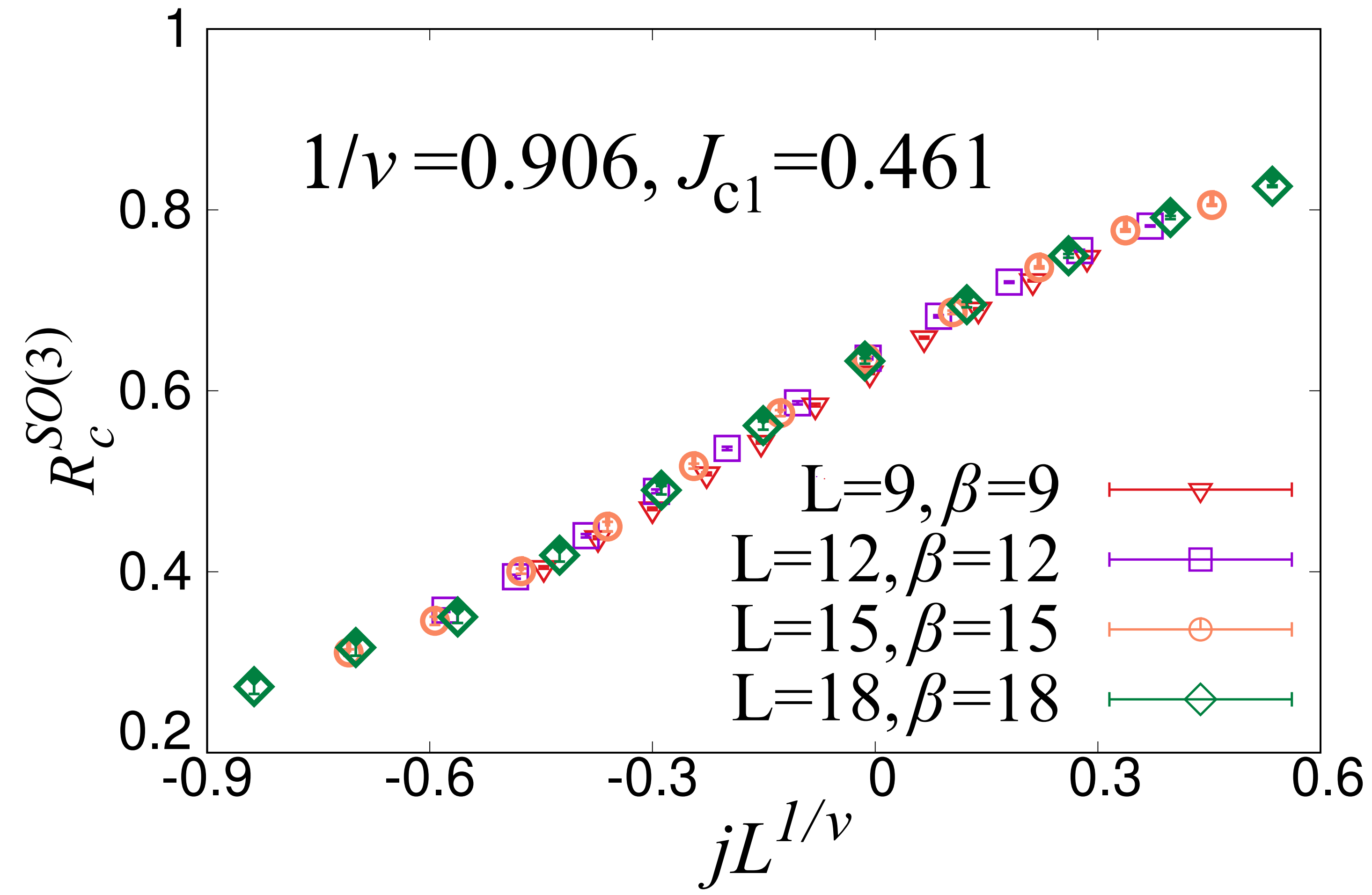
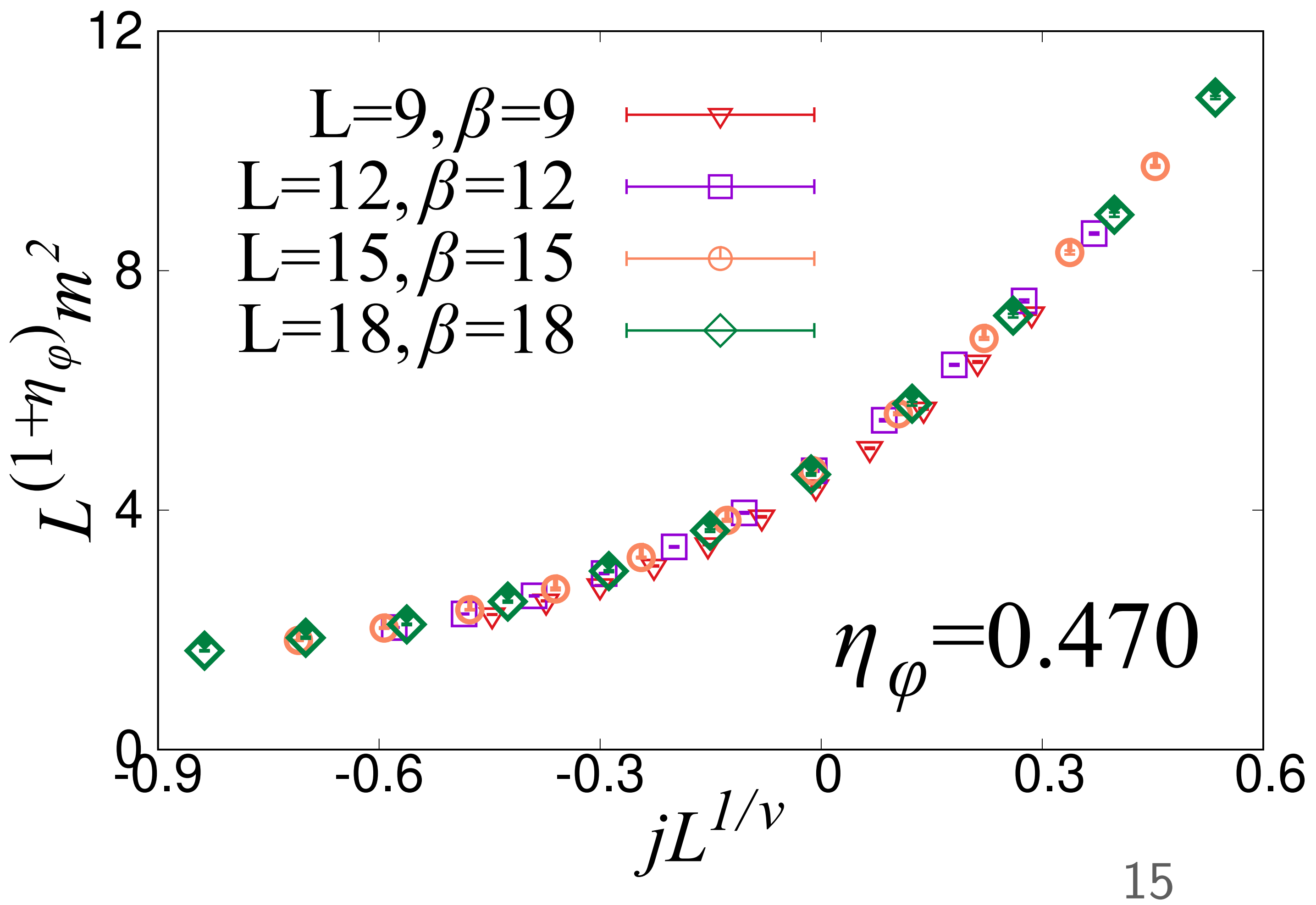




$\Rightarrow \quad 1/\nu = 0.906(35)$

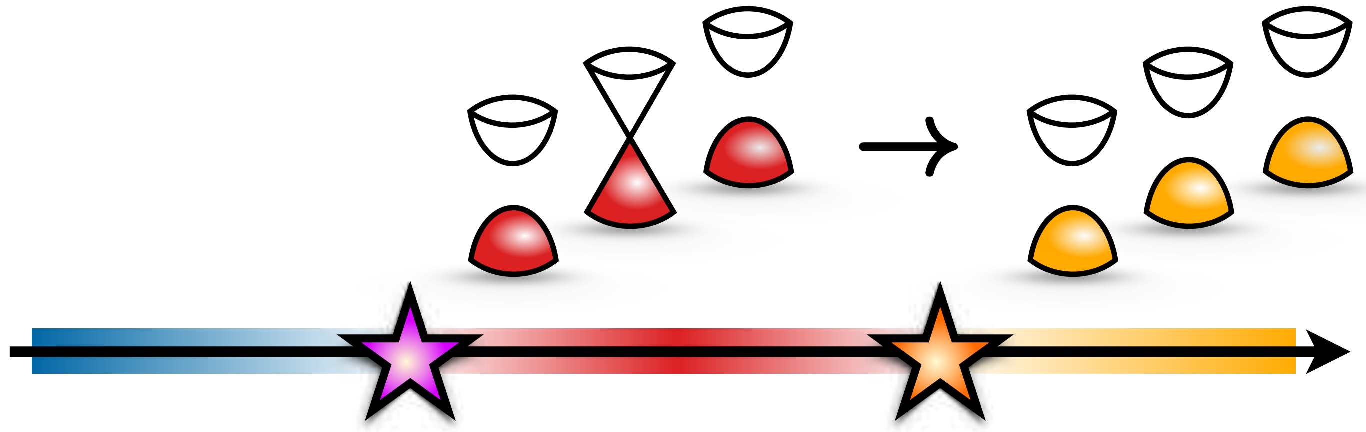
Order parameter:



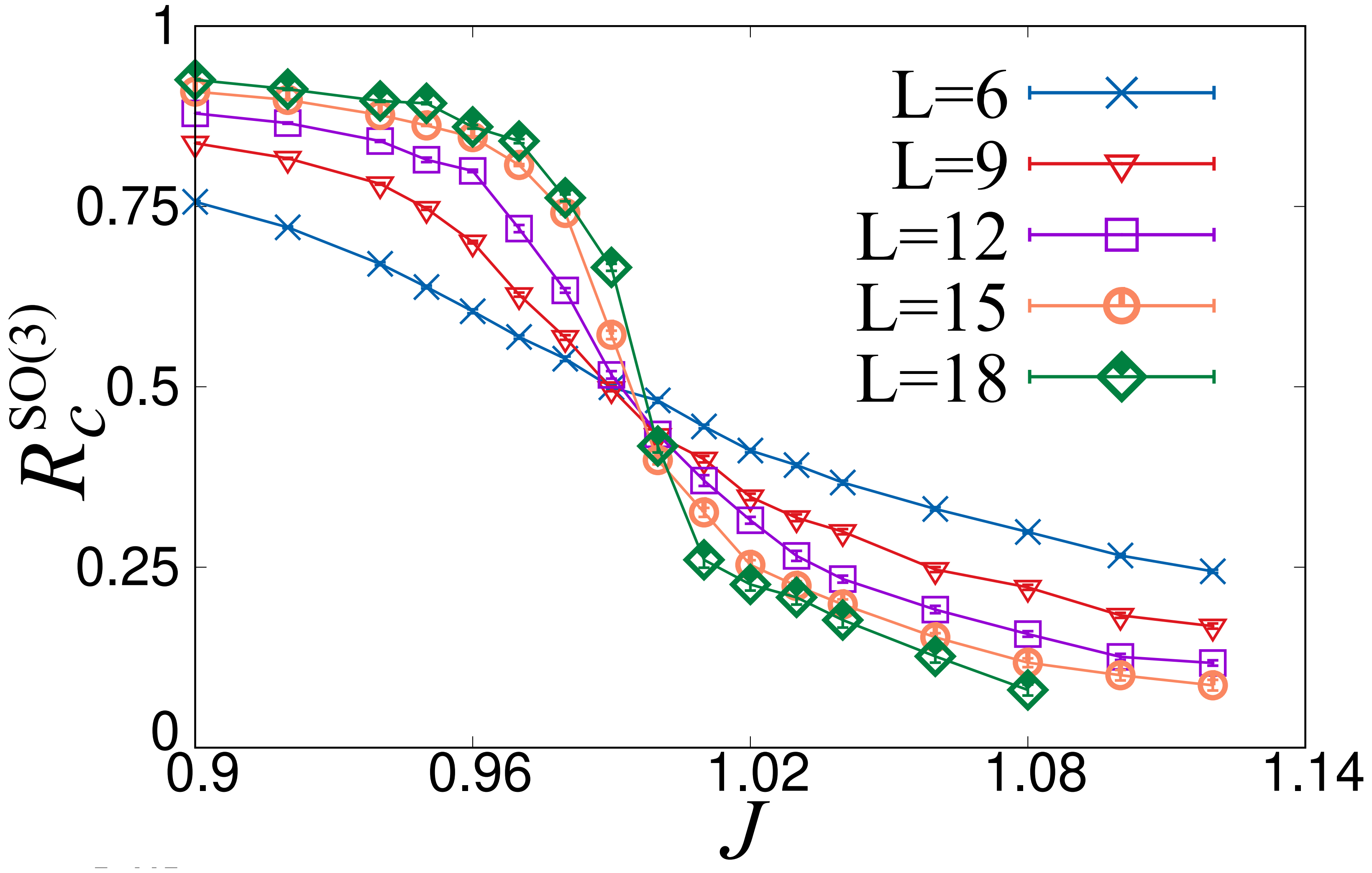
$\Rightarrow \quad \eta_\phi = 0.470(13)$

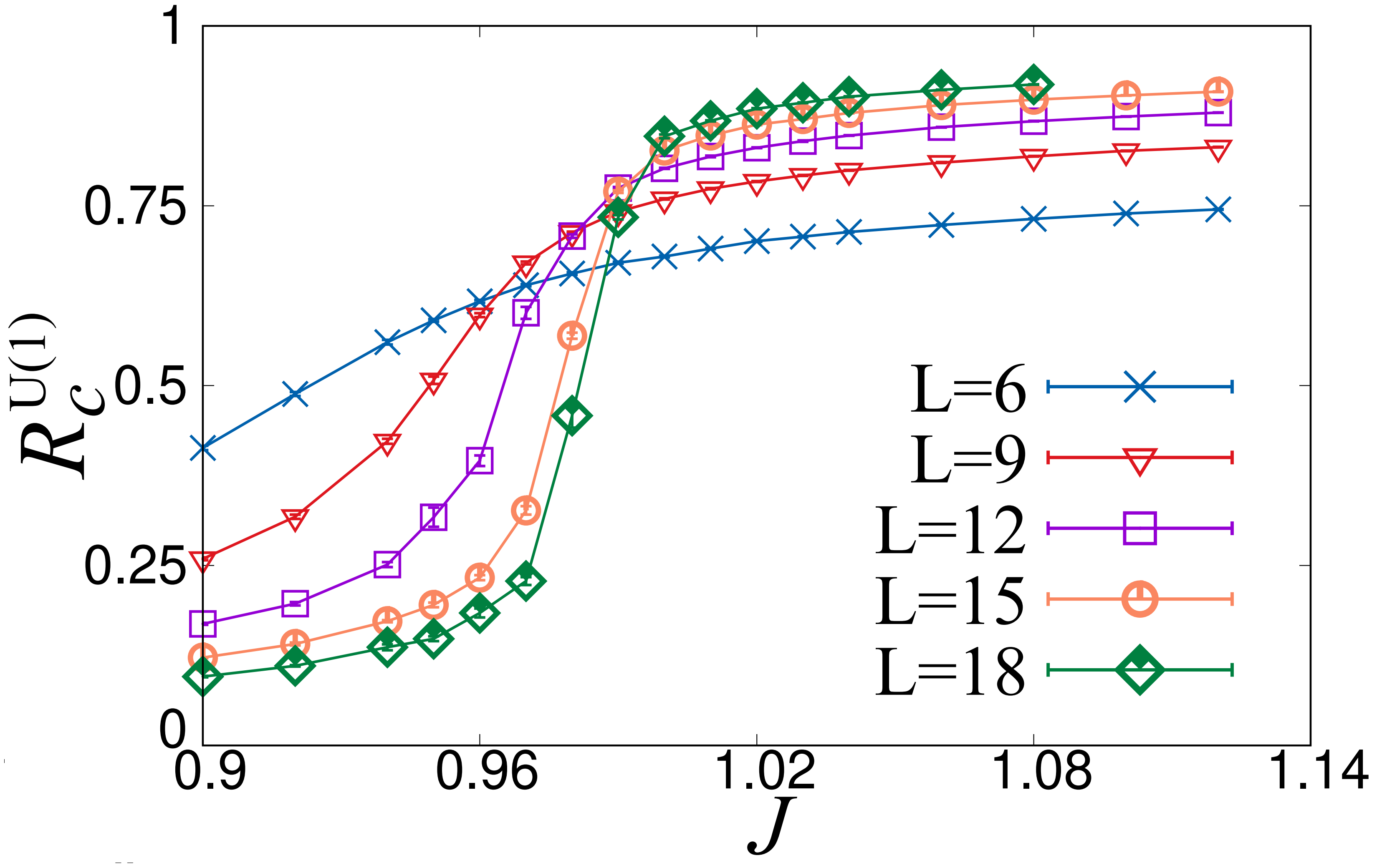
... cf. $1/\nu = 0.93(4)$ and $\eta_\phi = 0.83(4)$ from field theory ($N = 12$)
[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

Order-to-order transition at J_{c2}



Correlation ratios:





[Liu, Vojta, Assaad, LJ, PRL '22 (Editors' Suggestion)]

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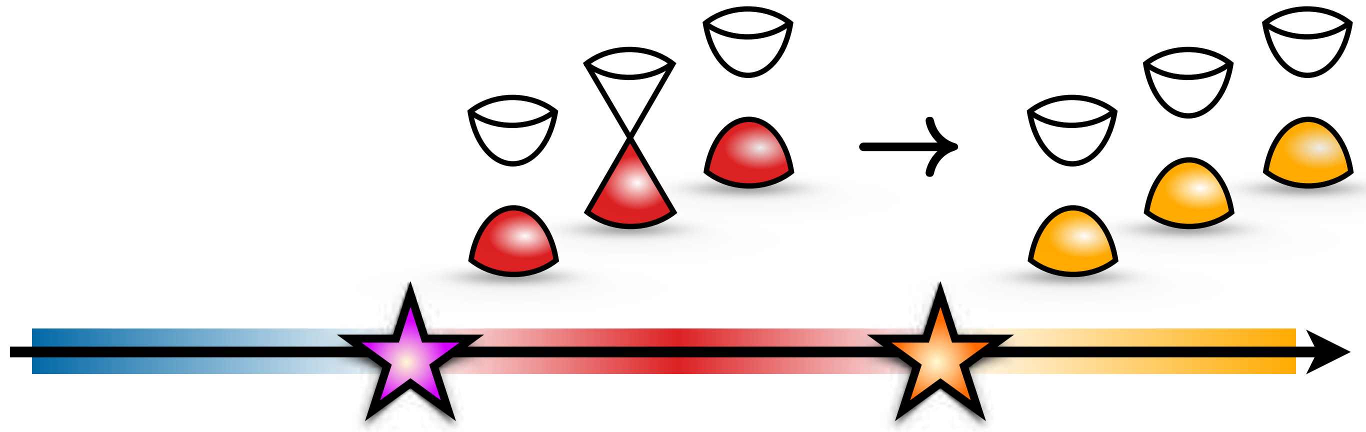

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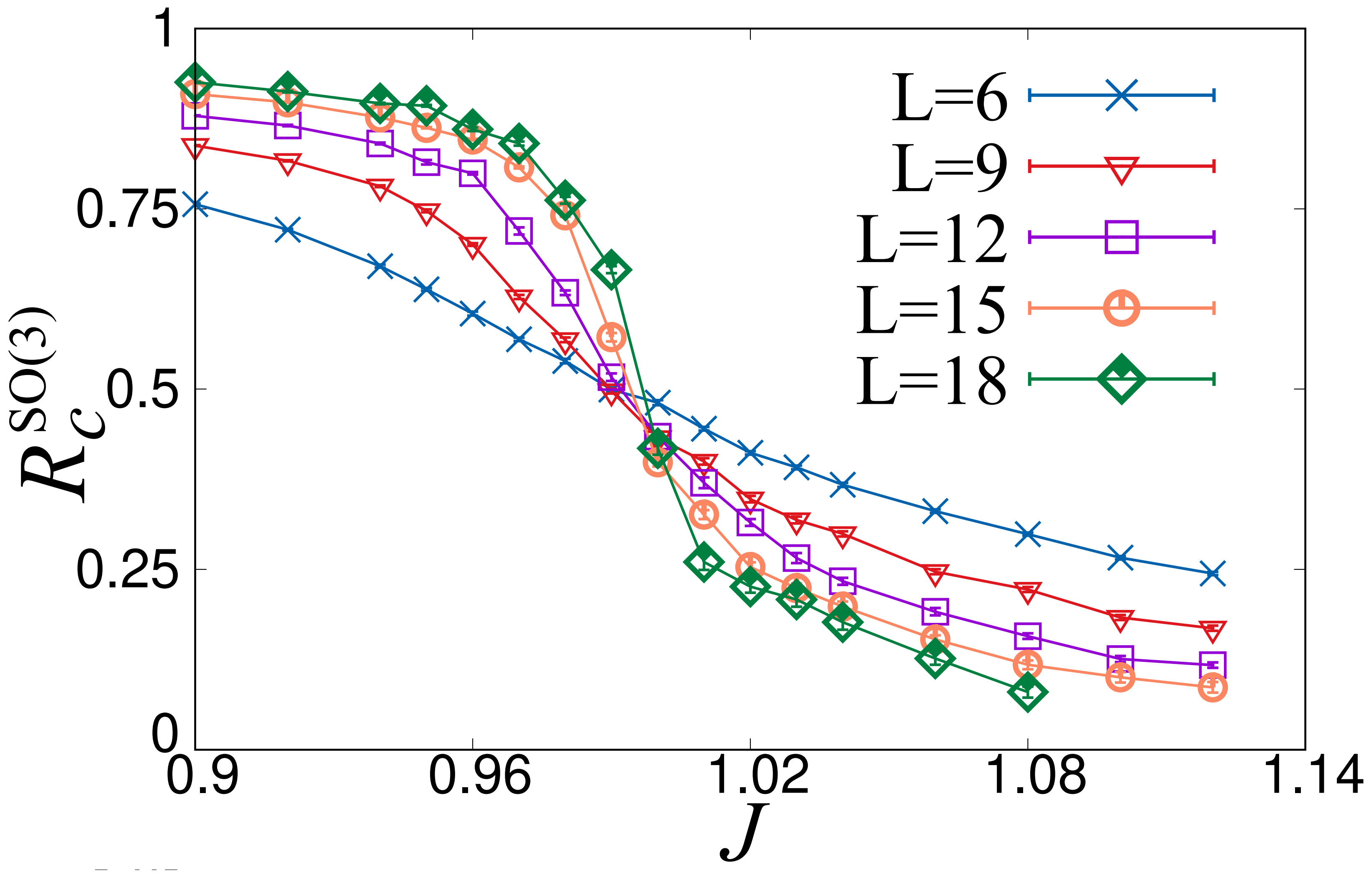
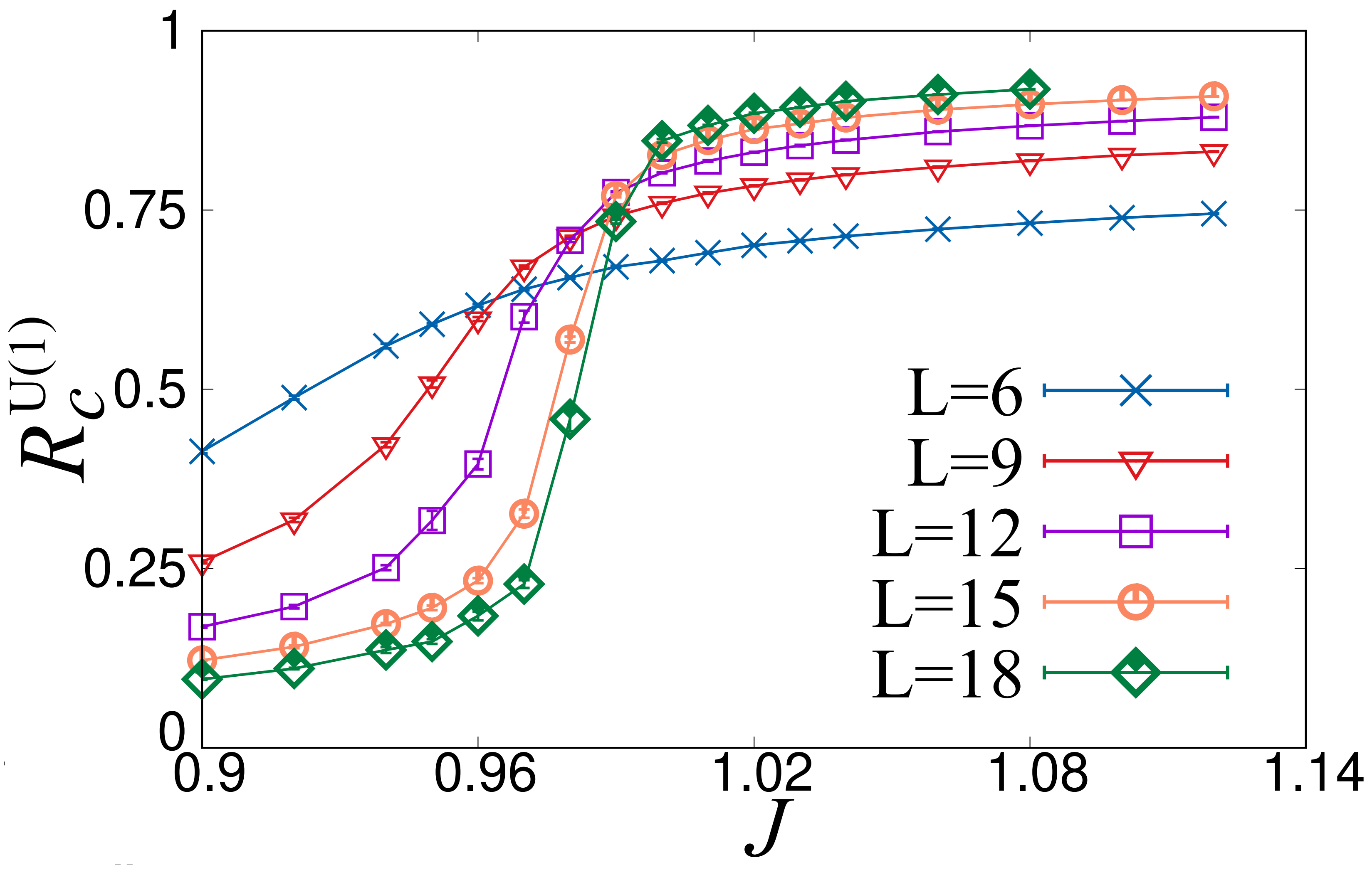
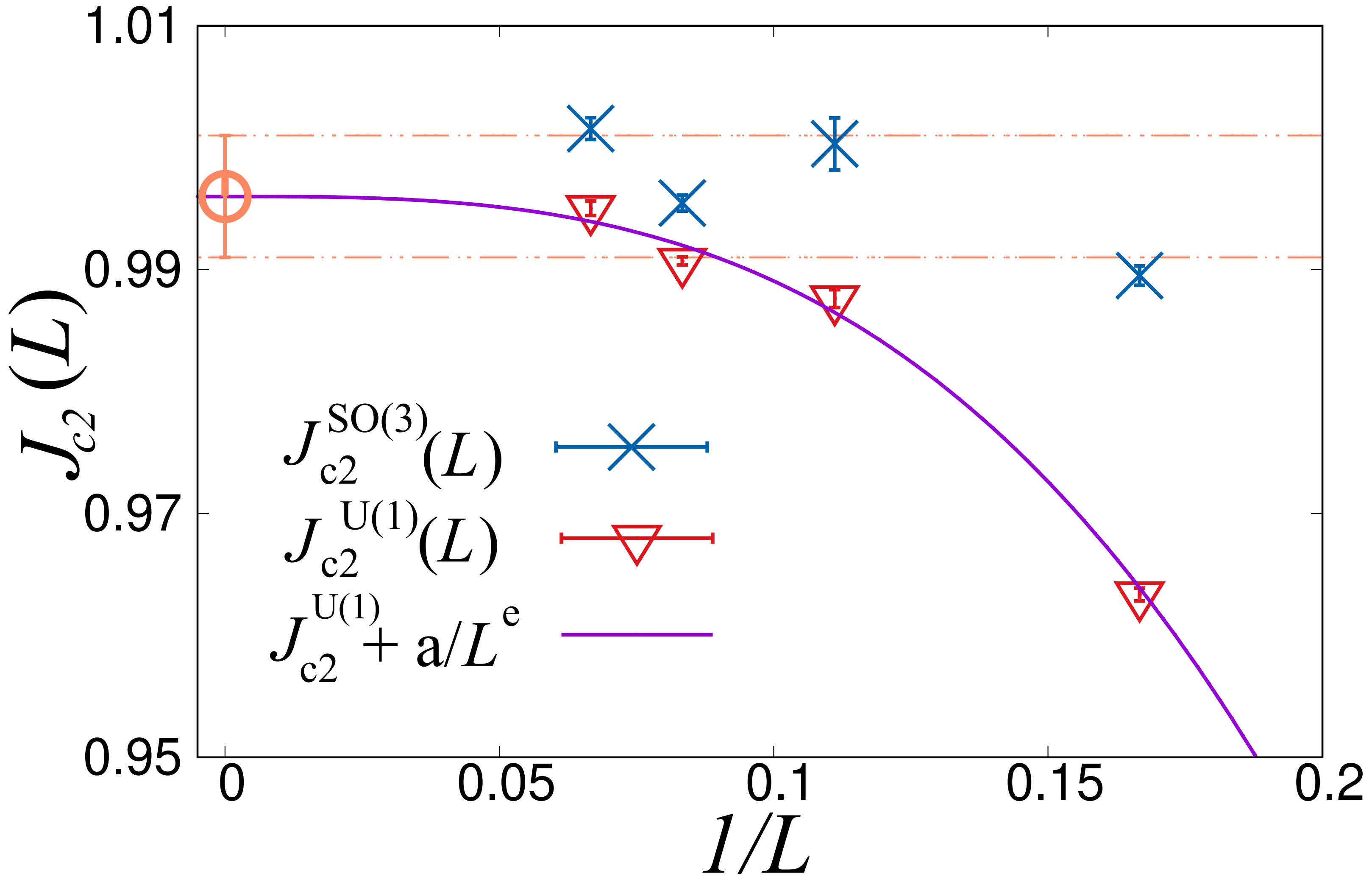




Critical couplings:



$\Rightarrow \quad J_{c2}^{SO(3)} = J_{c2}^{U(1)}$ unique!

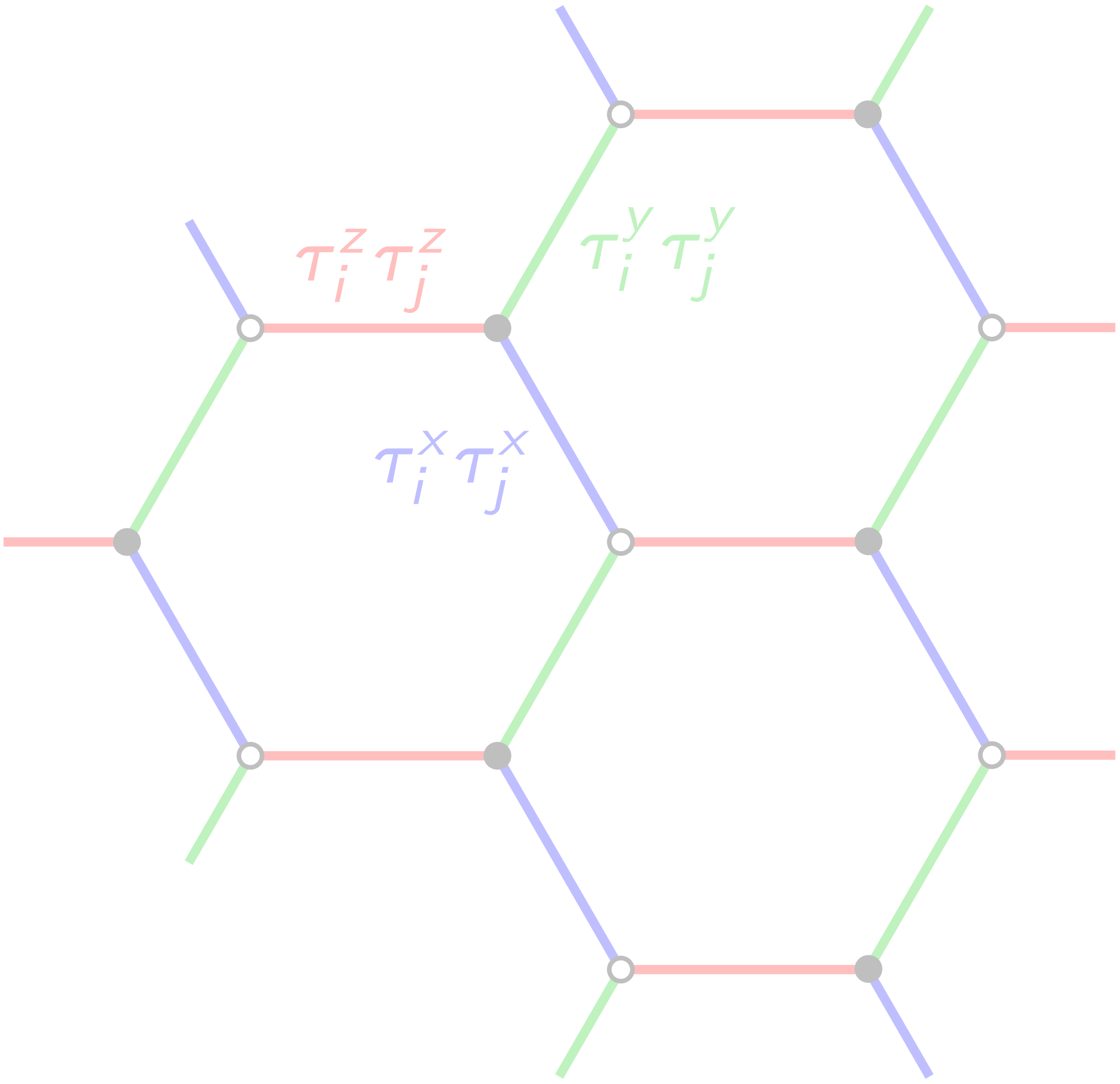
Metallic deconfined QCP?

[Liu, Vojta, Assaad, LJ, PRL '22 (Editors' Suggestion)]

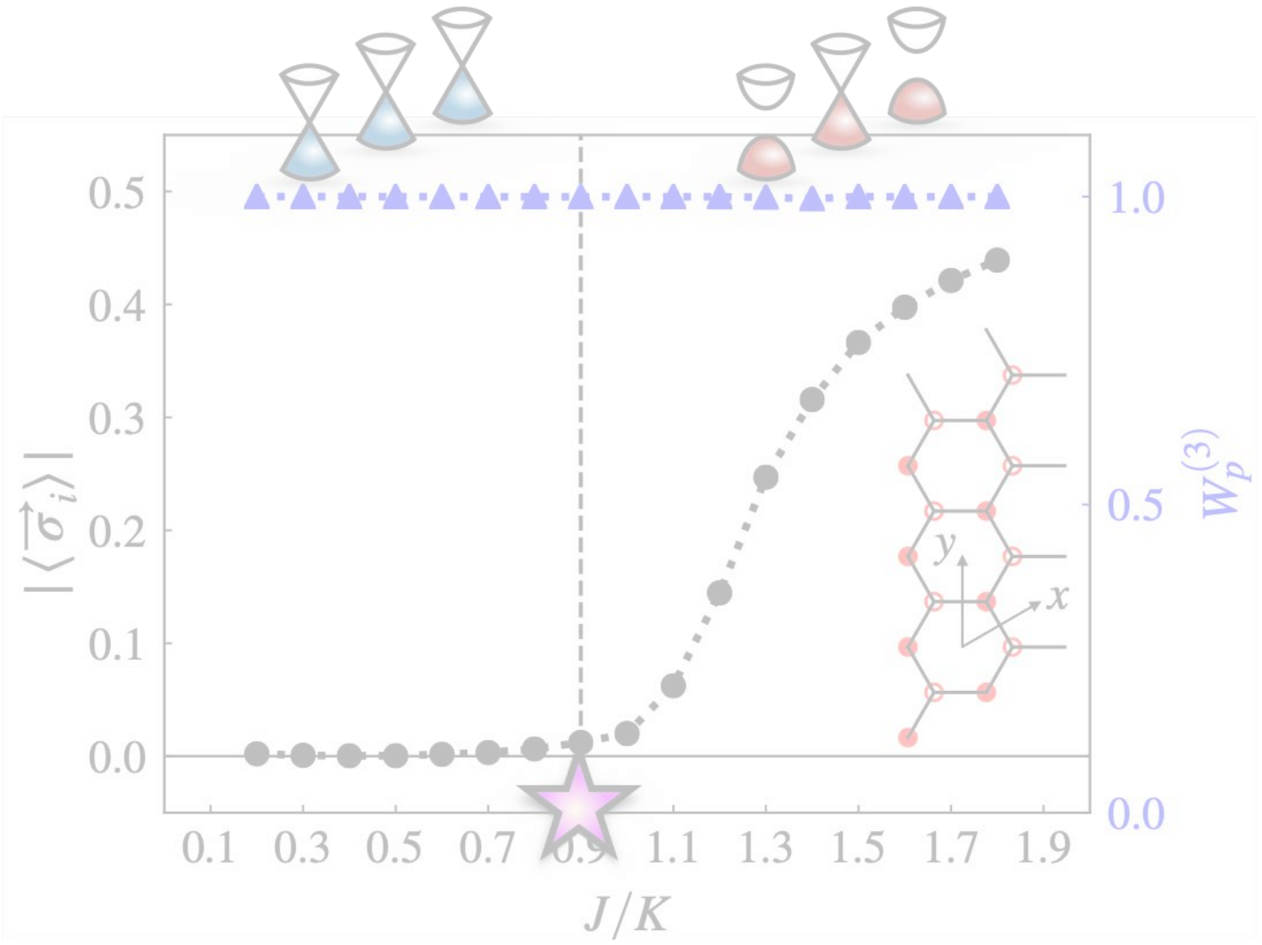
Outline

(1) Fractionalized quantum criticality

(2) From Kitaev to Kitaev-Kugel-Khomskii



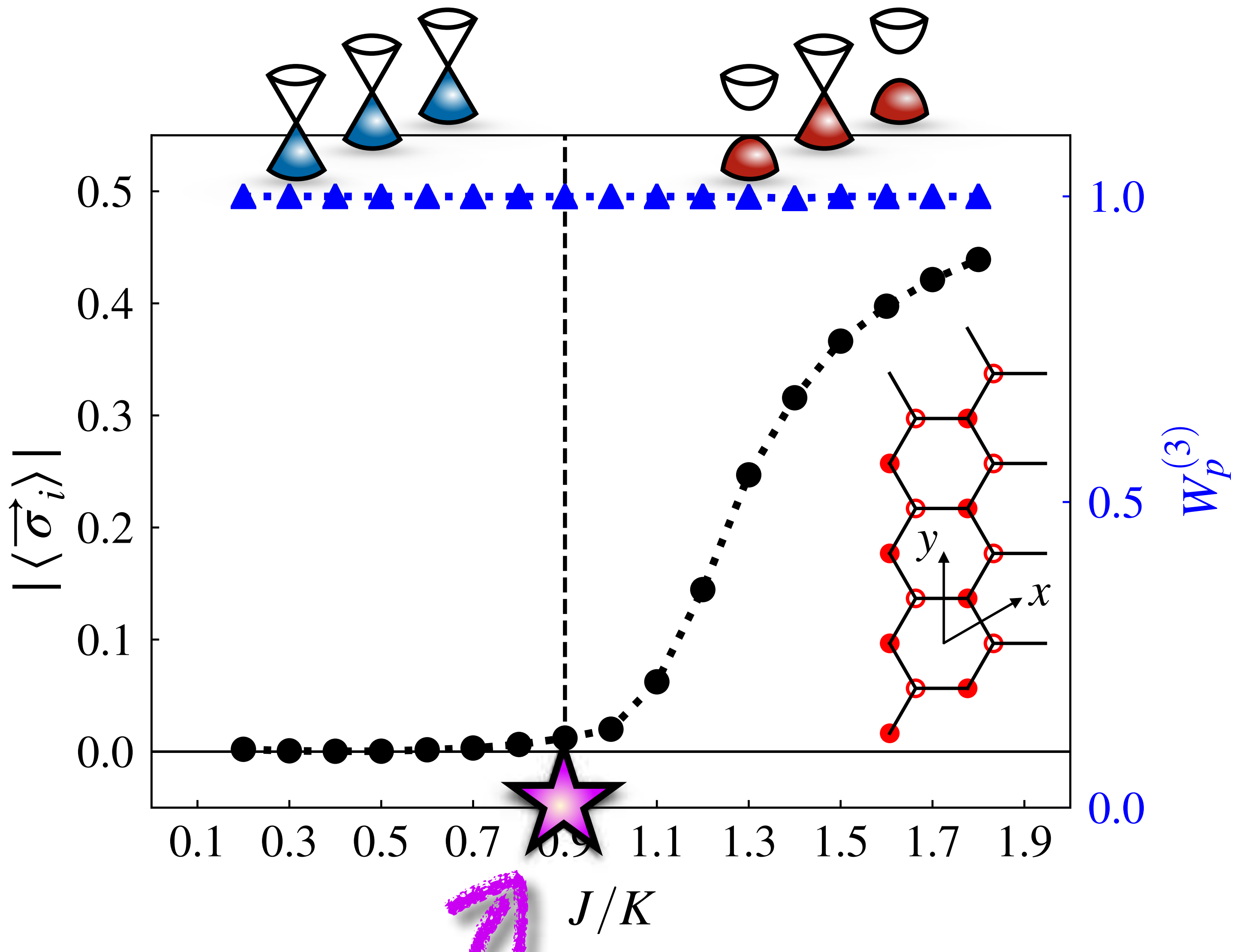
(3) Kitaev-Heisenberg spin-orbital models



(4) Conclusions

Conclusions

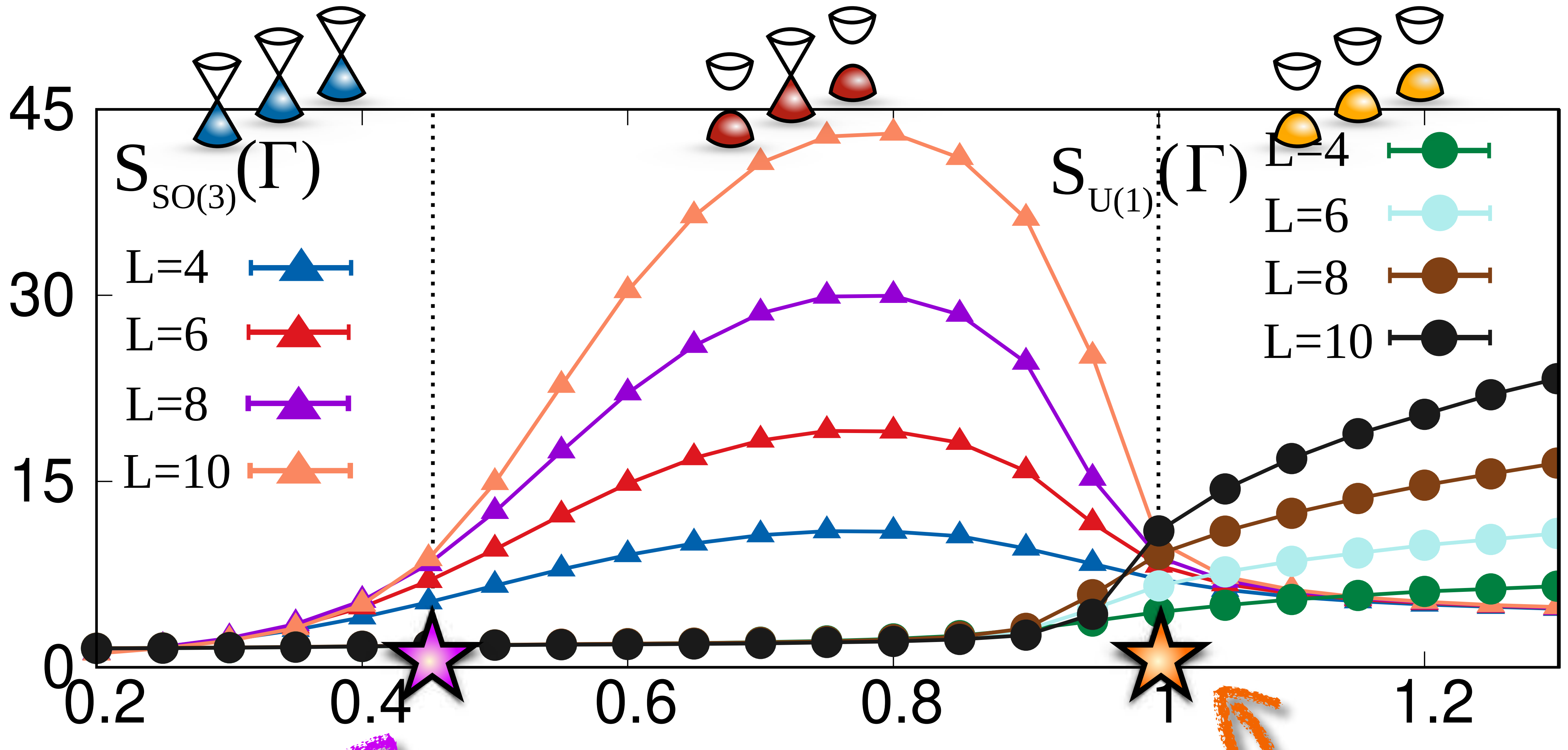
Kitaev-Heisenberg spin-orbital model:



Gross-Neveu-SO(3)*

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

Effective bilayer honeycomb model:

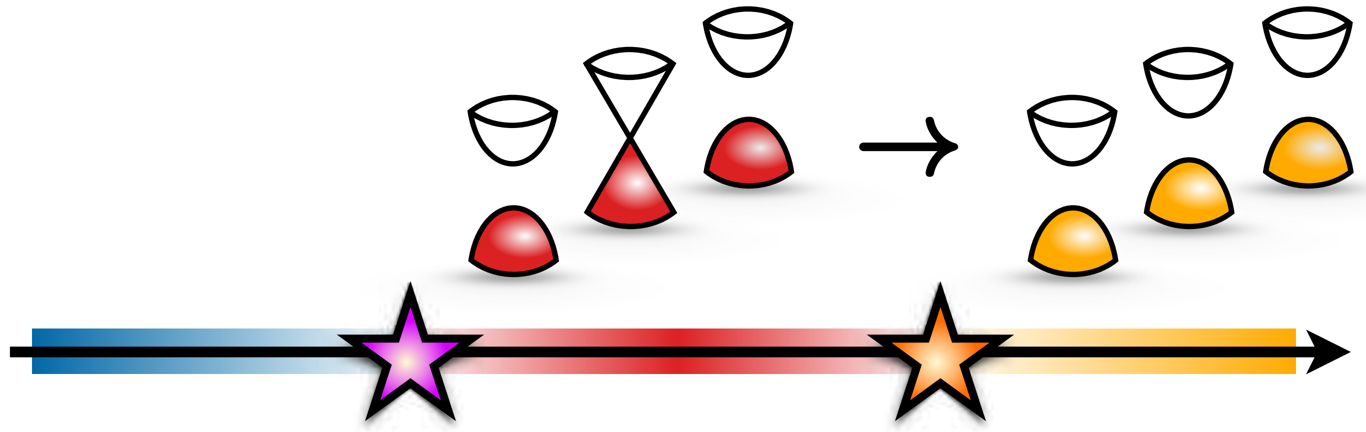


Gross-Neveu-SO(3)

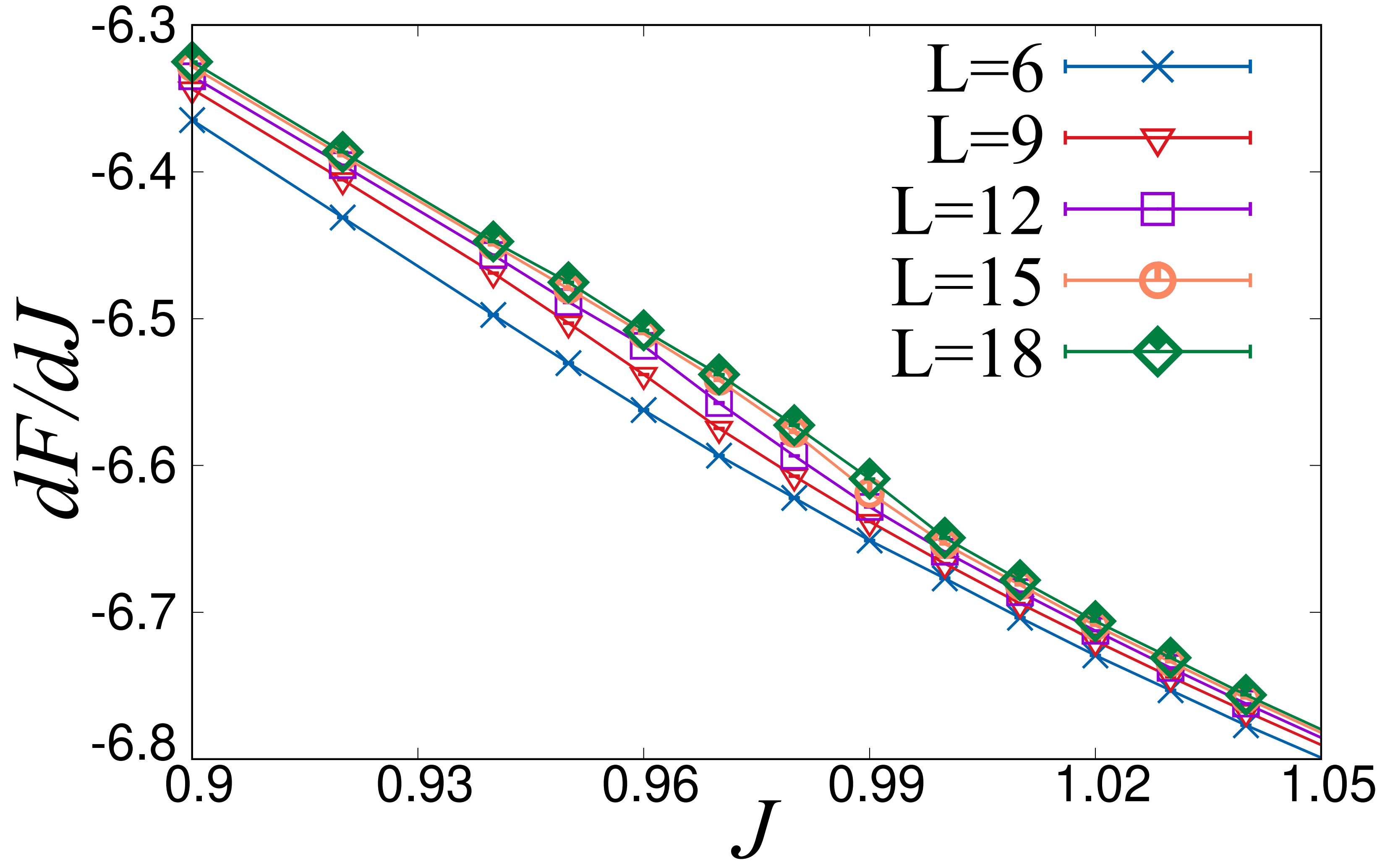
Metallic deconfined QCP?

[Liu, Vojta, Assaad, LJ, PRL '22 (Editors' Suggestion)]

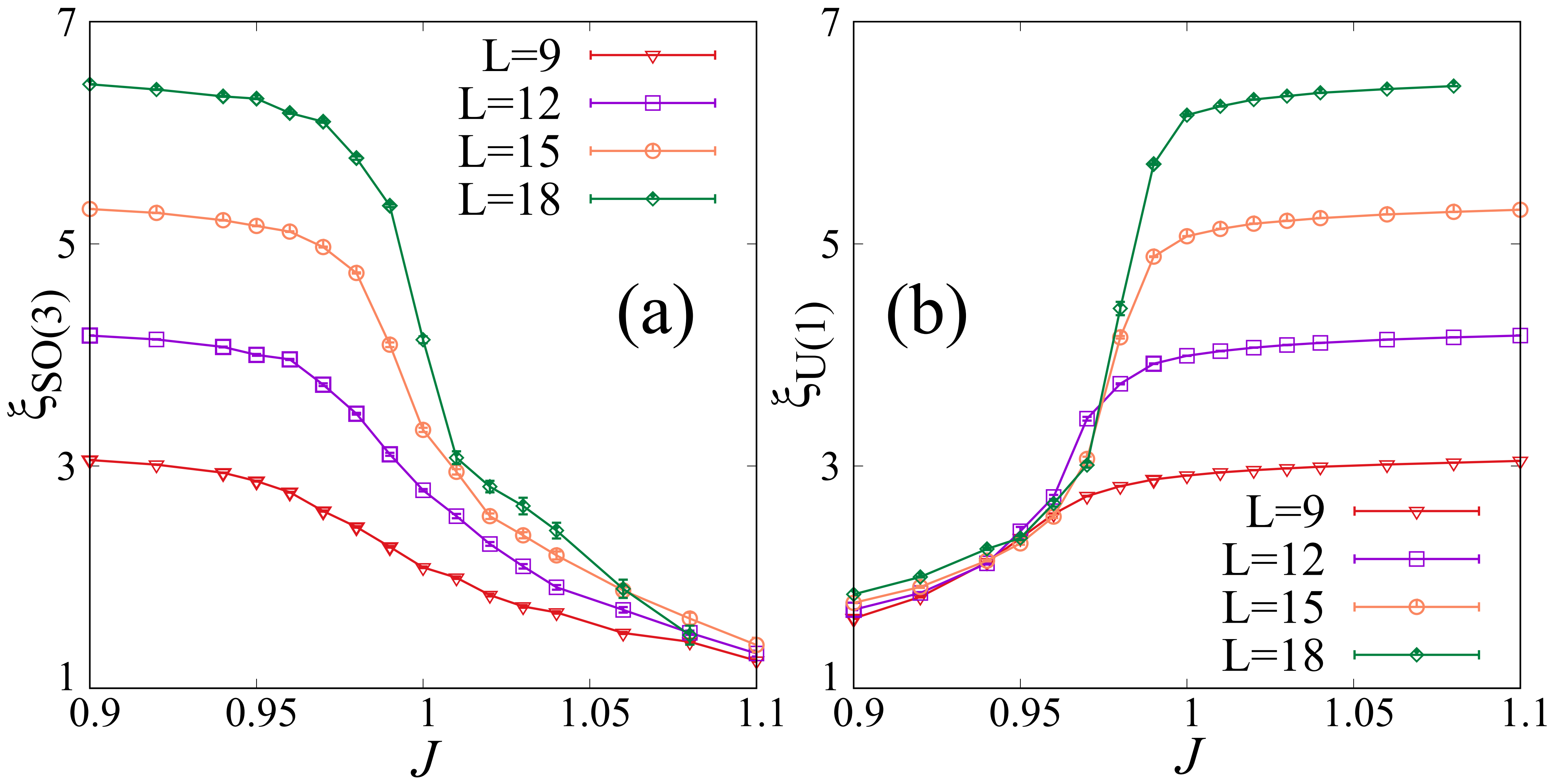
Order-to-order transition at J_{c2}



Free energy:



Correlation lengths:

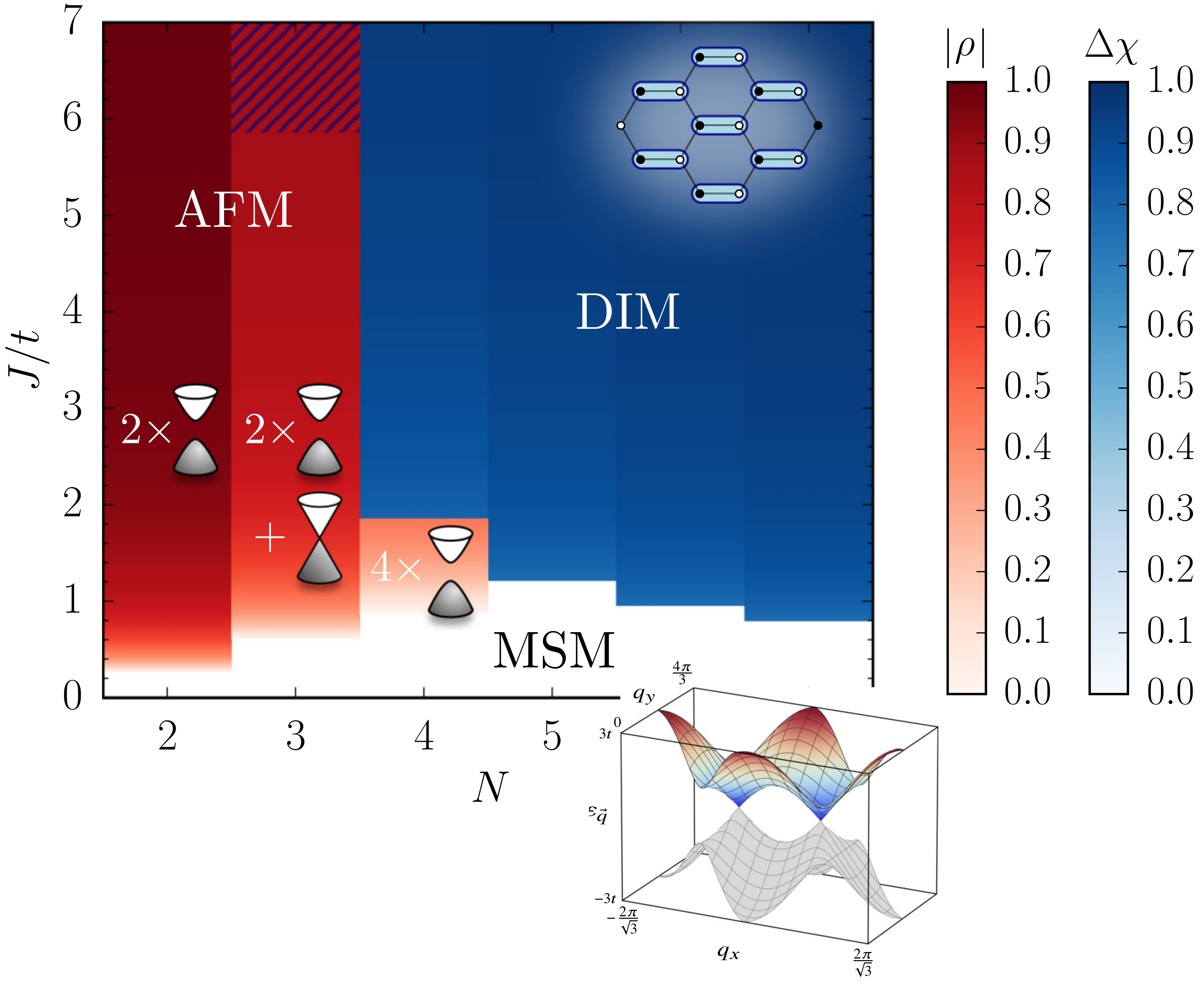


$$\xi^2 = \frac{1}{2d} \frac{\sum_{\vec{r}} |\vec{r}|^2 S(\vec{r})}{\sum_{\vec{r}} S(\vec{r})}$$

[Liu, Vojta, Assaad, LJ, PRL '22 (Editors' Suggestion)]

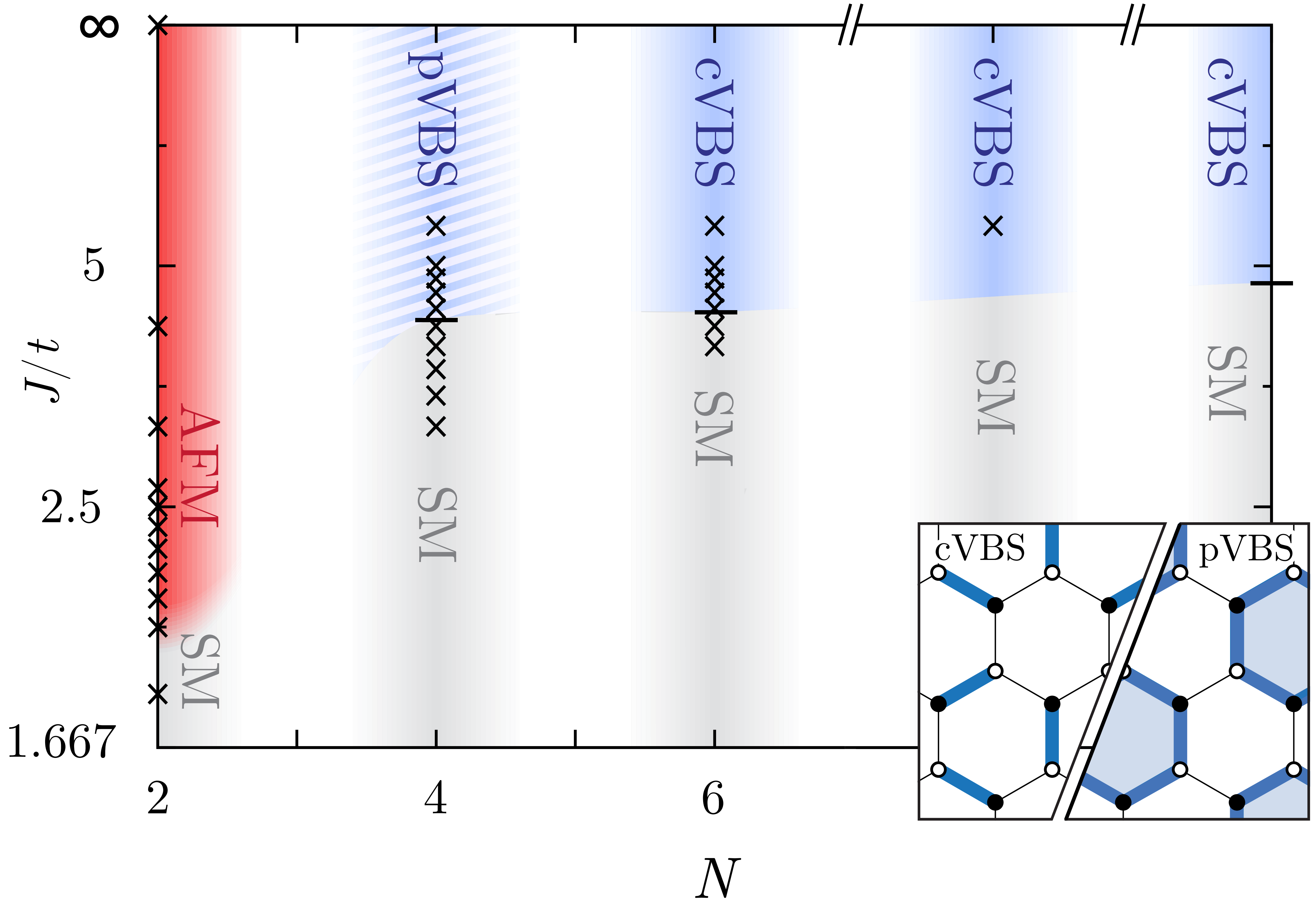
SO(*N*) generalization

SO(*N*) Majorana-Hubbard models



[LJ & Seifert, PRB '22]

SU(*N*) Hubbard-Heisenberg models

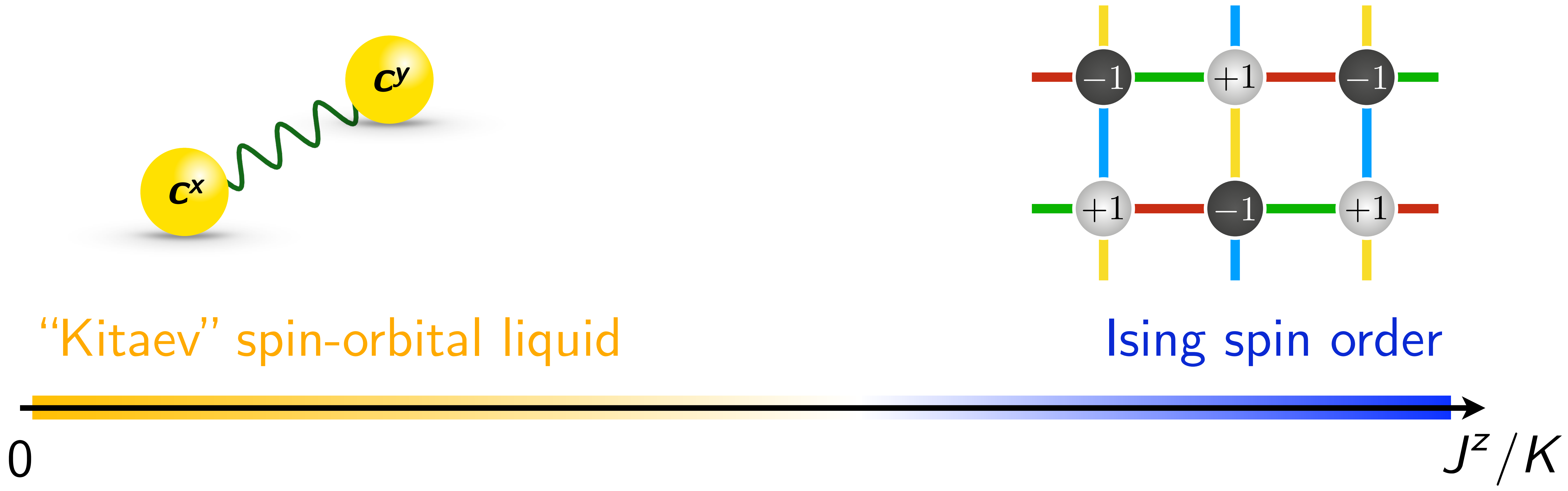


[Affleck & Marston, PRB '88]
[Read & Sachdev, NPB '89]
[Lang, Meng, Muramatsu, Wessel, Assaad, PRL '13]

Kitaev-Ising spin-orbital model

Ising perturbation:

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



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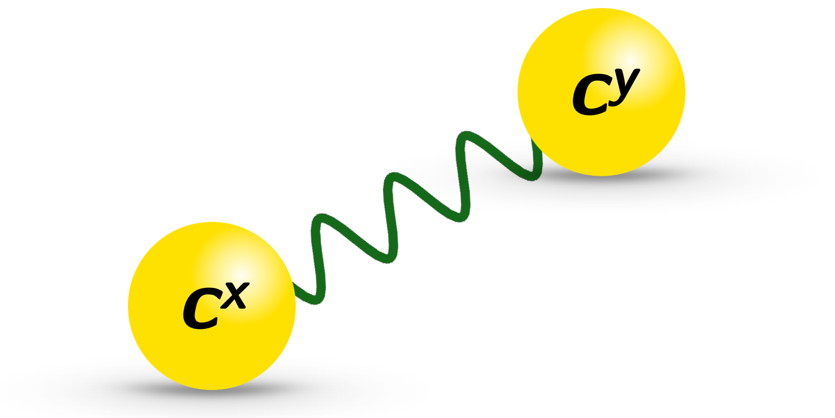
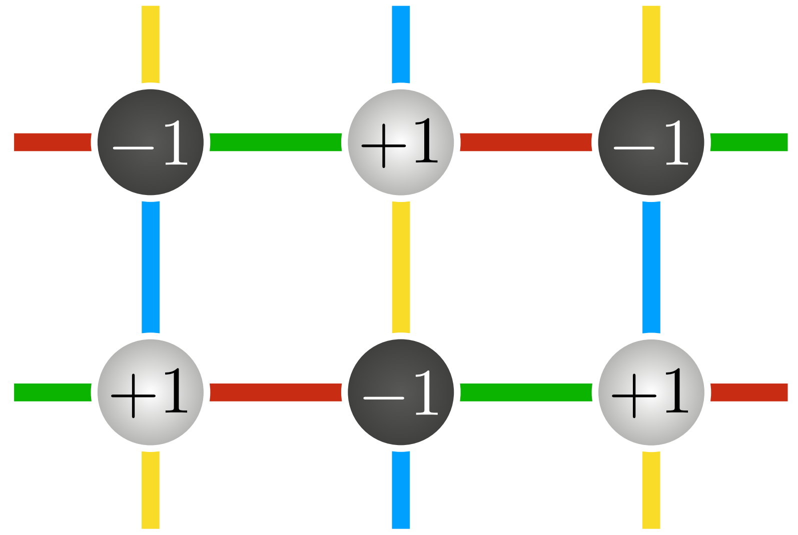




Parton representation:

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

hopping parameter $t = 2K$

π flux

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

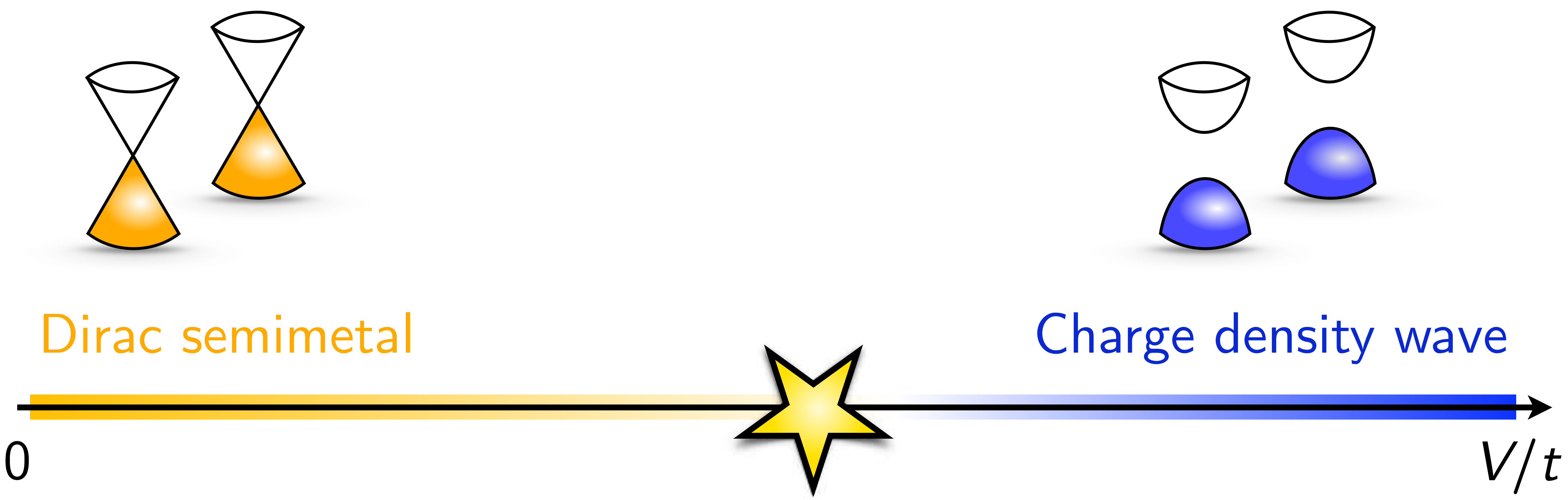
$f = \frac{1}{2}(c^x + ic^y)$

electron density $f^\dagger f$

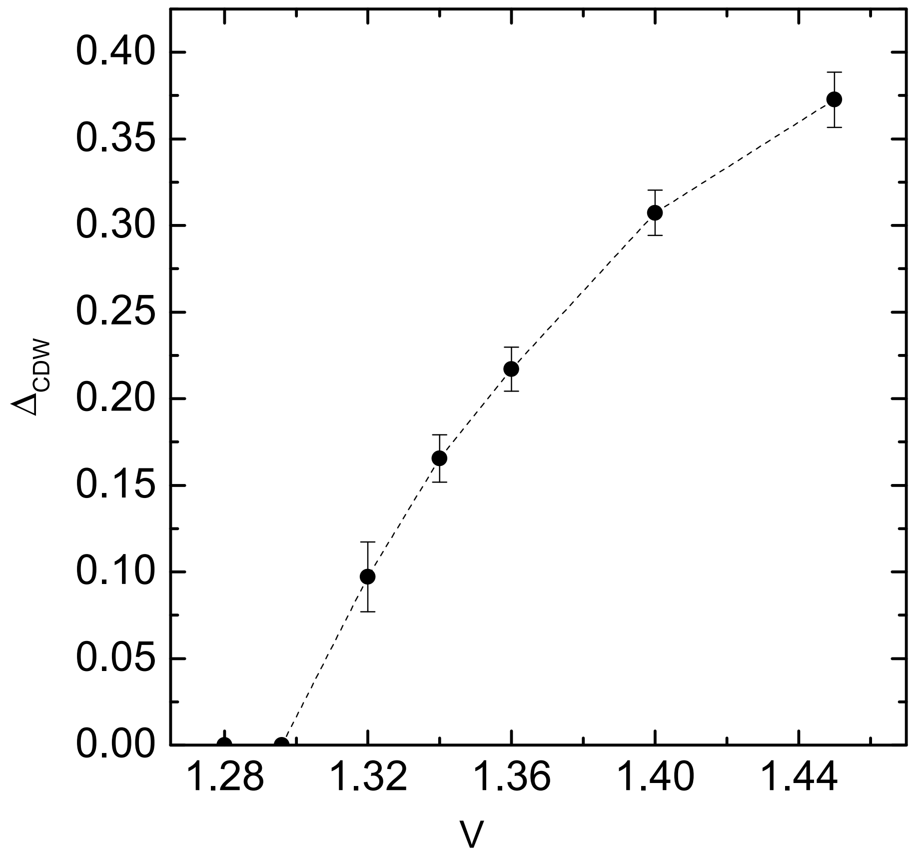
Ground-state flux pattern: [Lieb, PRL '94]

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

Spinless fermions on π-flux lattice: QMC



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

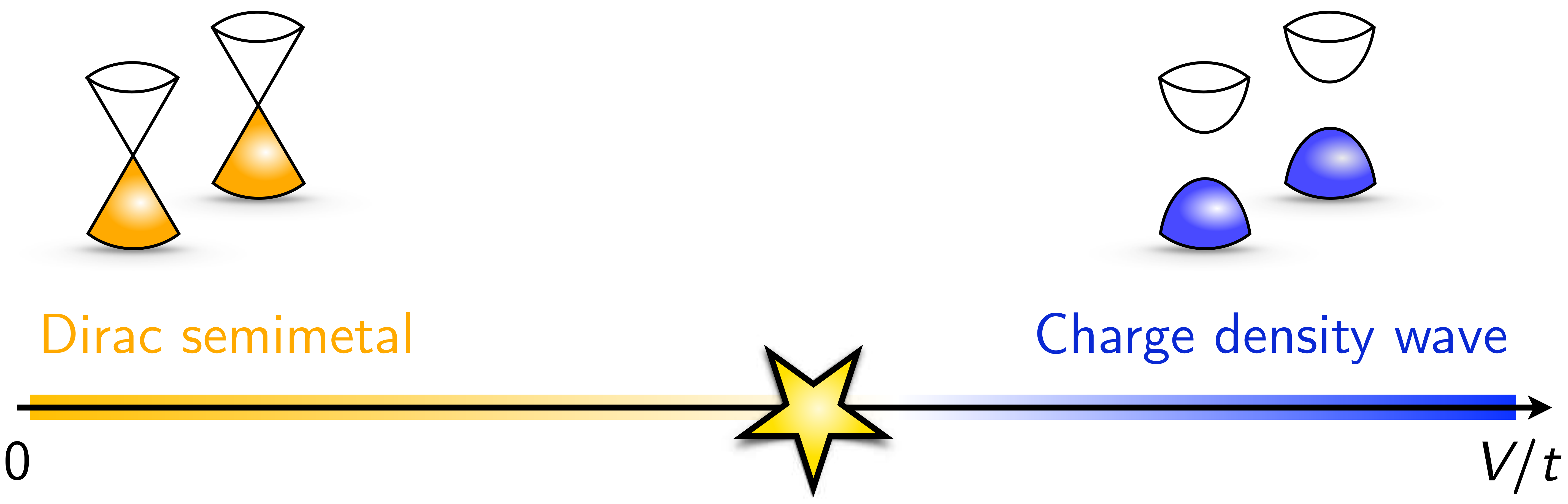


[Wang, Corboz, Troyer, NJP '14]
[Li, Jiang, Yao, NJP '15]
[Huffman & Chandrasekharan, PRD '17; PRD '20]

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

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

Spinless fermions on π-flux lattice: QMC



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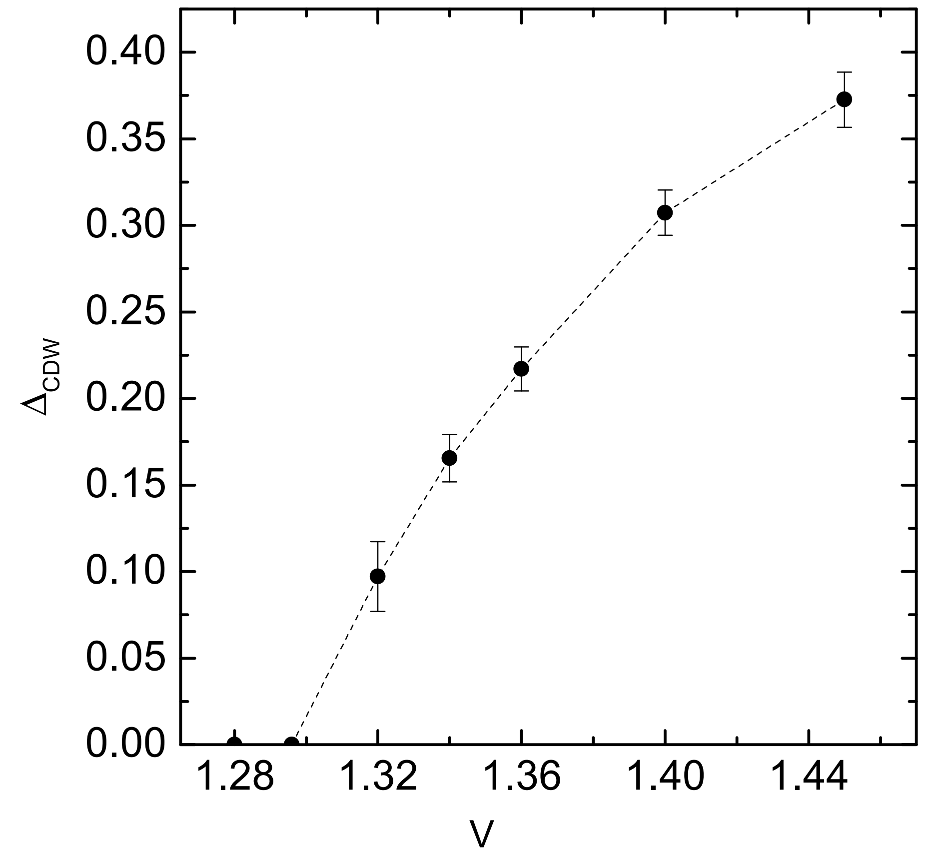

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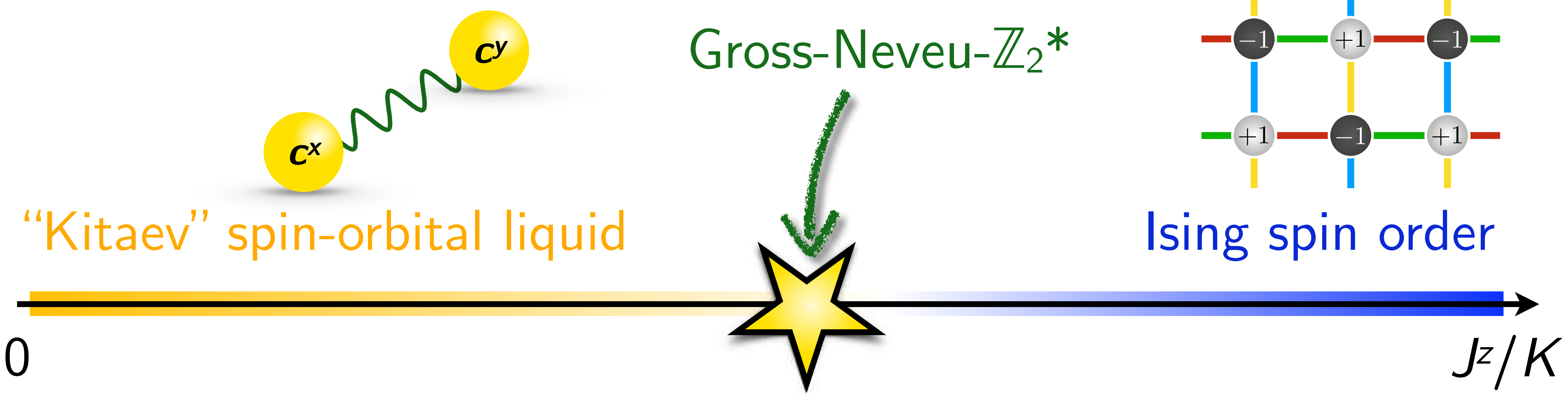
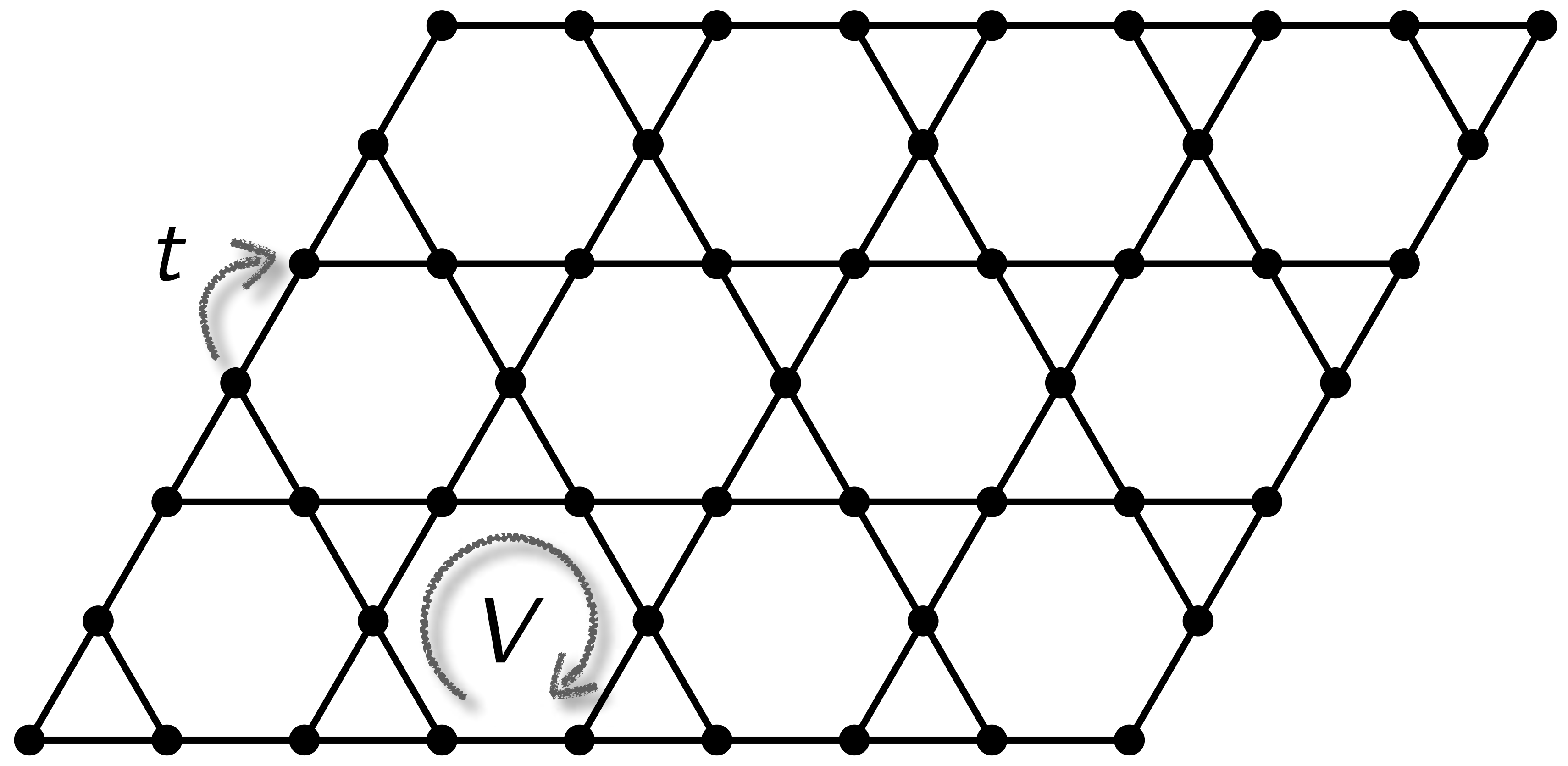
Spin-orbital model:



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

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

Example: Kagome-lattice Bose-Hubbard model



Hamiltonian:

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

... b_i hard-core bosons

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

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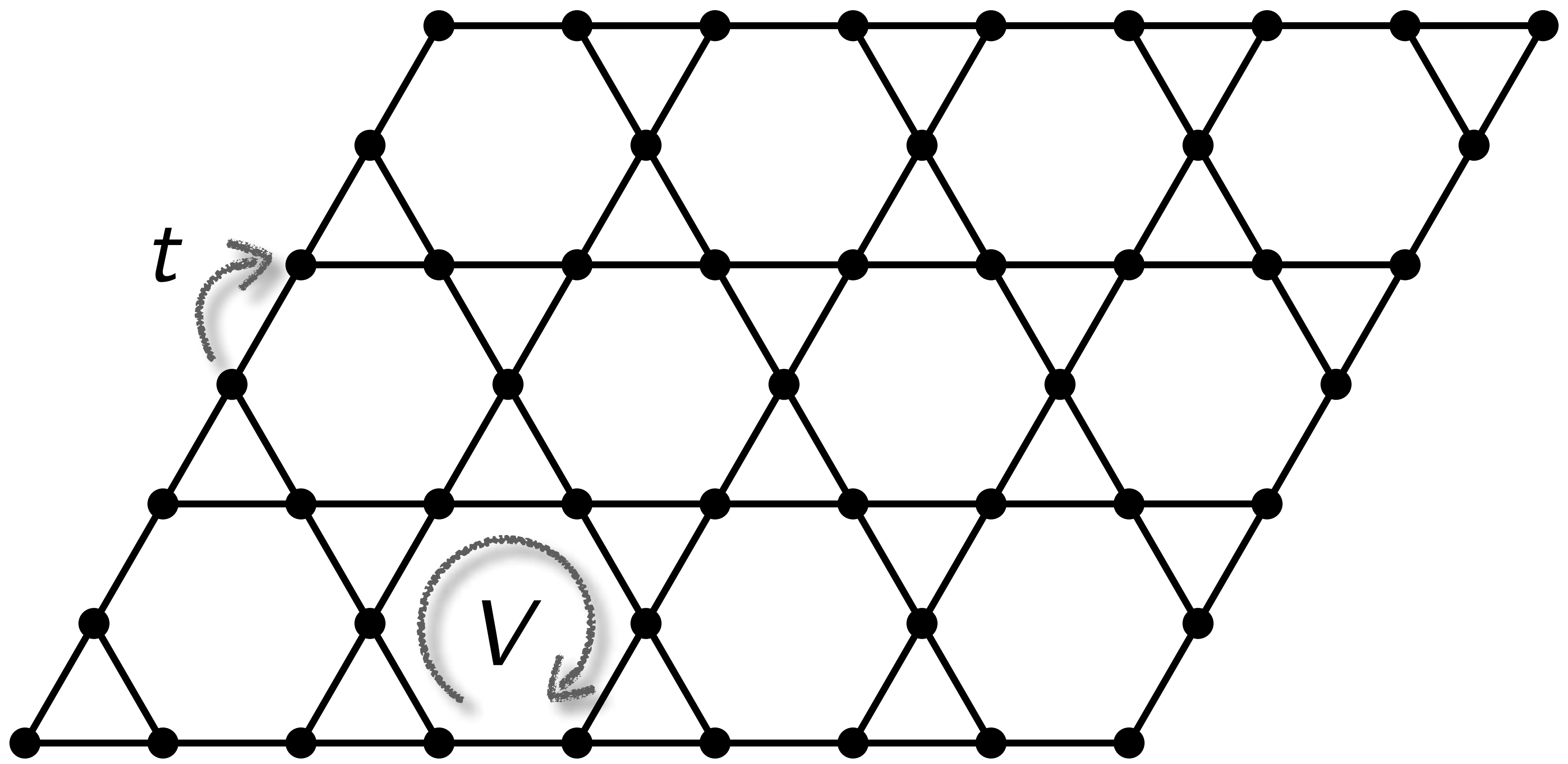

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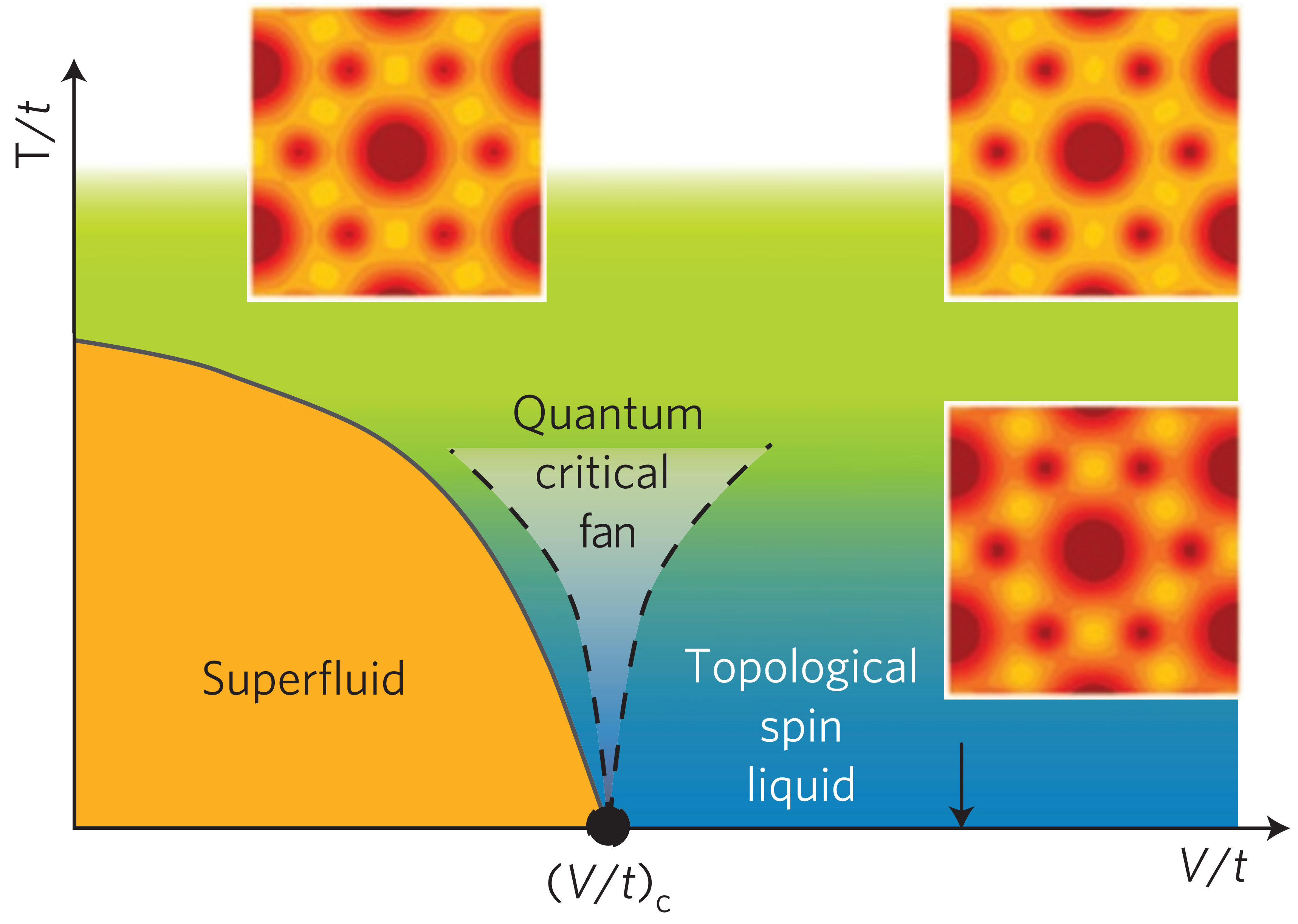

[Isakov, Hastings, Melko, Nat. Phys. '11]

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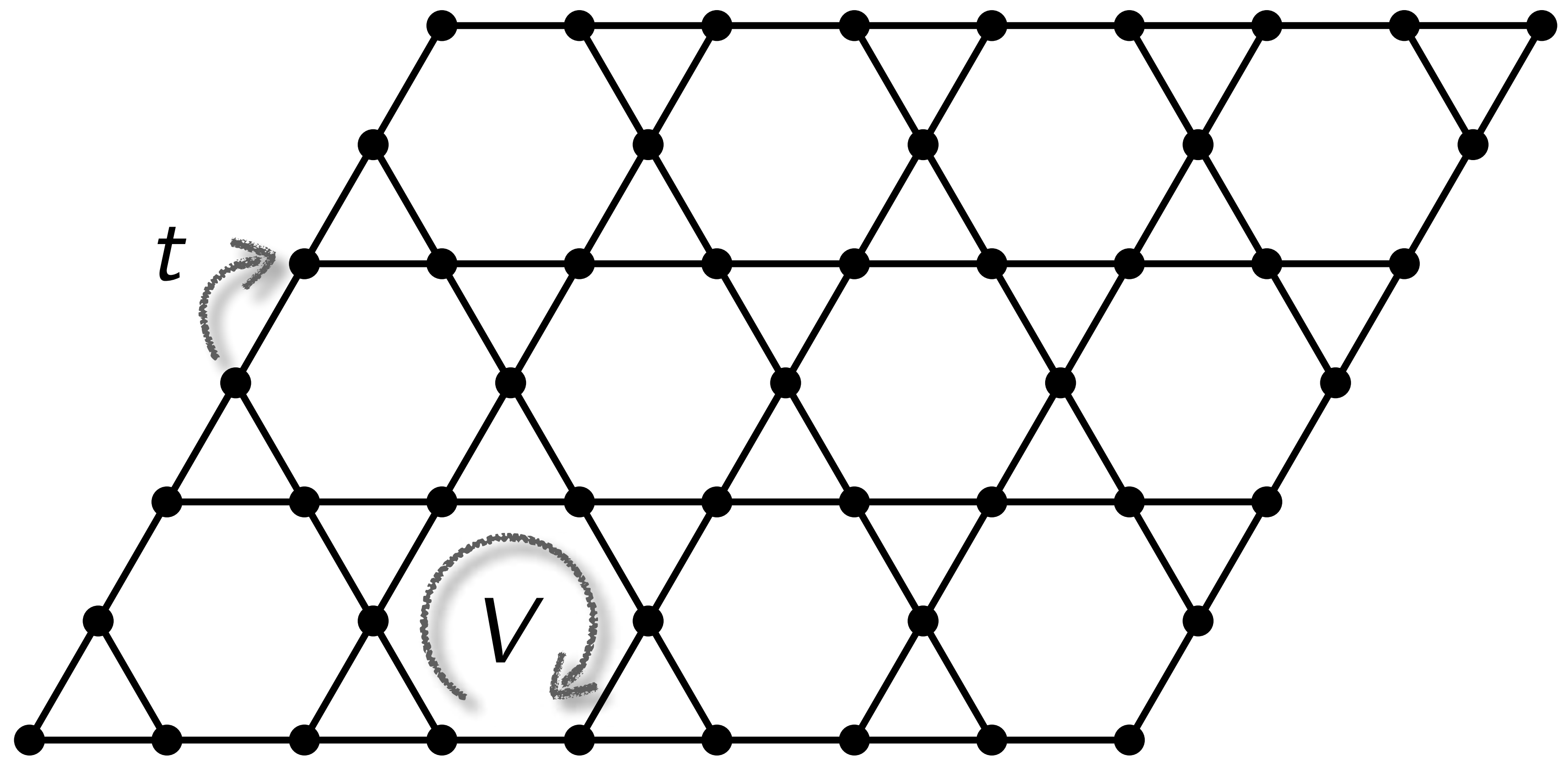

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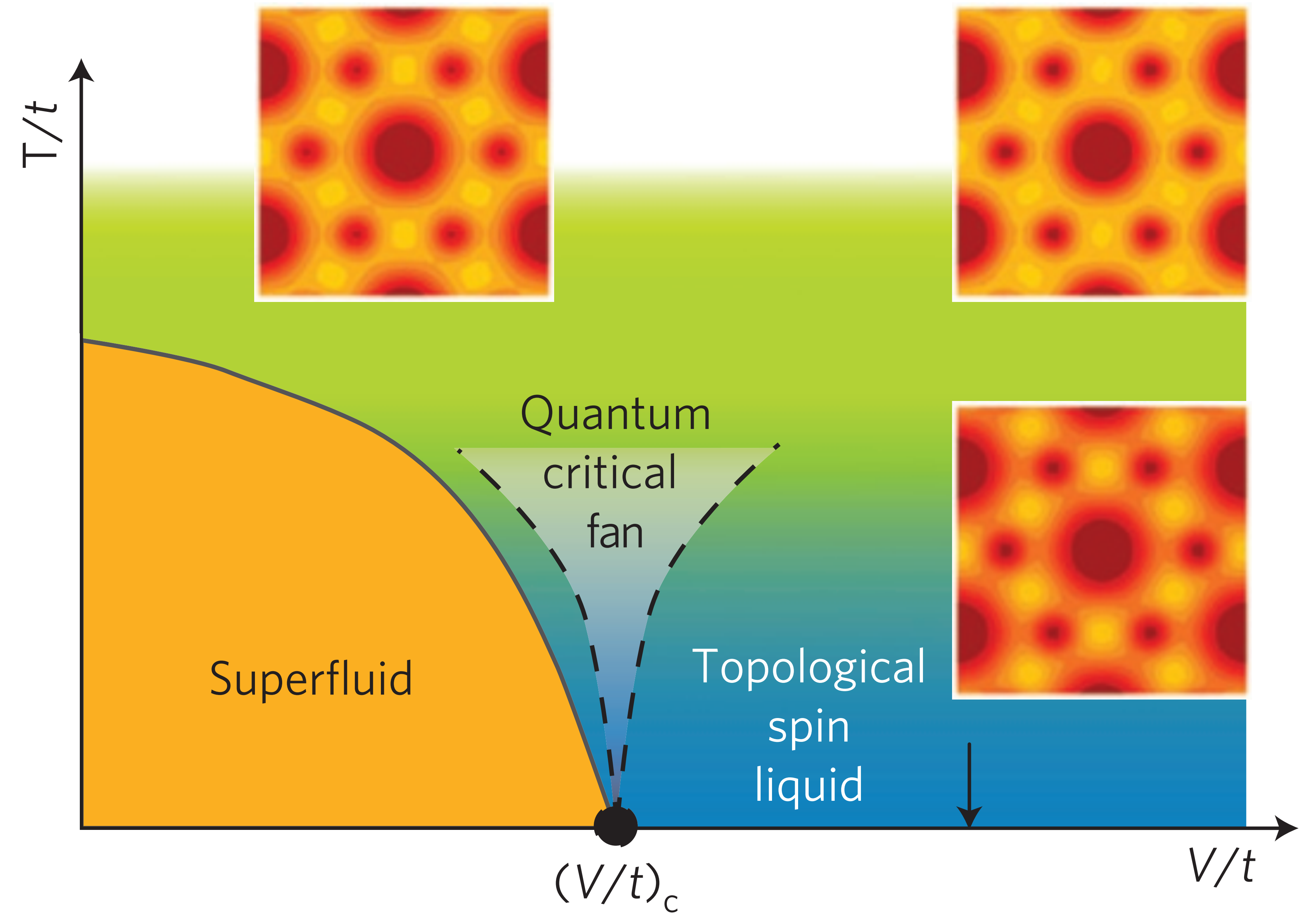
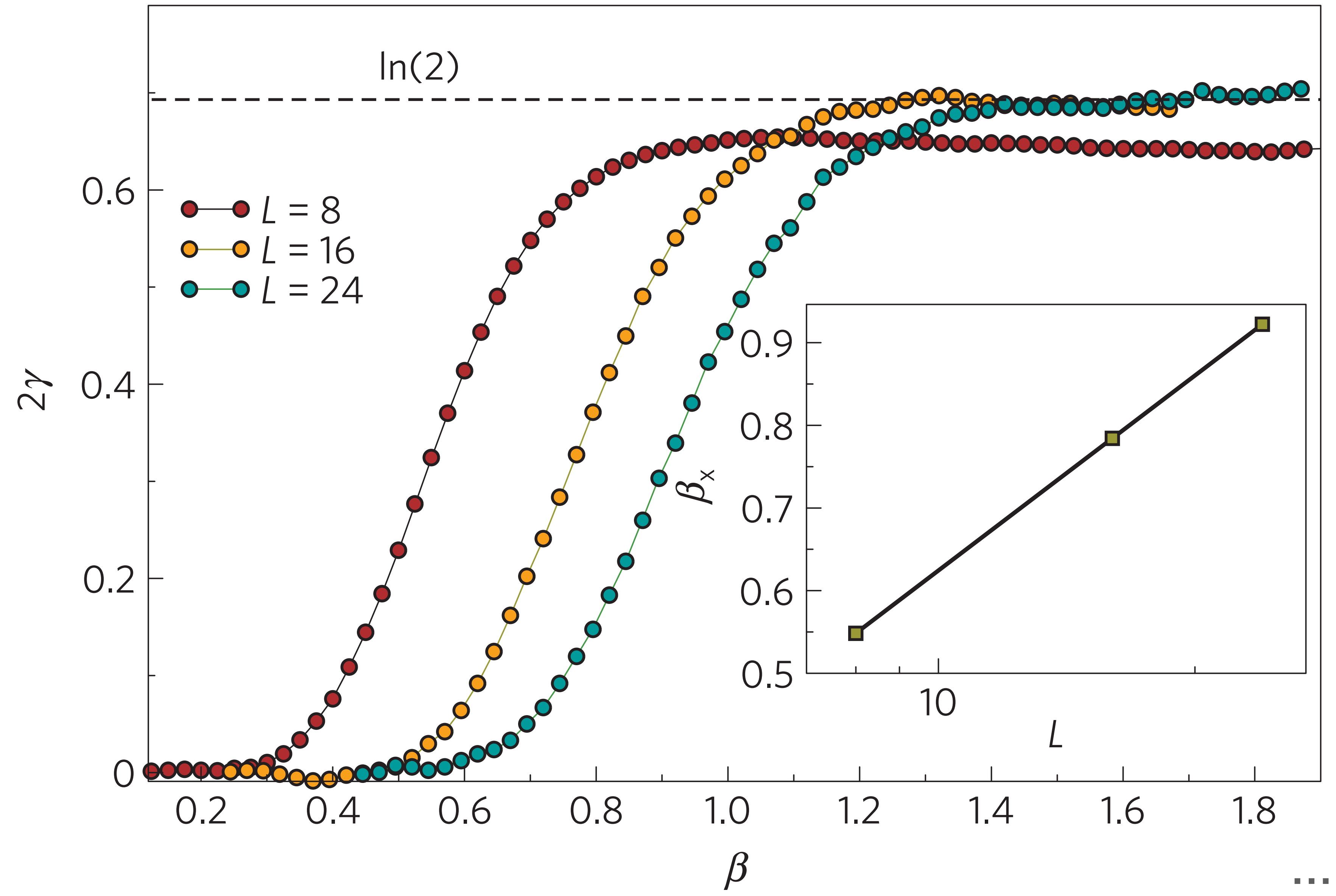


Entanglement entropy: $S_n(A) = a\ell - \gamma + \ldots$

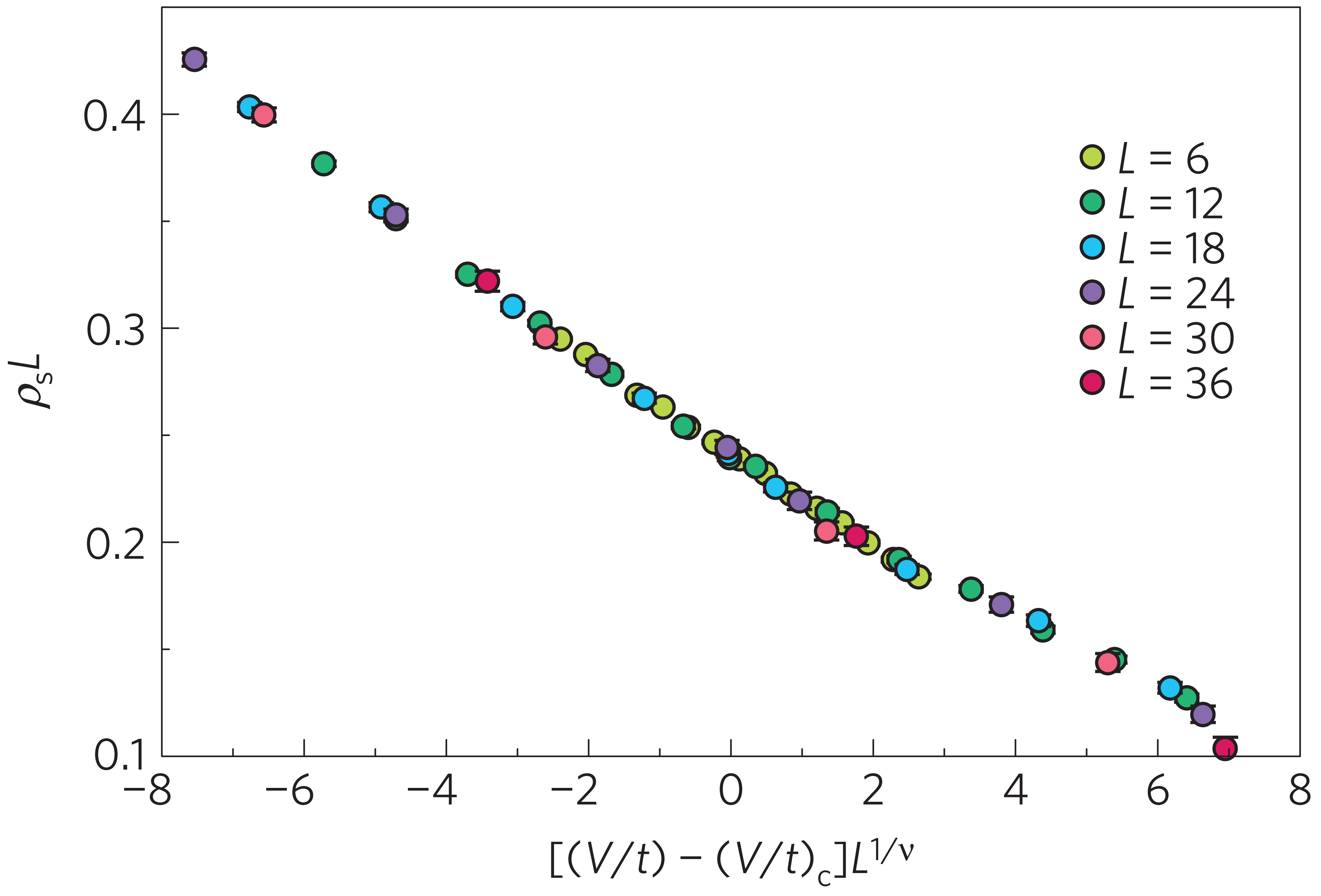


... in spin liquid phase

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

Quantum critical scaling: XY*

Superfluid density:



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

$$\nu \approx 0.67 = \nu_{XY}$$

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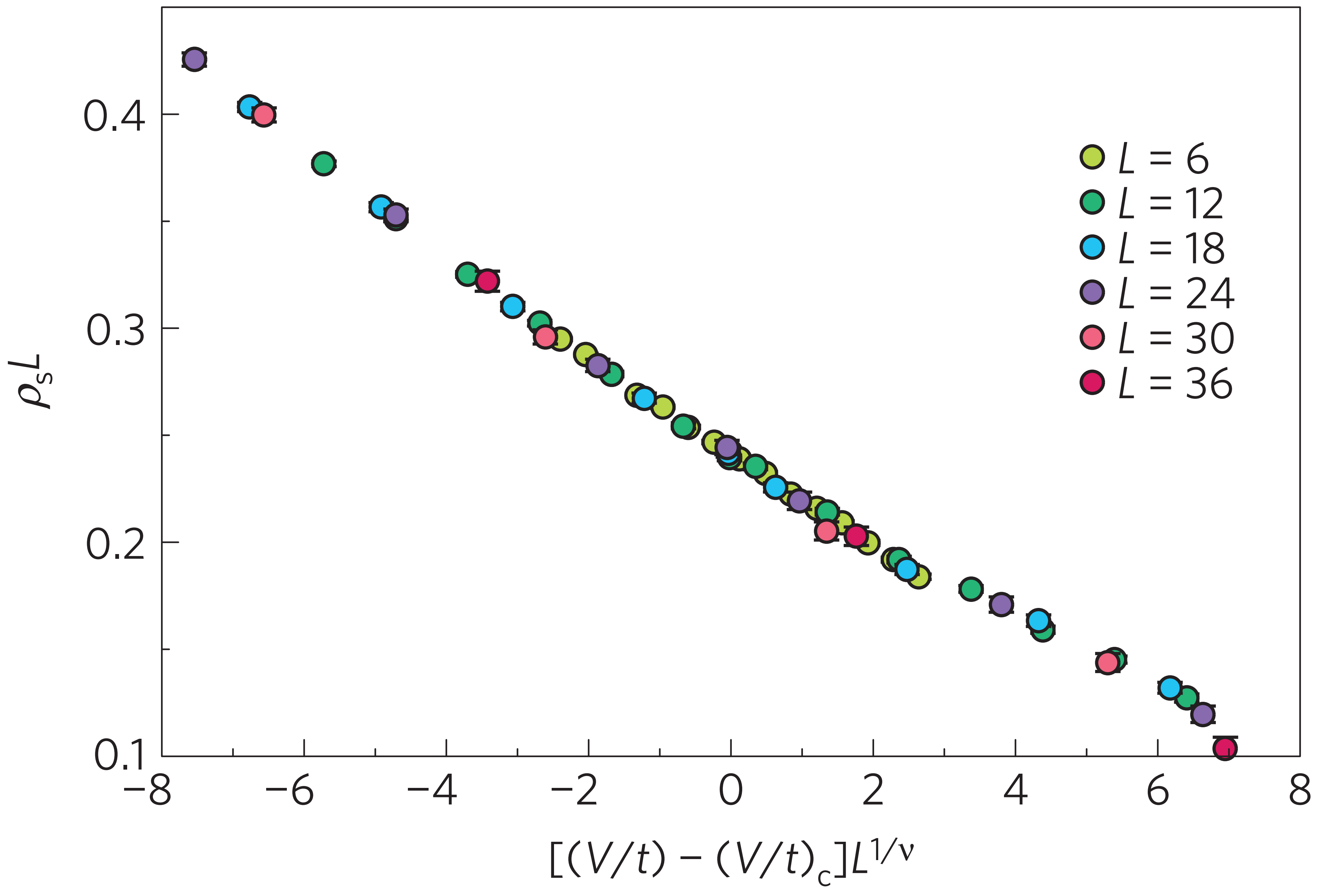

[Isakov, Hastings, Melko, Nat. Phys. '11]

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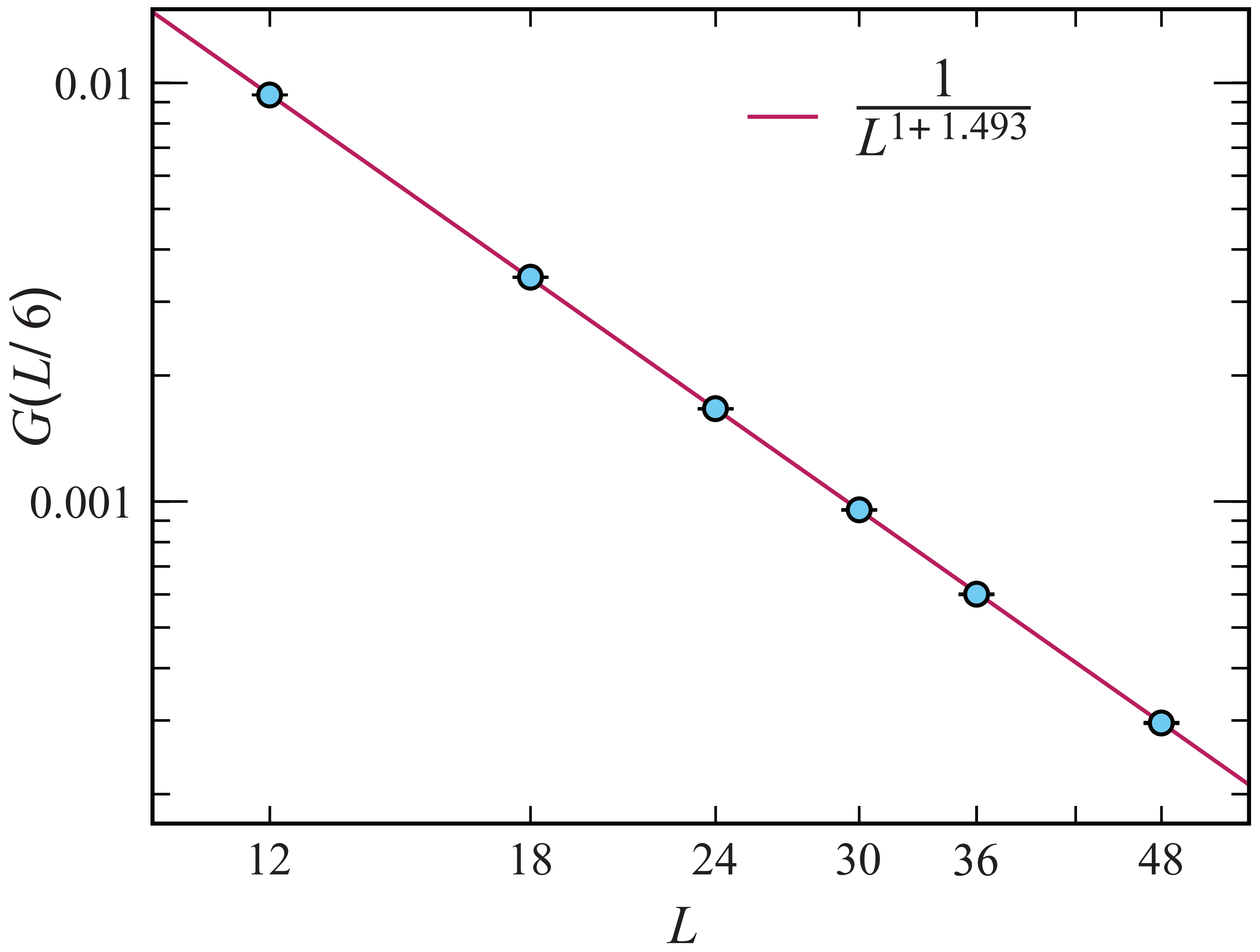
Two-point superfluid correlator:



[Isakov, Melko, Hastings, Science '12]

$$\eta \approx 1.49 \neq \eta_{XY} \approx 0.038$$

Order parameter *composite* of fractionalized particles!

... cf. $\eta_T \approx 1.47$ from XY field theory
[Calabrese, Pelissetto, Vicari, PRE '02]

Finite-size spectroscopy: Ising vs Ising*

Transverse-field Ising:

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

Transverse-field toric code:

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

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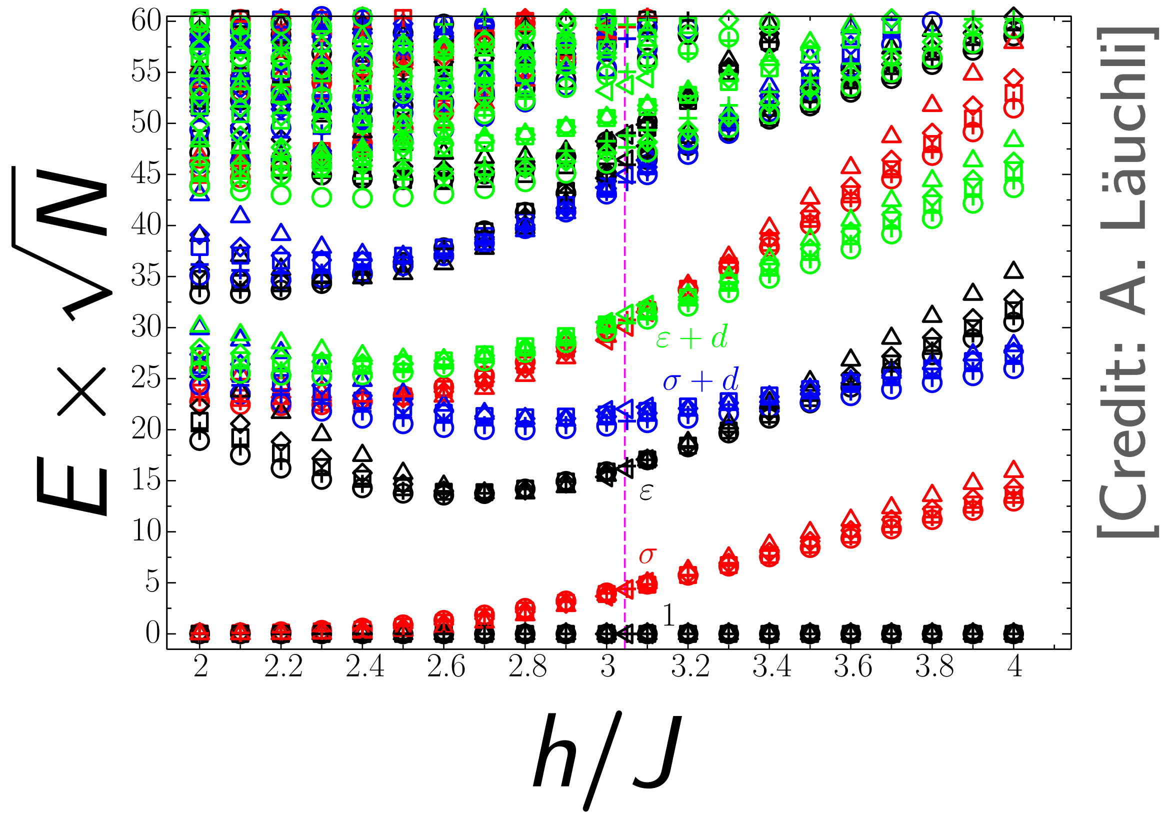
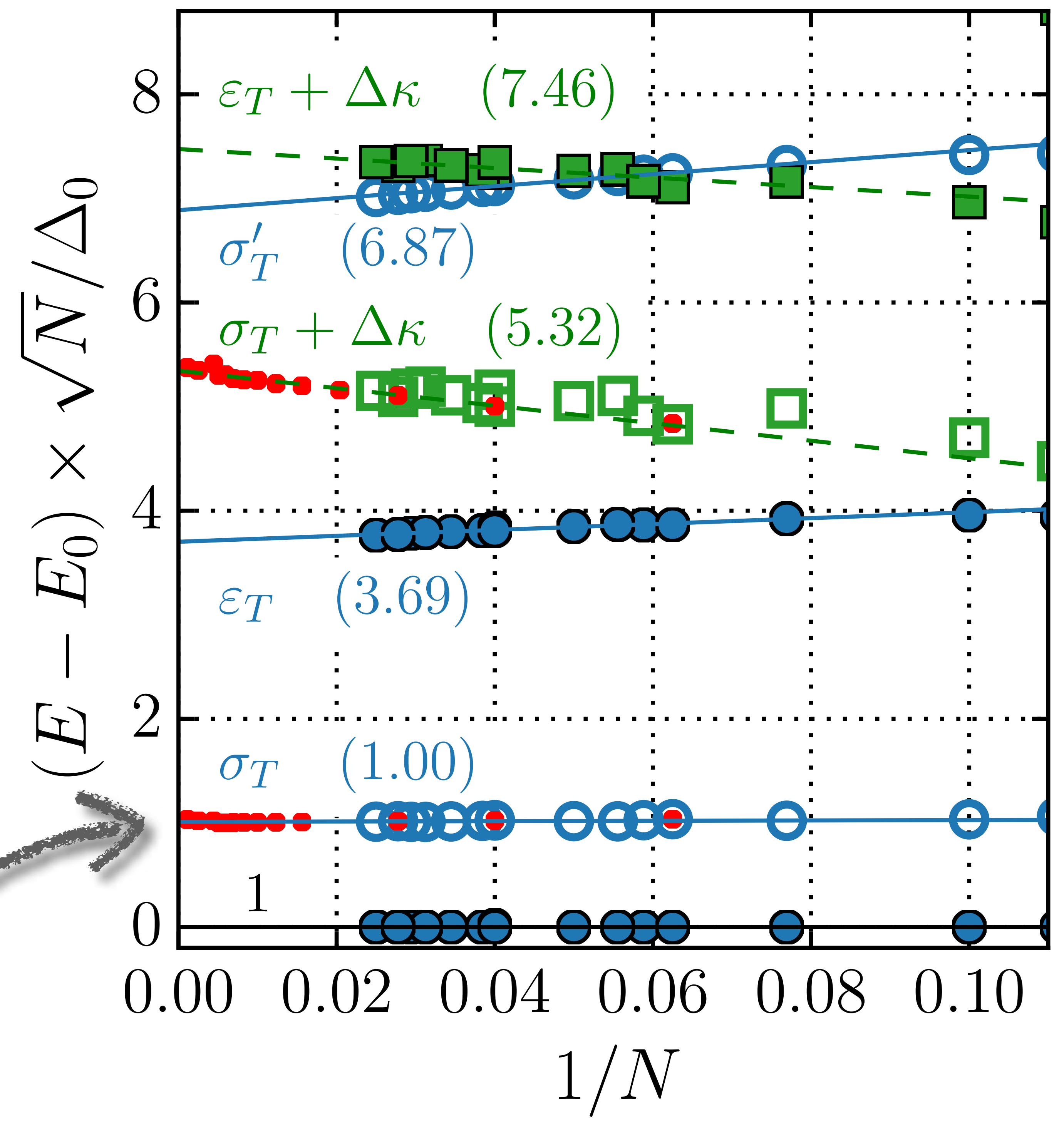
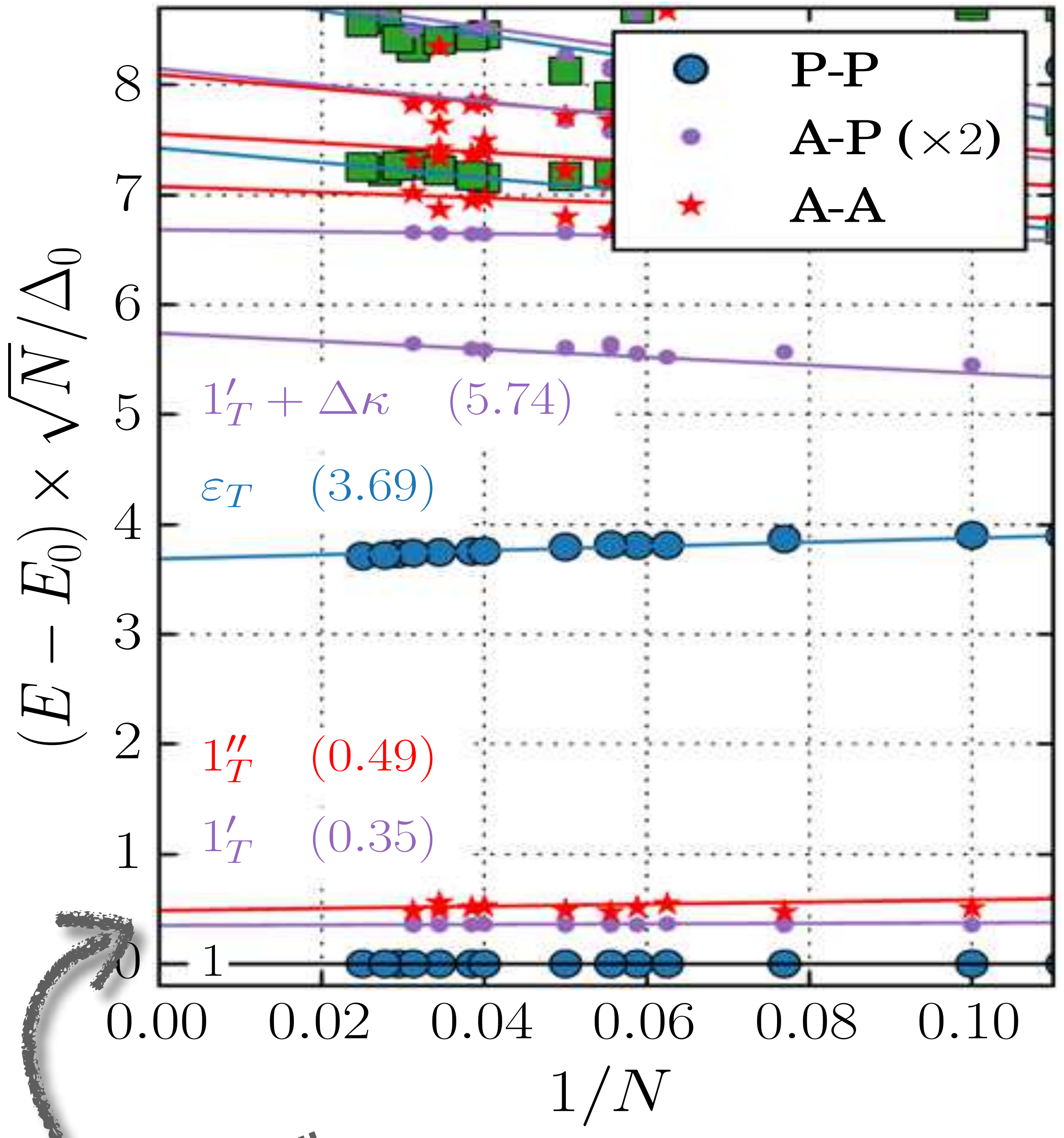


Ising
$h = h_c$

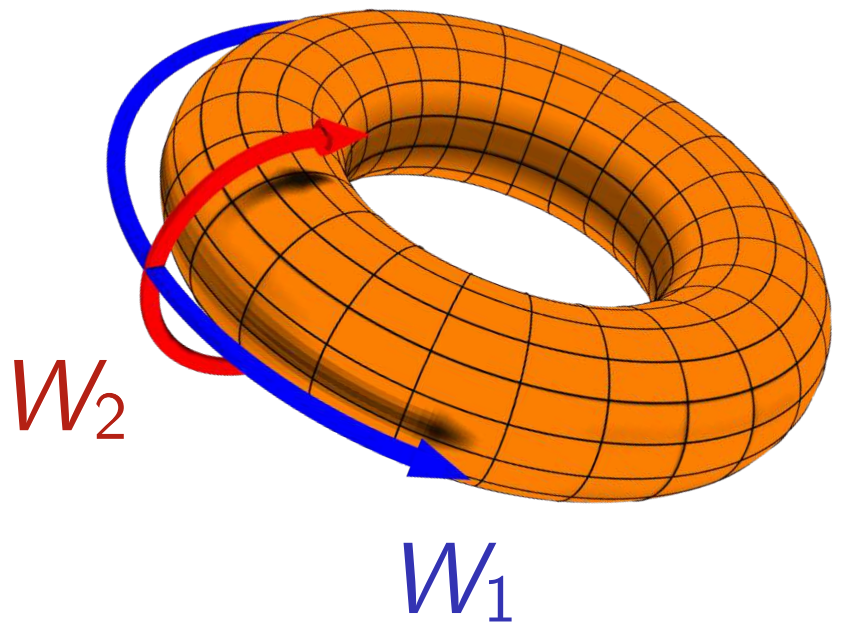


missing in Ising*

Ising*
$h = h_c$

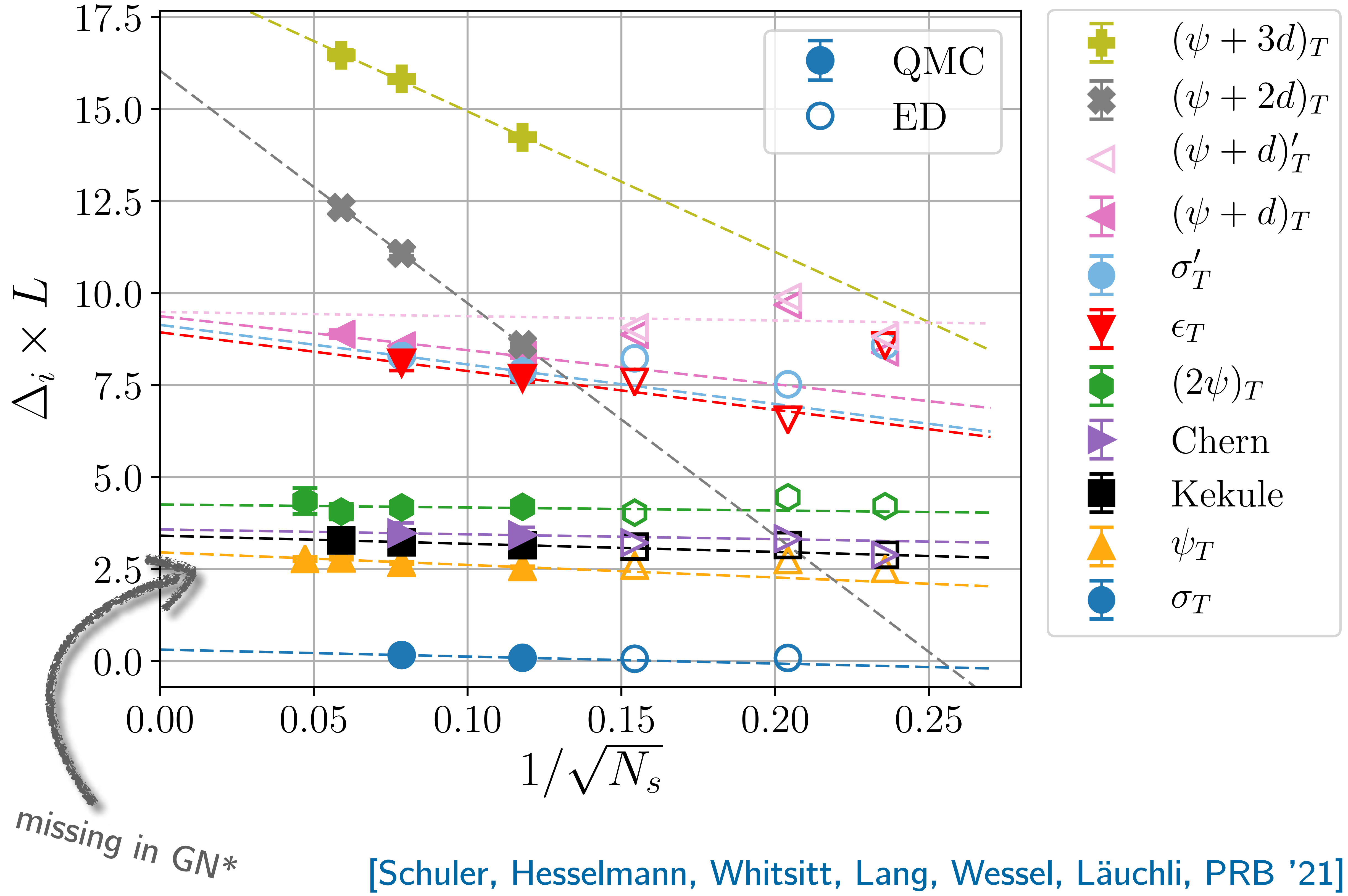


topological "copies"

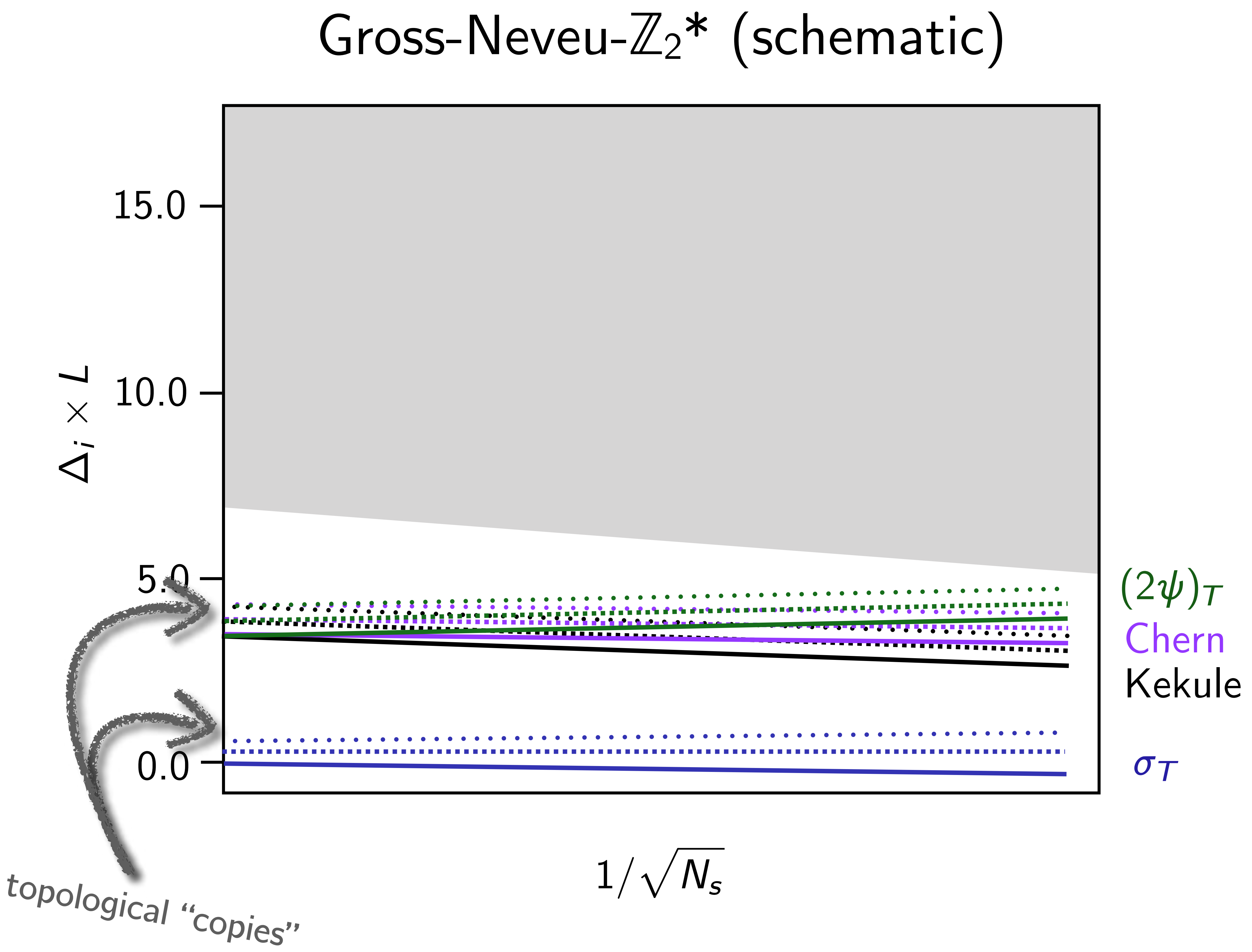


[Schuler, Whitsitt, Henry, Sachdev, Läuchli, PRL '16]

Gross-Neveu vs Gross-Neveu*



[Schuler, Hesselmann, Whitsitt, Lang, Wessel, Läuchli, PRB '21]



... testable in future simulations

Gross-Neveu-SO(3) criticality

Field theory:

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

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

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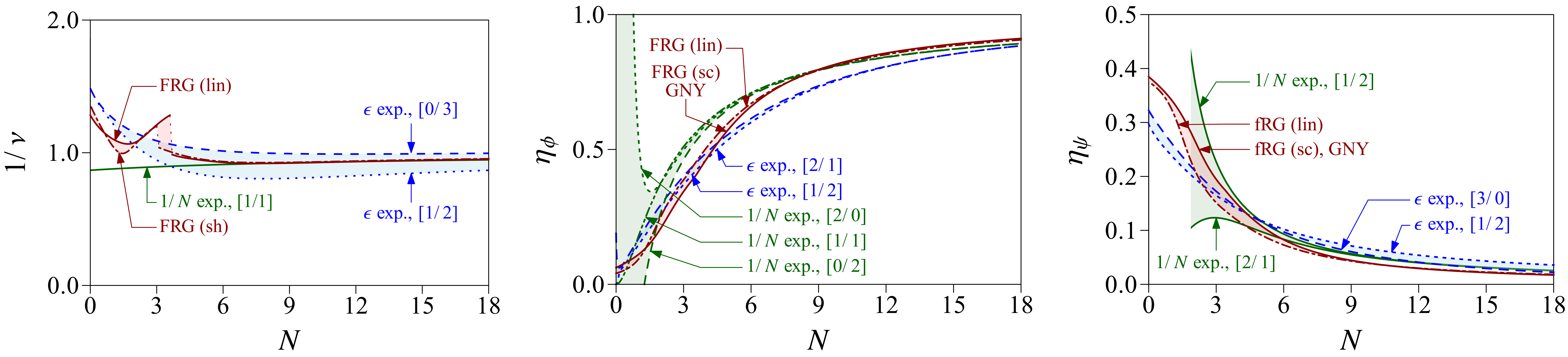
Critical exponents:



... from three-loop ε expansion,
second/third-order $1/N$ expansion,
functional RG in local potential approximation

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

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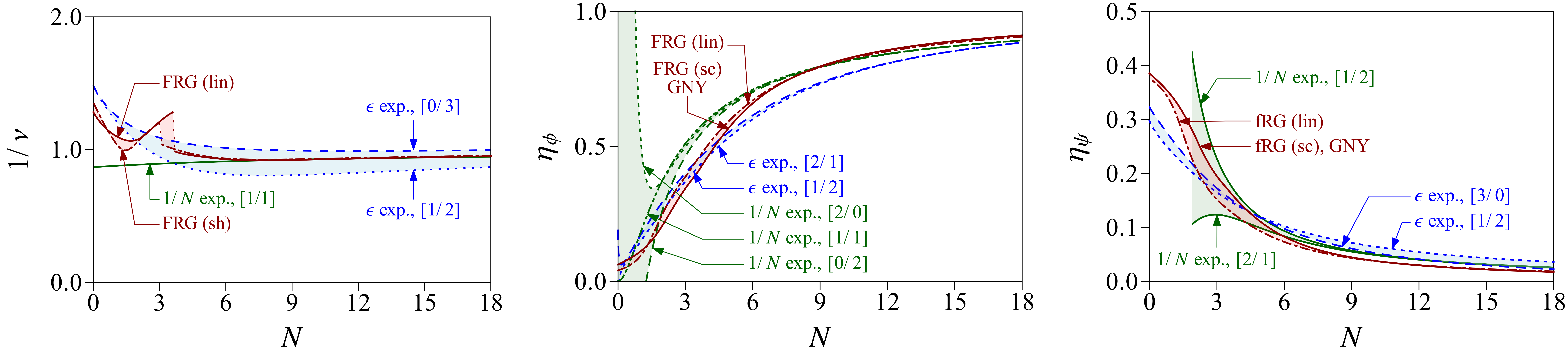


... from three-loop ε expansion,
second/third-order $1/N$ expansion,
functional RG in local potential approximation

Spin-orbital realization ($N = 3$):

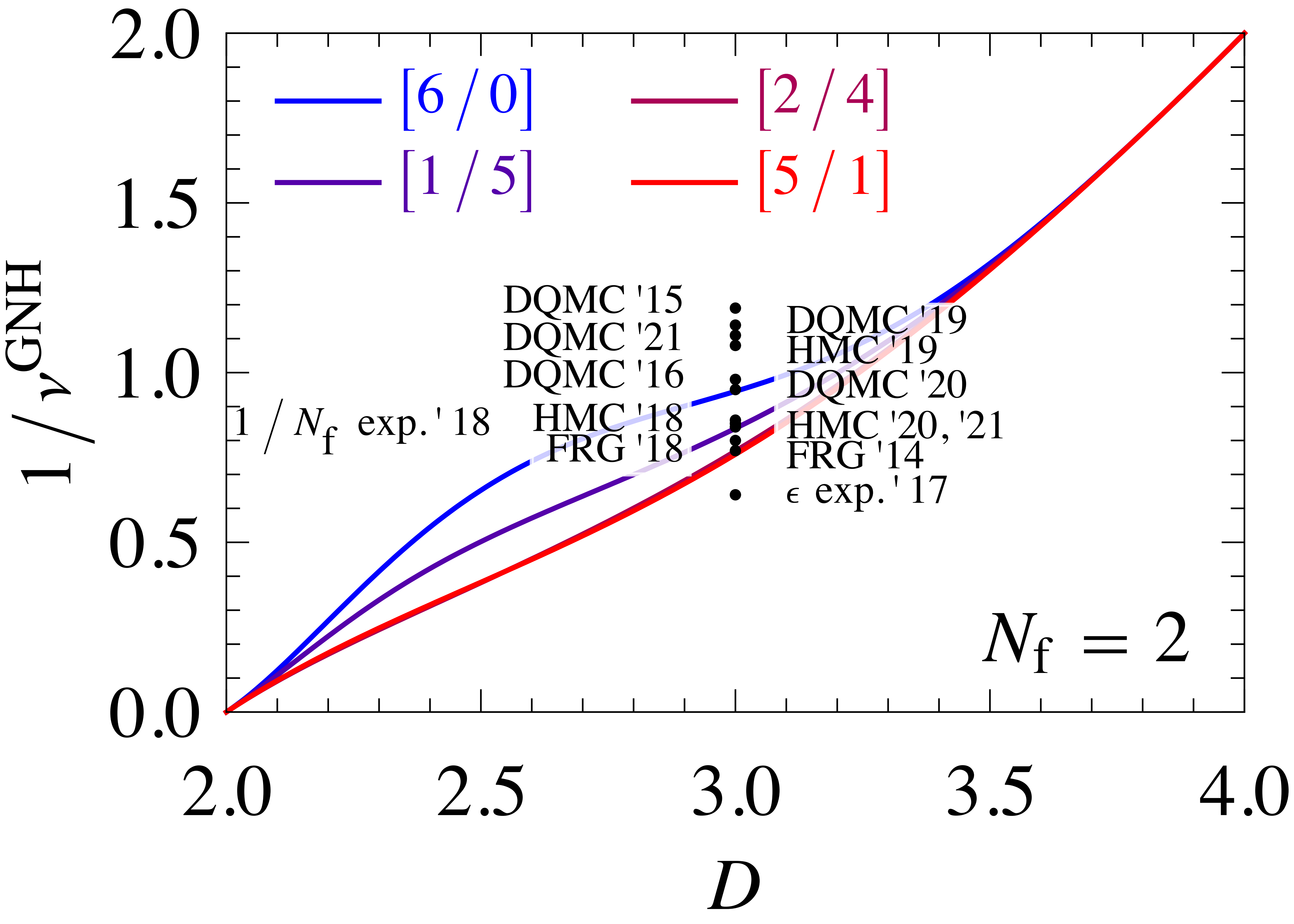
$$1/\nu = 1.03(15)$$
$$\eta_\phi = 0.42(7)$$
$$\eta_\psi = 0.180(10)$$

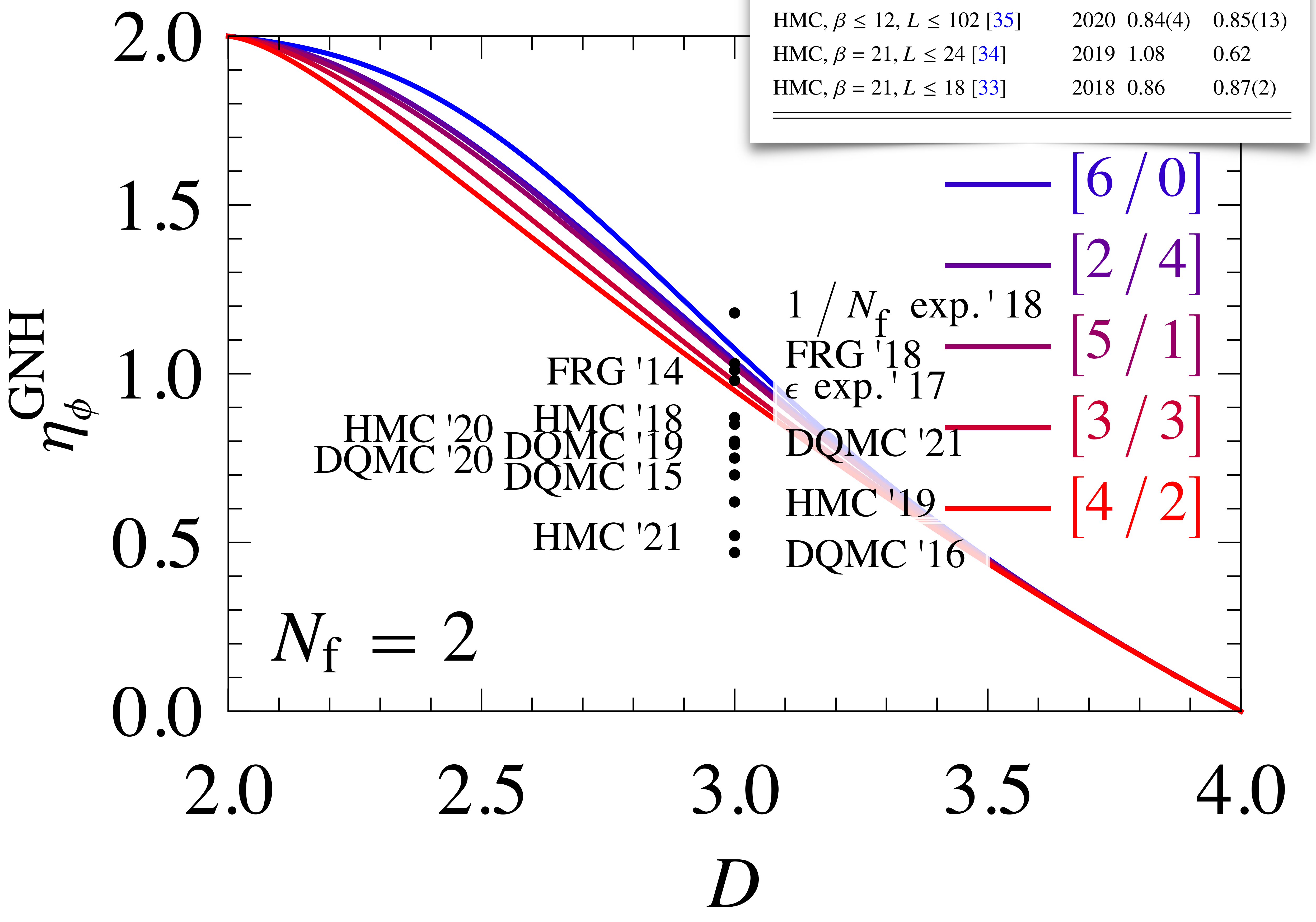
... different from Gross-Neveu-Heisenberg

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

Comparison of exponents: Gross-Neveu-Heisenberg

$N_f = 2$	Year	$1/\nu$	η_ϕ
Interpolation (this work)	2022	0.83(12)	1.01(6)
$4-\varepsilon$ expansion, $O(\varepsilon^4)$ [13]	2017	0.64	0.98
$1/N_f$ expansion, $O(1/N_f^{2,3})$ [39]	2018	0.85	1.18
functional RG, NLO [38]	2018	0.80	1.03
functional RG, LPA' [16]	2014	0.77	1.01
DQMC, $\tau \sim L \leq 40$ [31]	2020	0.95(5)	0.75(4)
DQMC, $\tau \sim L \leq 40$ [30]	2016	0.98(1)	0.47(7)
DQMC, $\beta = L \leq 24$ [29]	2021	1.11(4)	0.80(9)
DQMC, $\beta = L \leq 21$ [28]	2019	1.14(9)	0.79(5)
DQMC, $\tau = 60$, $L \leq 18$ [27]	2015	1.19(6)	0.70(15)
DQMC, $\beta = L \leq 20$ [32]	2021	1.01(8)	0.55(2)
HMC, $\beta \leq 12$, $L \leq 102$ [36]	2021	0.84(4)	0.52(1)
HMC, $\beta \leq 12$, $L \leq 102$ [35]	2020	0.84(4)	0.85(13)
HMC, $\beta = 21$, $L \leq 24$ [34]	2019	1.08	0.62
HMC, $\beta = 21$, $L \leq 18$ [33]	2018	0.86	0.87(2)





[Ladovrechis, Ray, Meng, LJ, arXiv:2209.02734]