TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Functional approaches to quantum magnets

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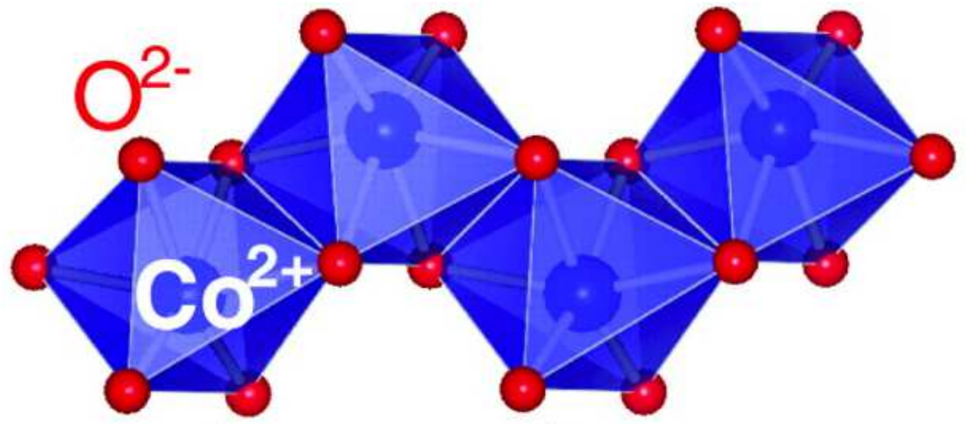
Michael Scherer

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

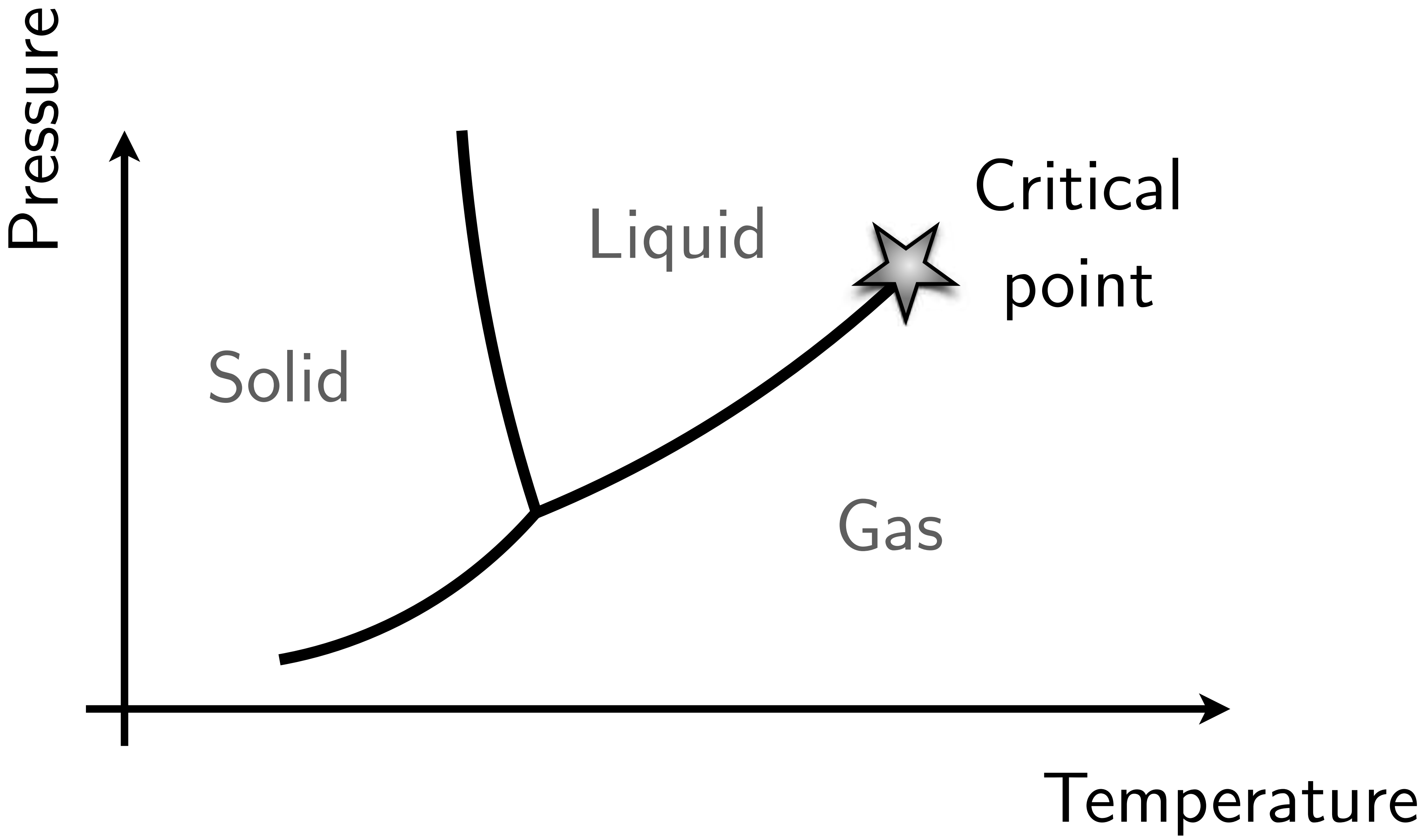
ct.qmat
Complexity and Topology in Quantum Matter
Würzburg-Dresden Cluster of Excellence

SFB 1143

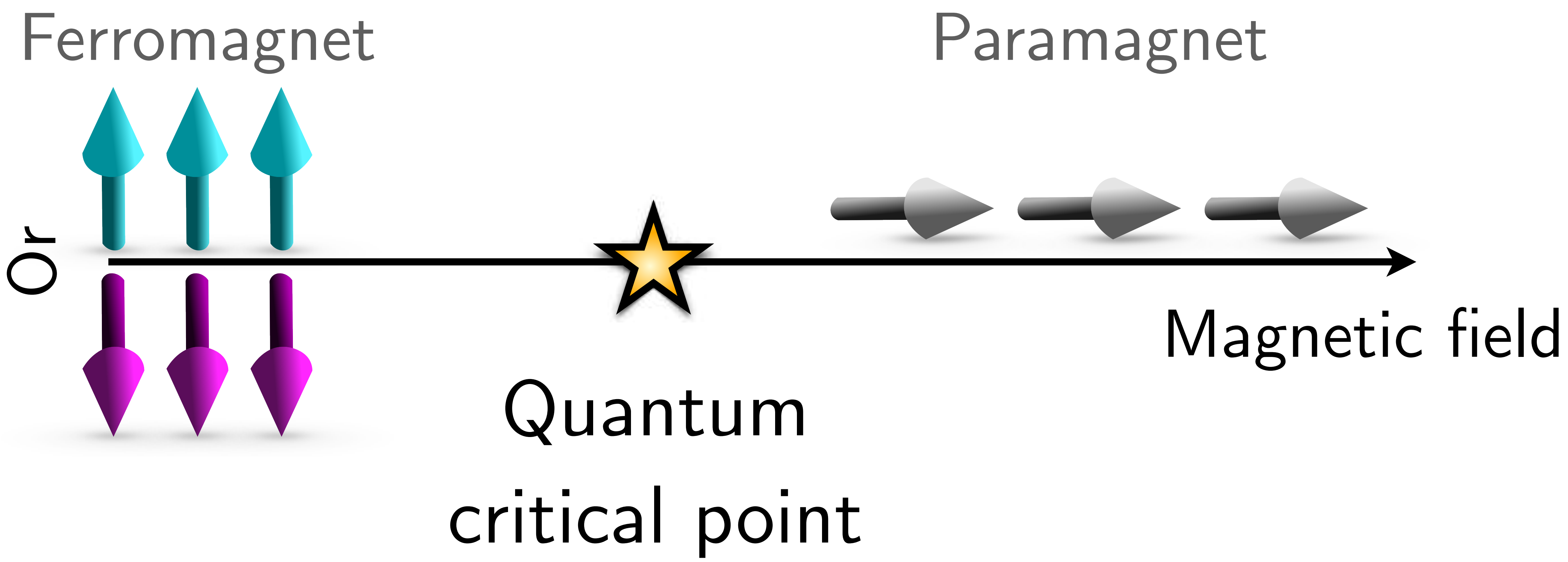
Classical vs quantum criticality



H_2O $\boldsymbol{T > 0}$



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

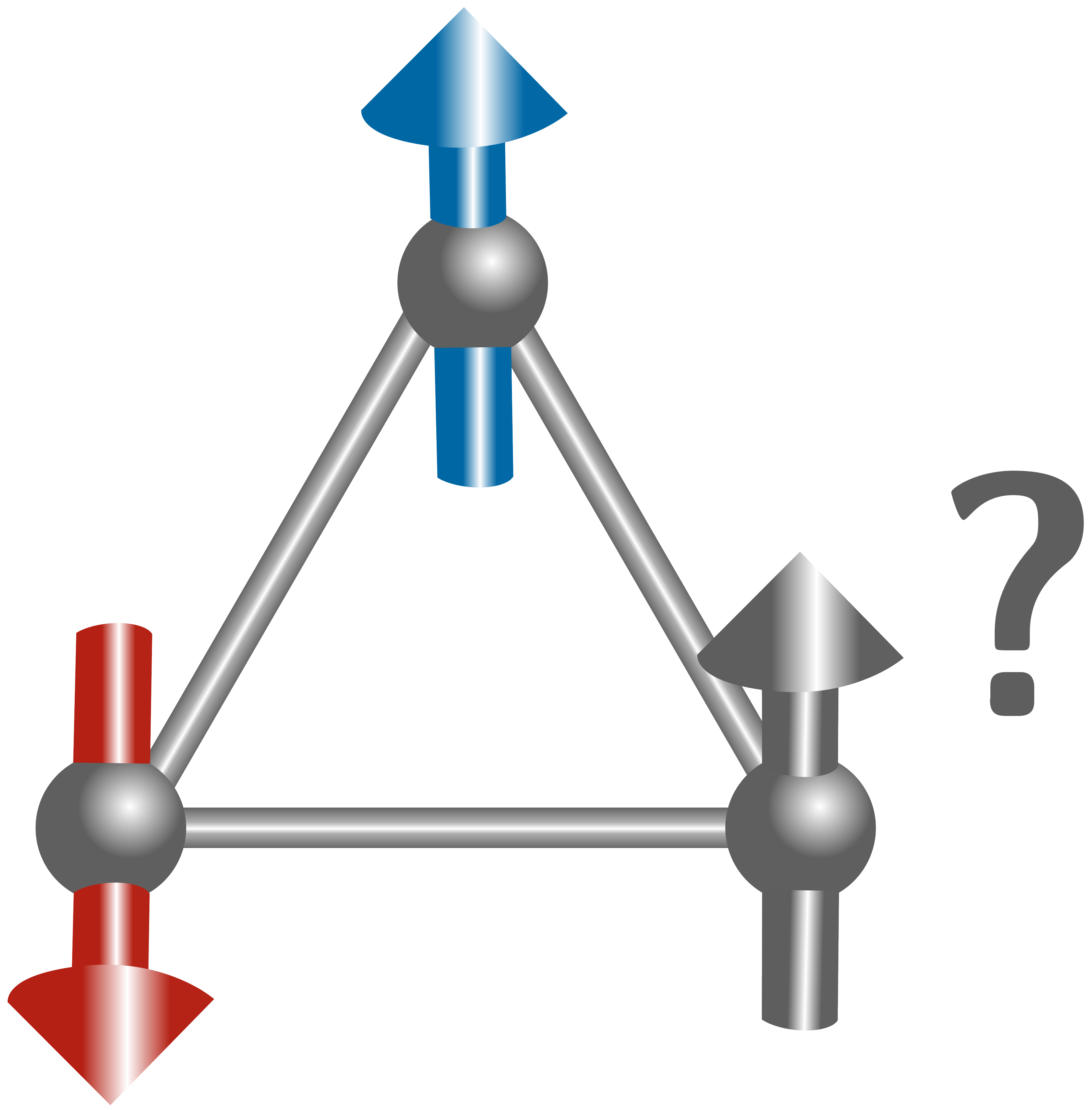


[Coldea *et al.*, Science '10]
[Kinross *et al.*, PRX '14]
[Morris *et al.*, Kaul, Armitage, Nat. Phys. '21]
...

Magnetic frustration

Antiferromagnetic interaction:

$$\mathcal{H}_{ij} = J S_i^z S_j^z \qquad\qquad J > 0$$



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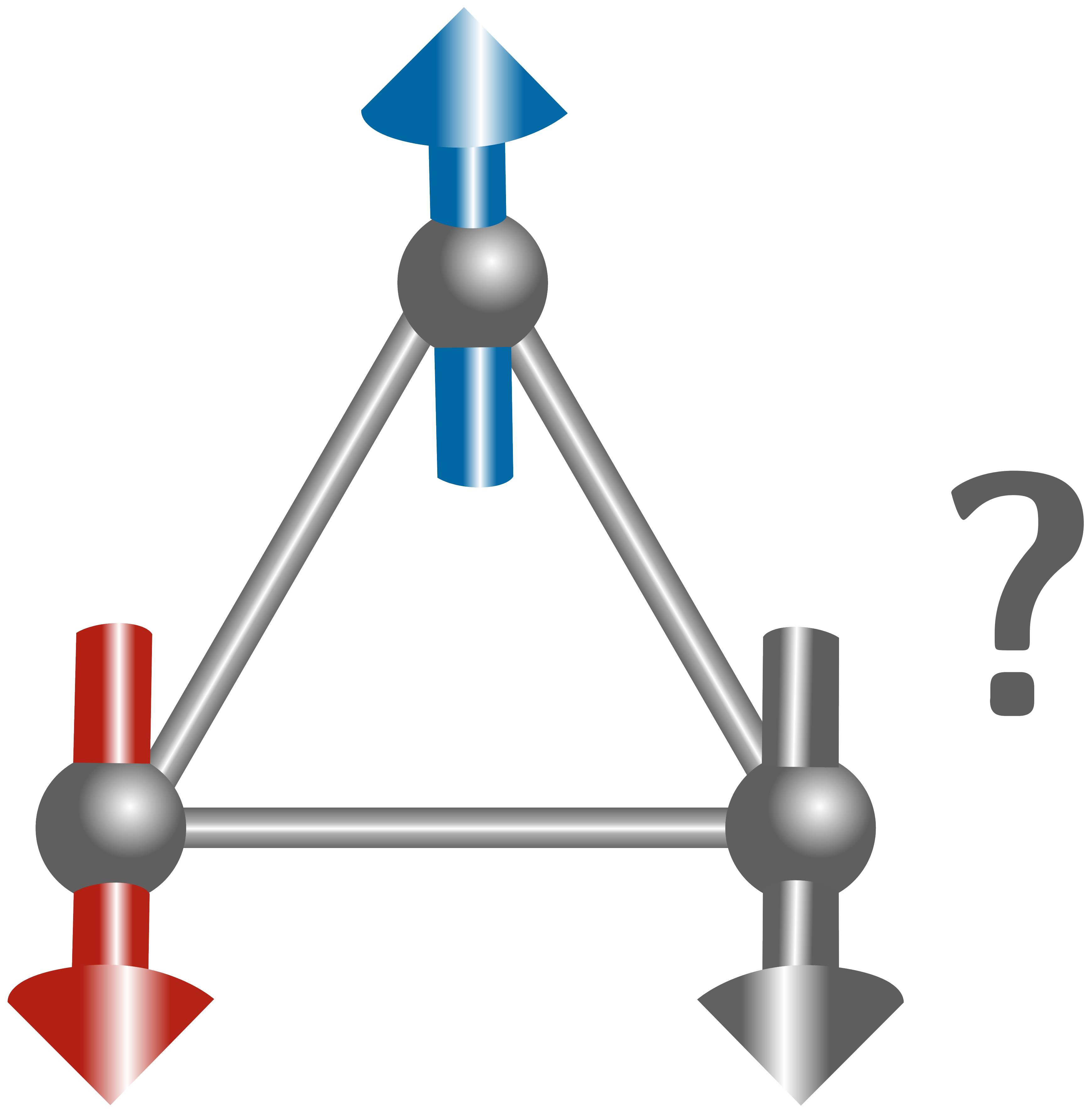

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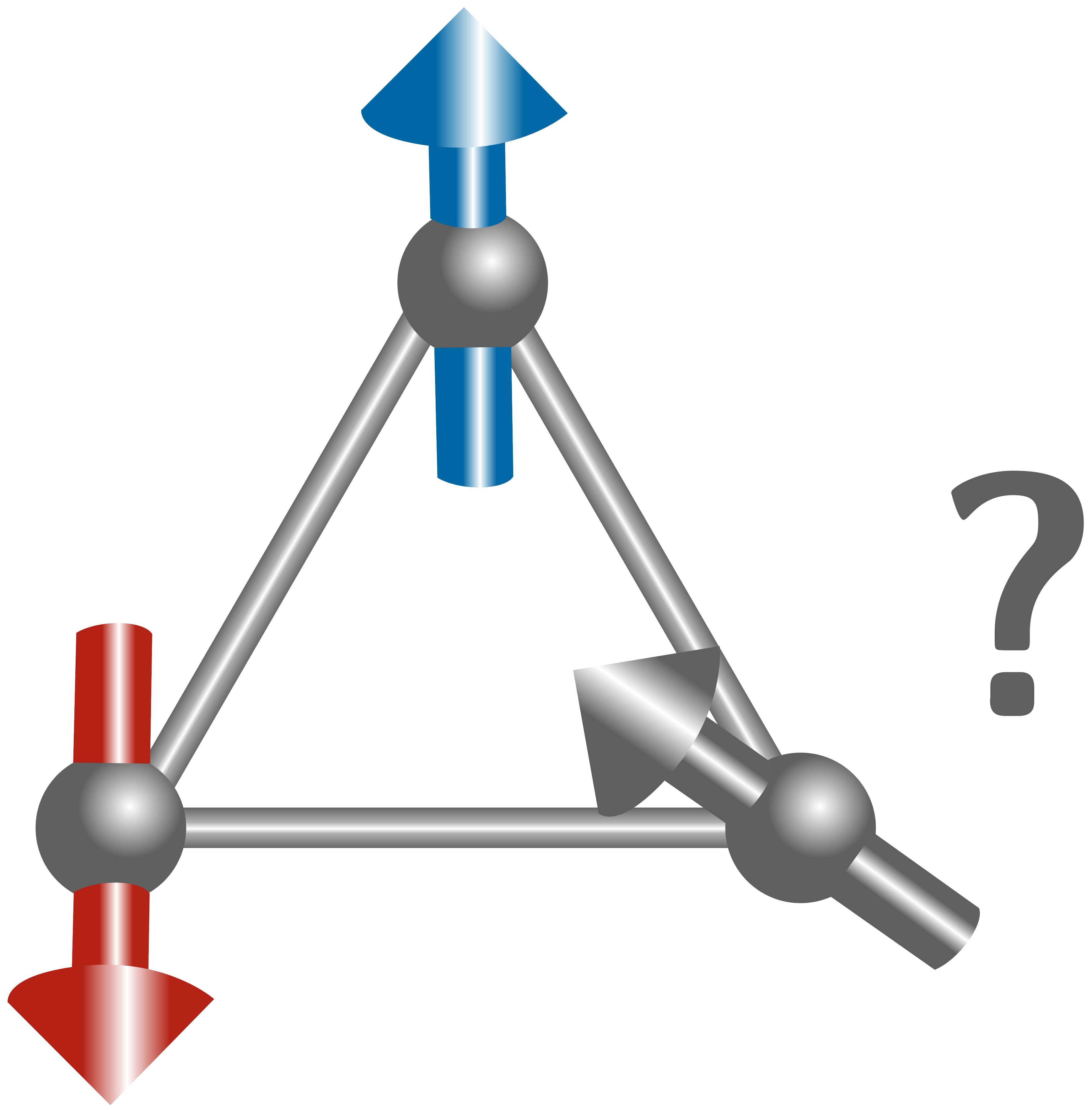

Magnetic frustration

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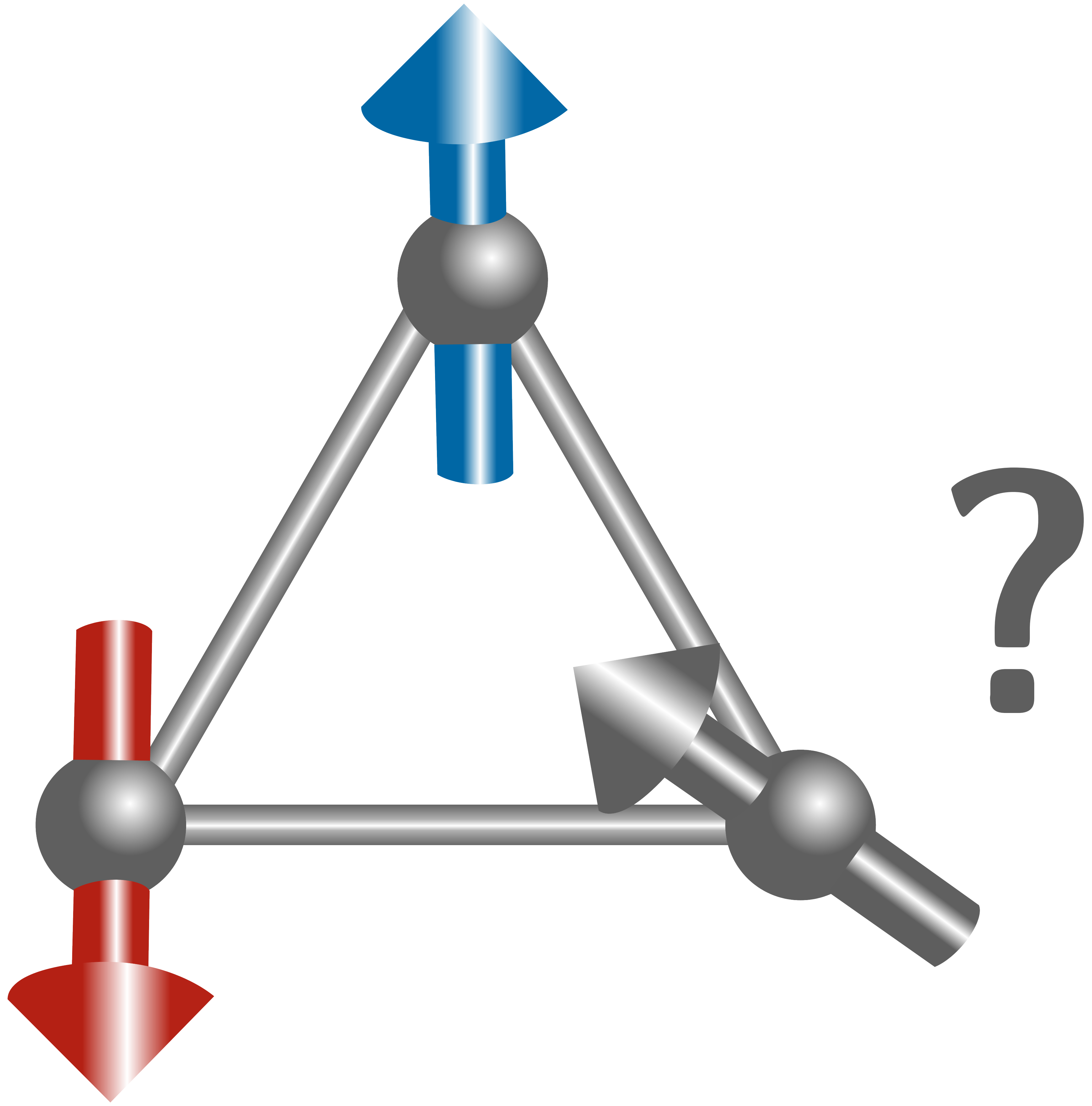
Frustration:

Incompatible interactions



Magnetic frustration

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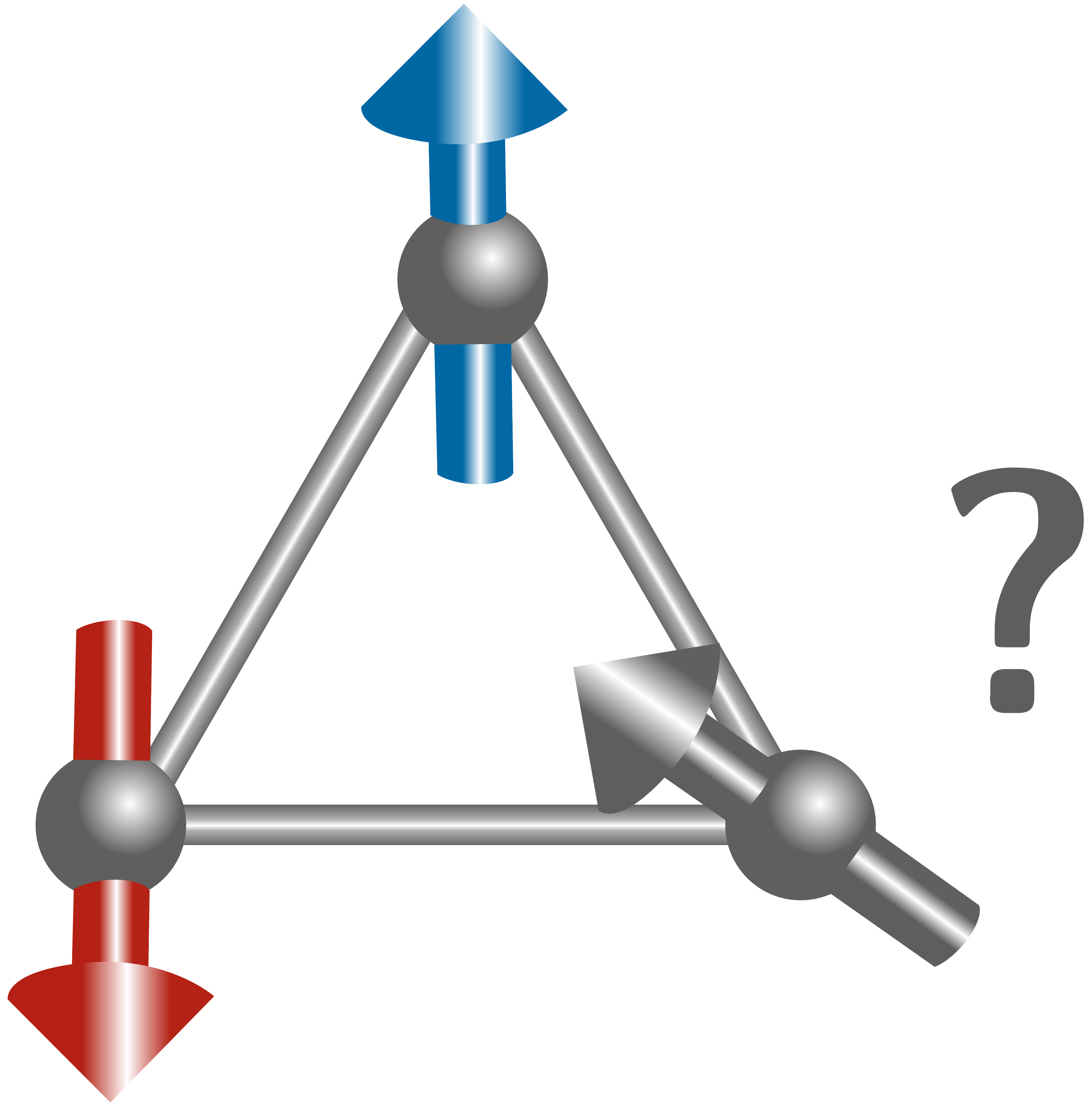


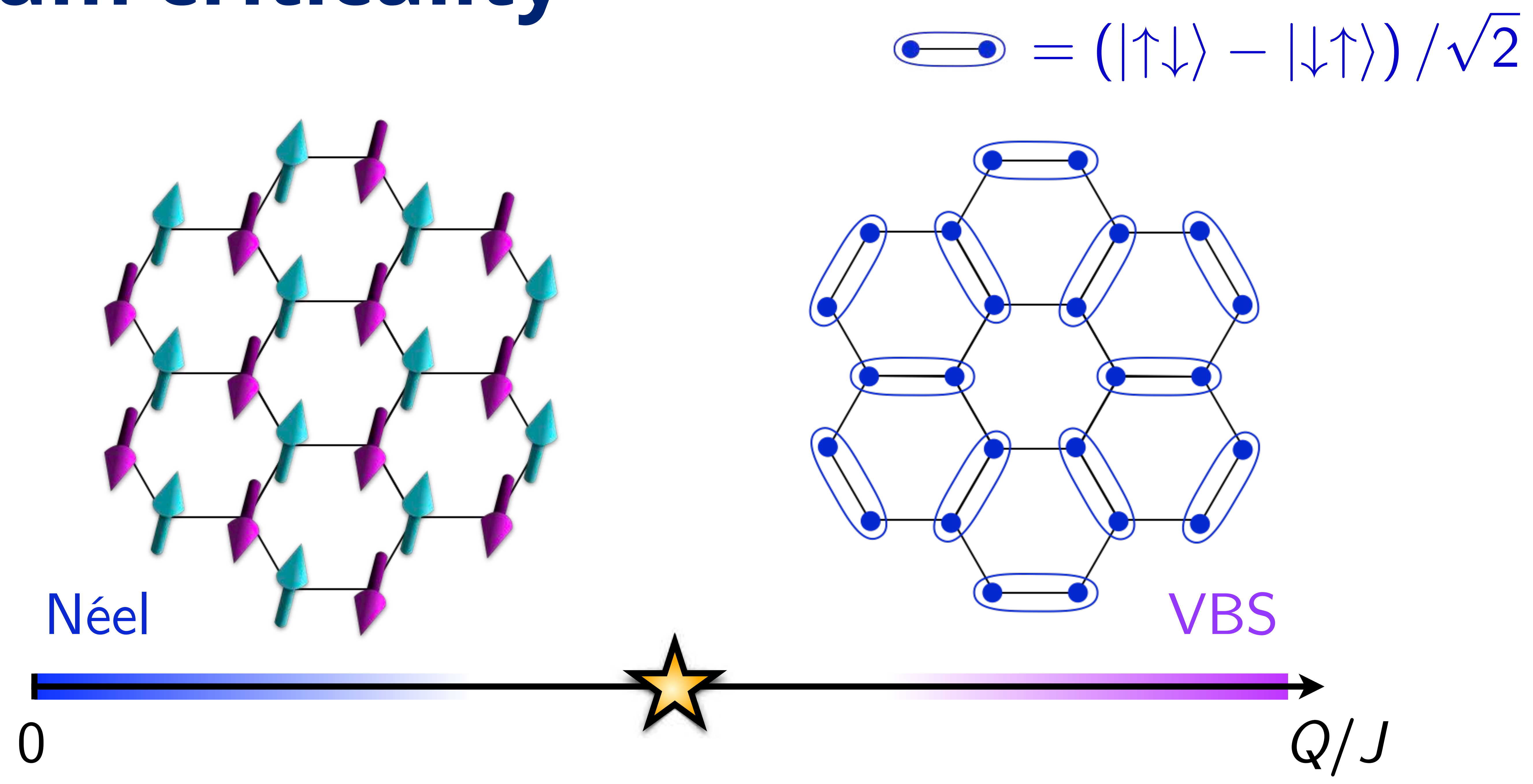
Frustration:

Incompatible interactions

⇓

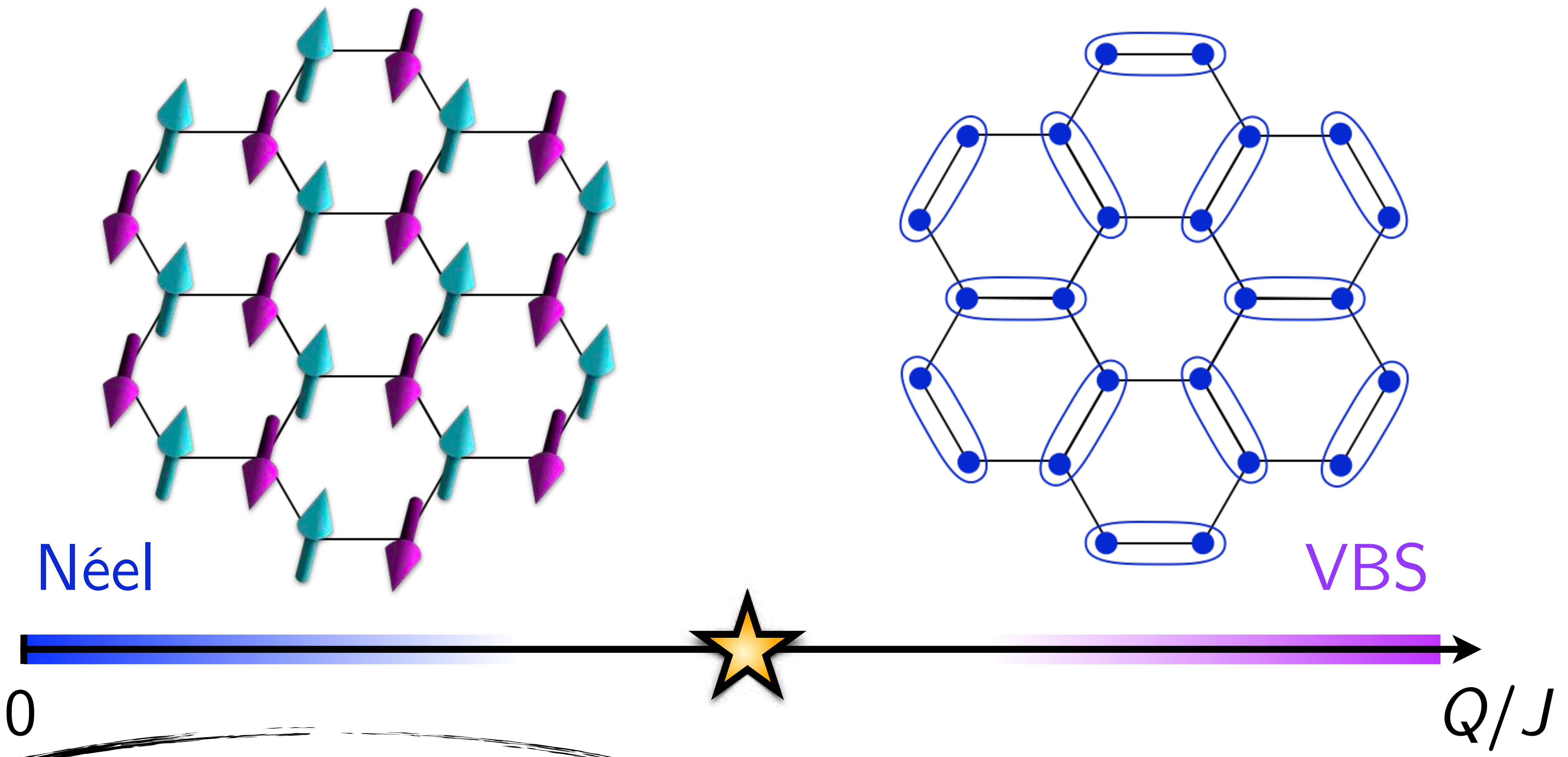
New states of matter
with exotic excitations?

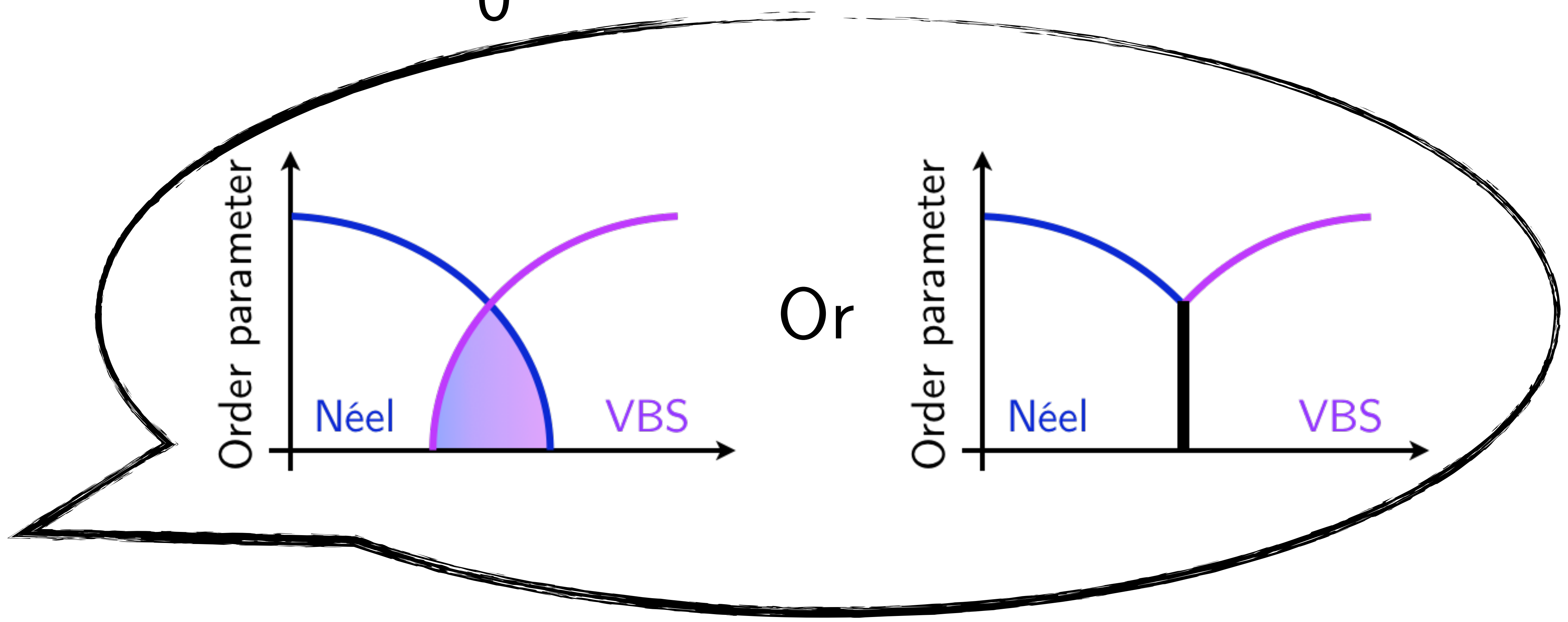
Deconfined quantum criticality

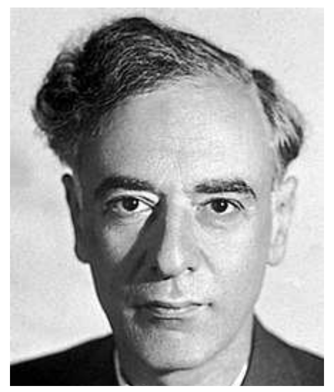


Deconfined quantum criticality

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



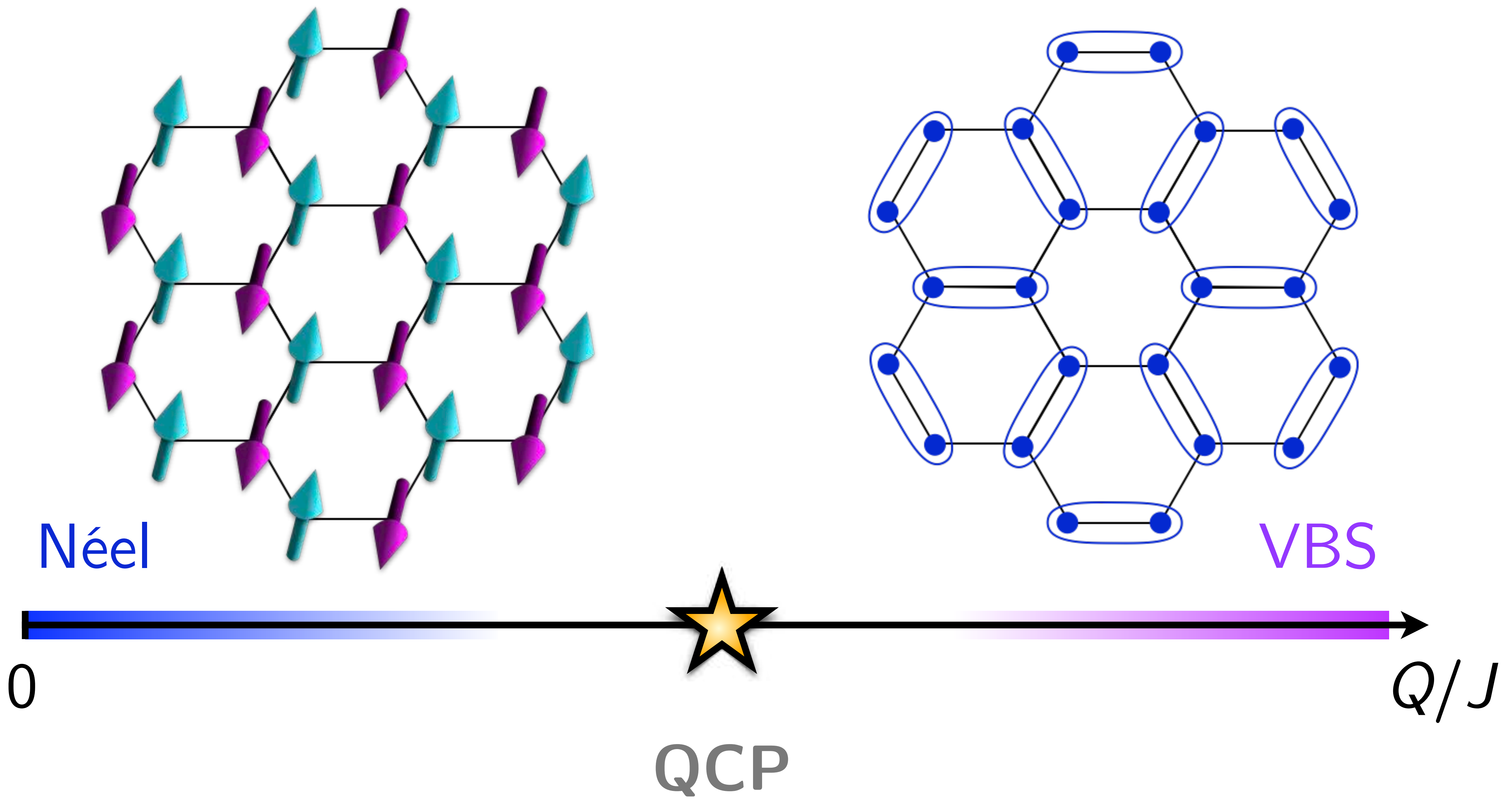


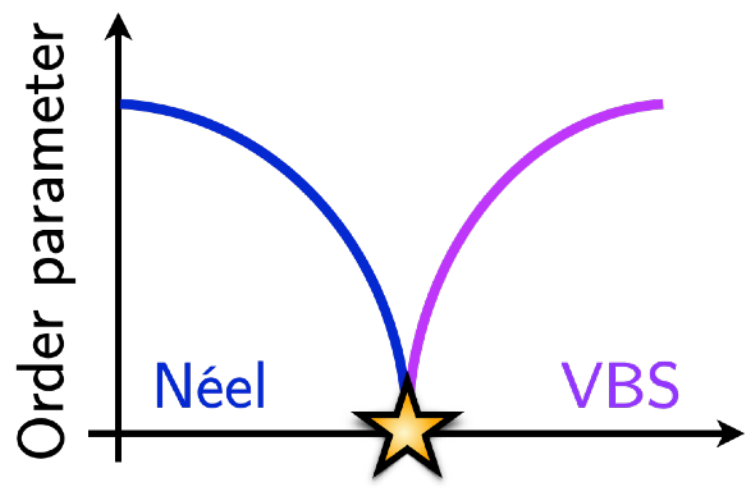


Landau

Deconfined quantum criticality

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





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

Deconfined quantum criticality

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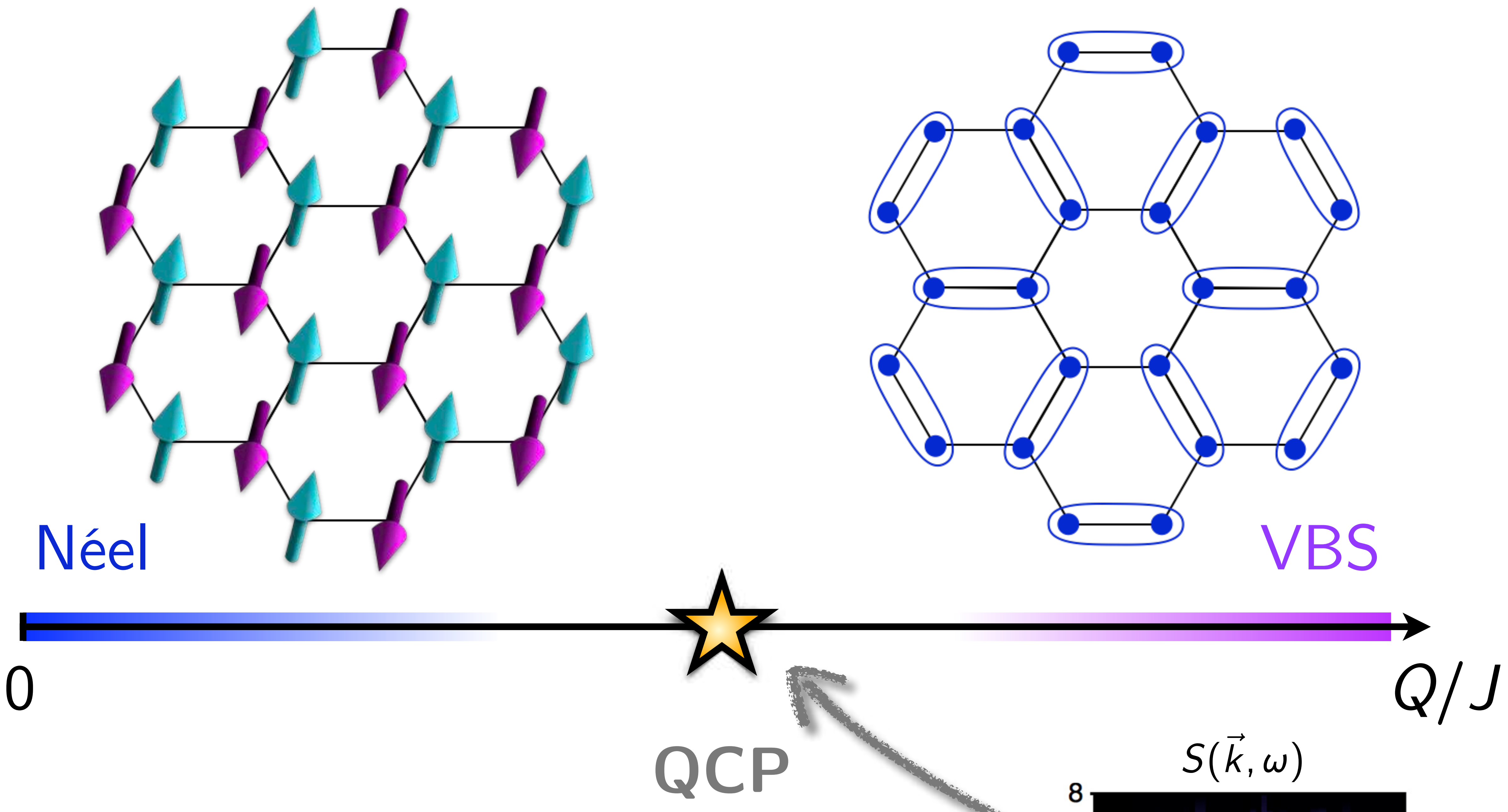
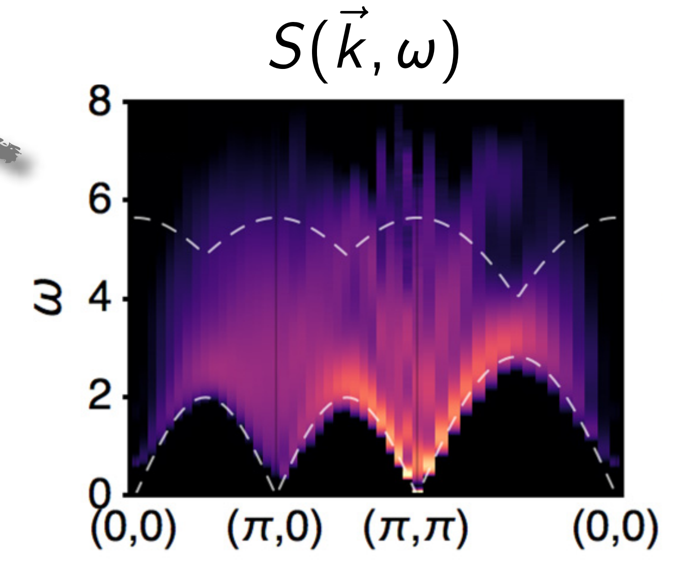
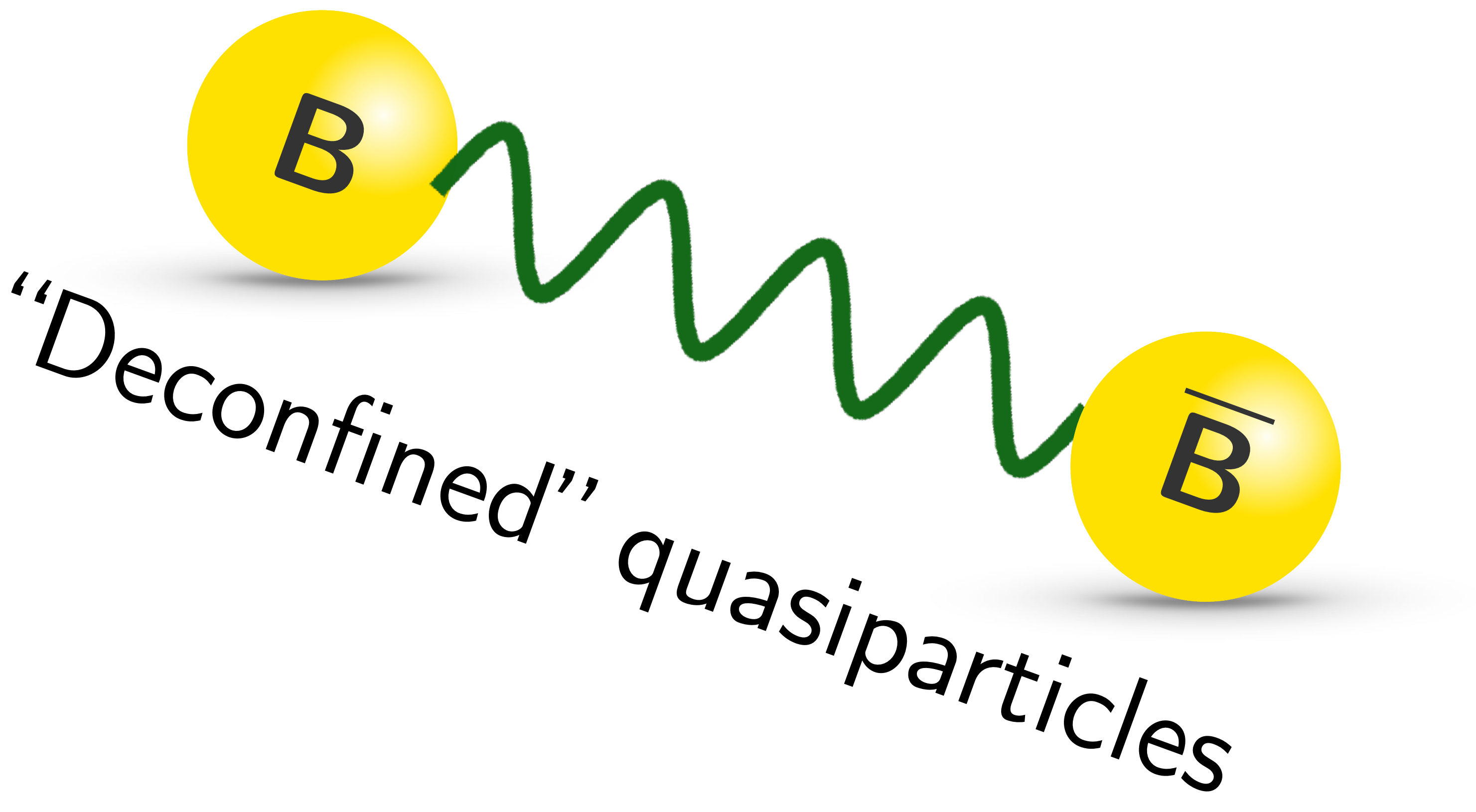
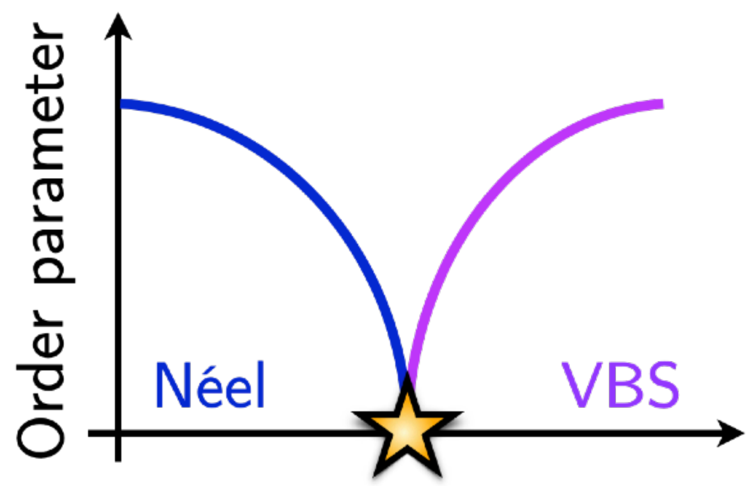




[Ma *et int.*, Meng, PRB '18]





[Senthil *et al.*, Science '04]
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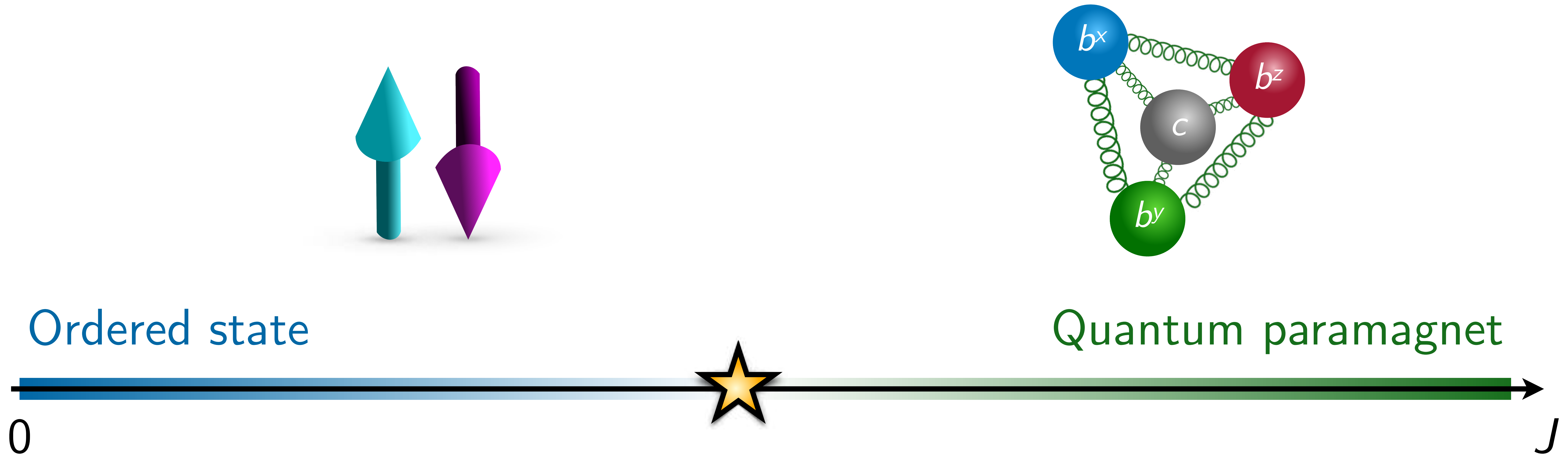
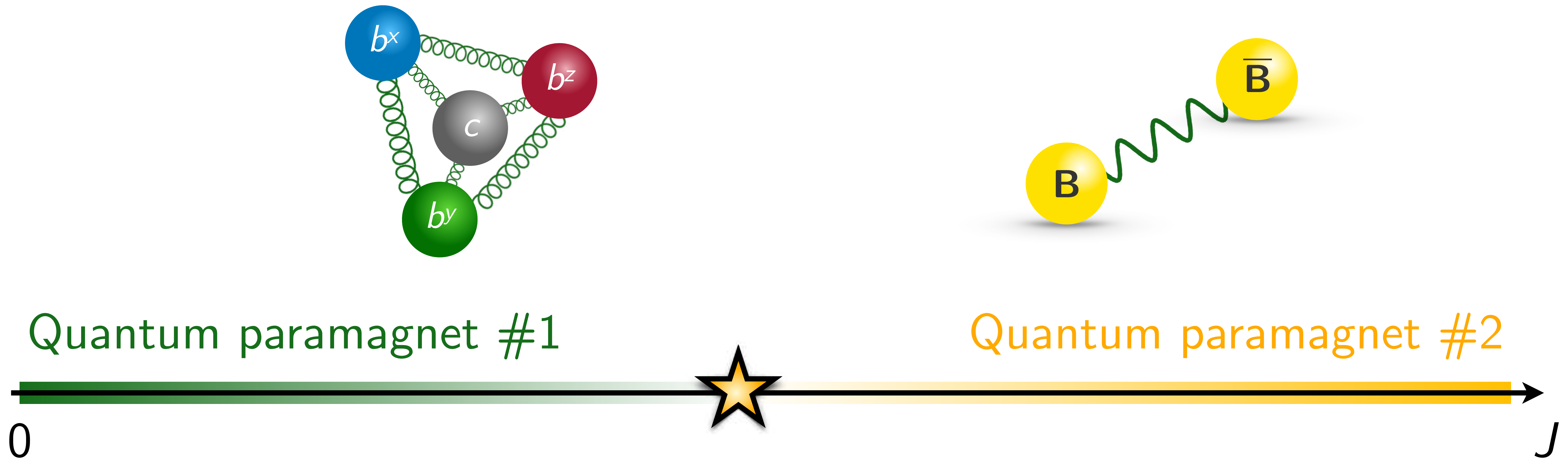
...

Fractionalized quantum criticality



[Assaad & Grover, PRX '16]
[Xu,, Qi, Zhang, Assaad, Xu, Meng, PRX '19]
[LJ, Wang, Scherer, Meng, Xu, PRB '20]
...

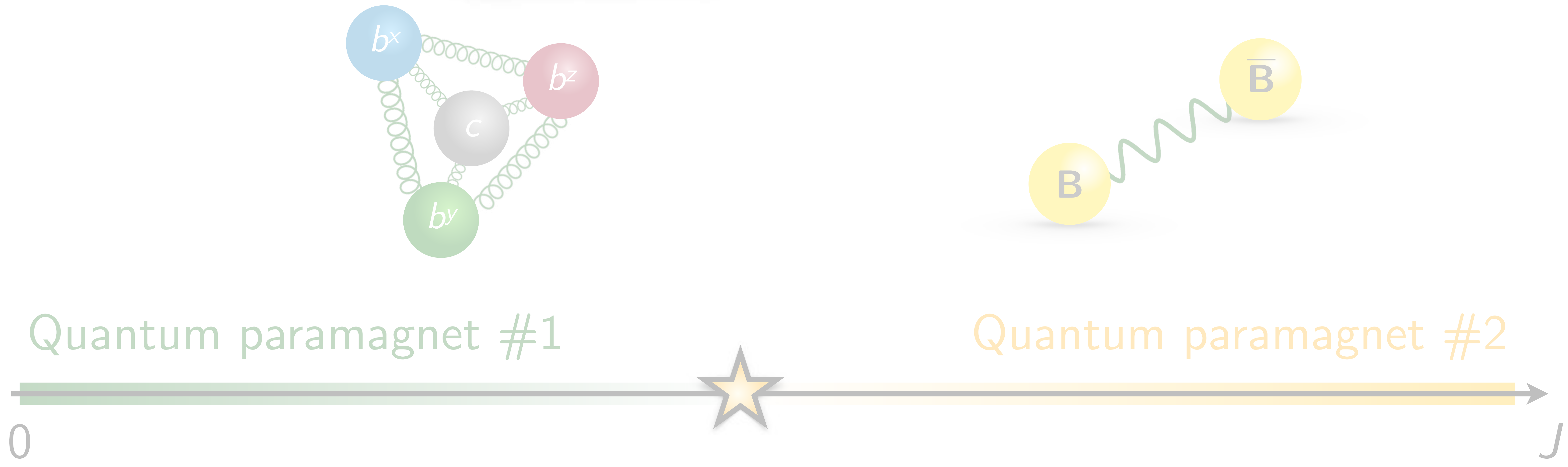


[Metlitski, Mross, Sachdev, Senthil, PRB '15]
[LJ & He, PRB '17]
[Boyack, Lin, Zerf, Rayyan, Maciejko, PRB '18]
...

Fractionalized quantum criticality

[Assaad & Grover, PRX '16]
[Xu,, Qi, Zhang, Assaad, Xu, Meng, PRX '19]
[LJ, Wang, Scherer, Meng, Xu, PRB '20]
...

Functional approaches can help!



[Metlitski, Mross, Sachdev, Senthil, PRB '15]
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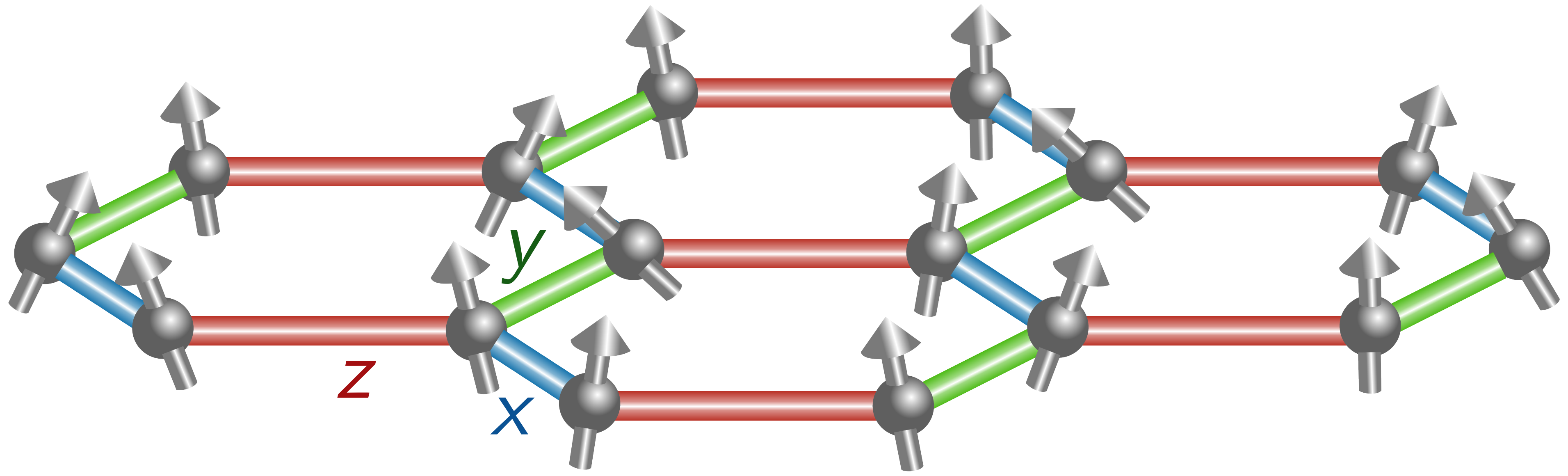
...

Kitaev spin-1/2 model

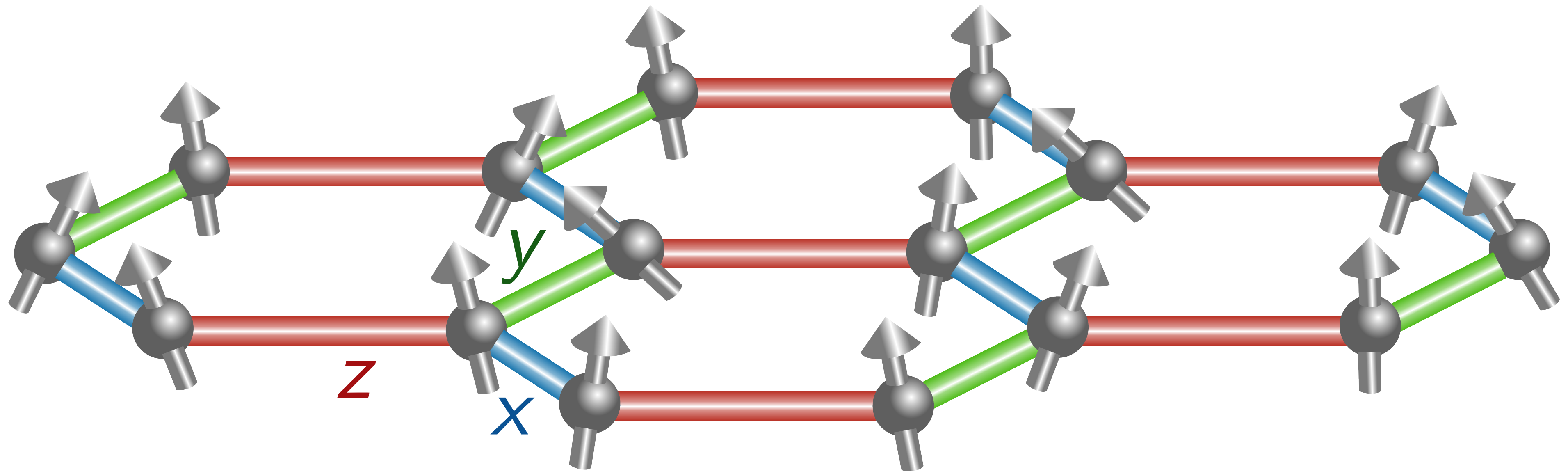


Hamiltonian:

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

[Kitaev, Ann. Phys. '06]

Kitaev spin-1/2 model



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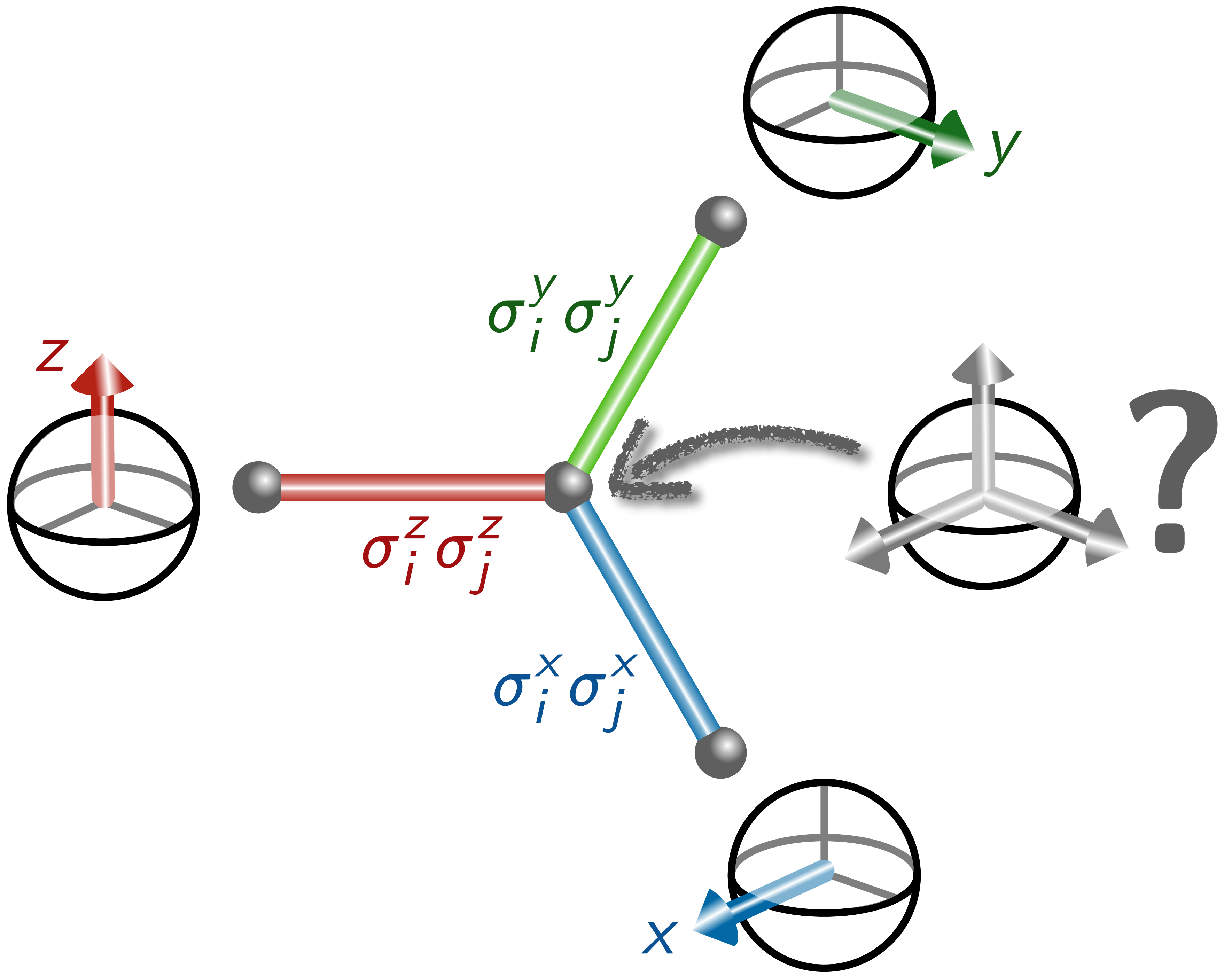
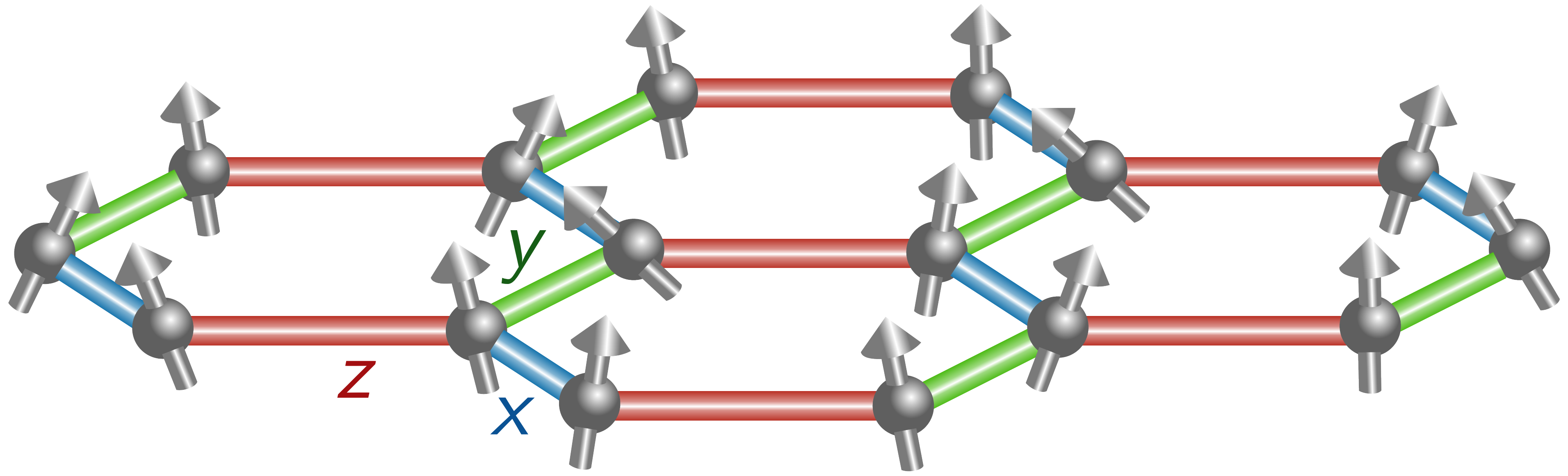
[Kitaev, Ann. Phys. '06]

Frustration:



Kitaev spin-1/2 model



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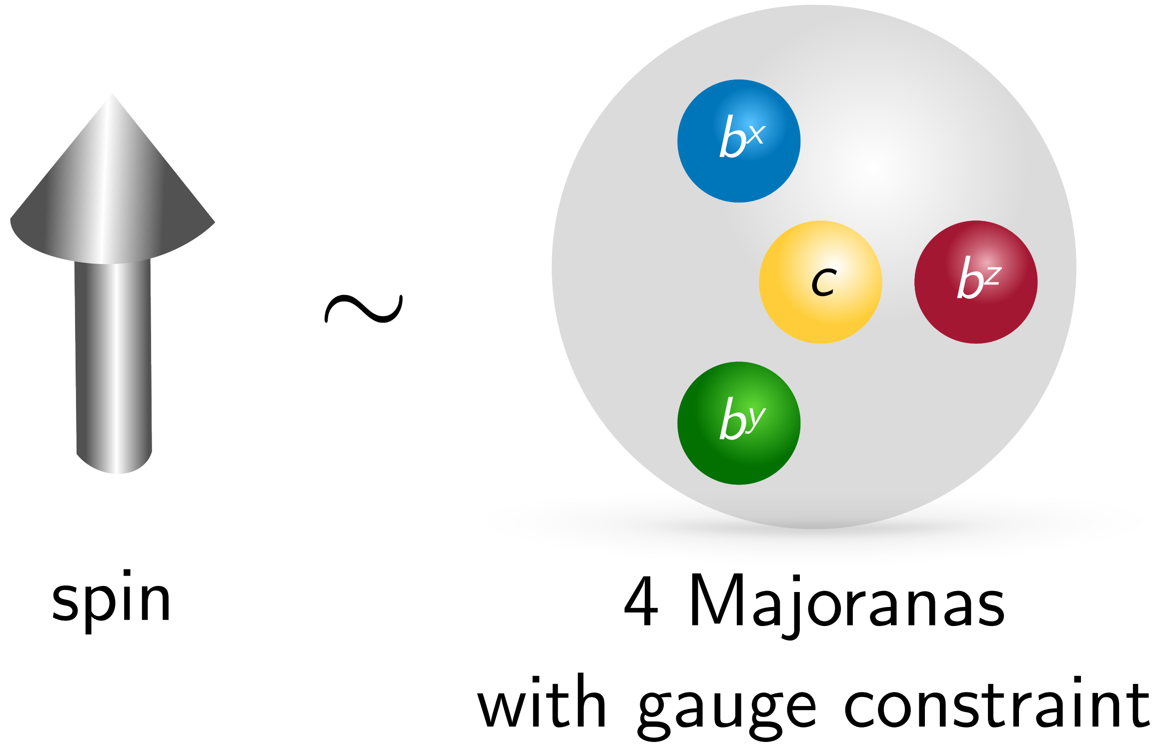
[Kitaev, Ann. Phys. '06]

Majorana representation:

$$\sigma^x \sim i b^x c$$
$$\sigma^y \sim i b^y c$$
$$\sigma^z \sim i b^z c$$



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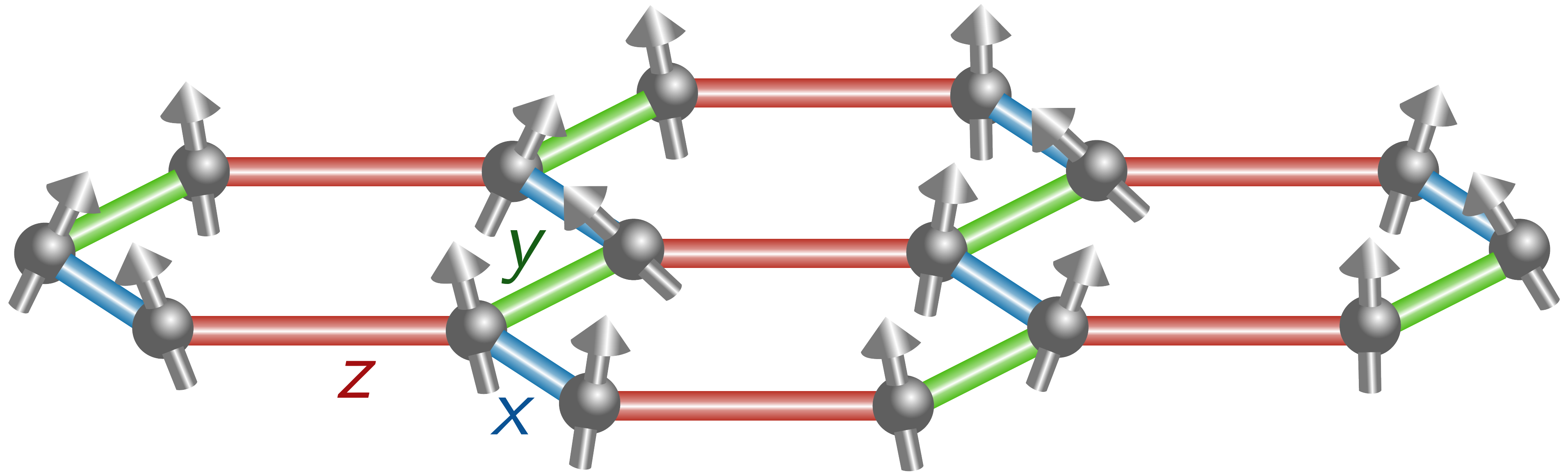

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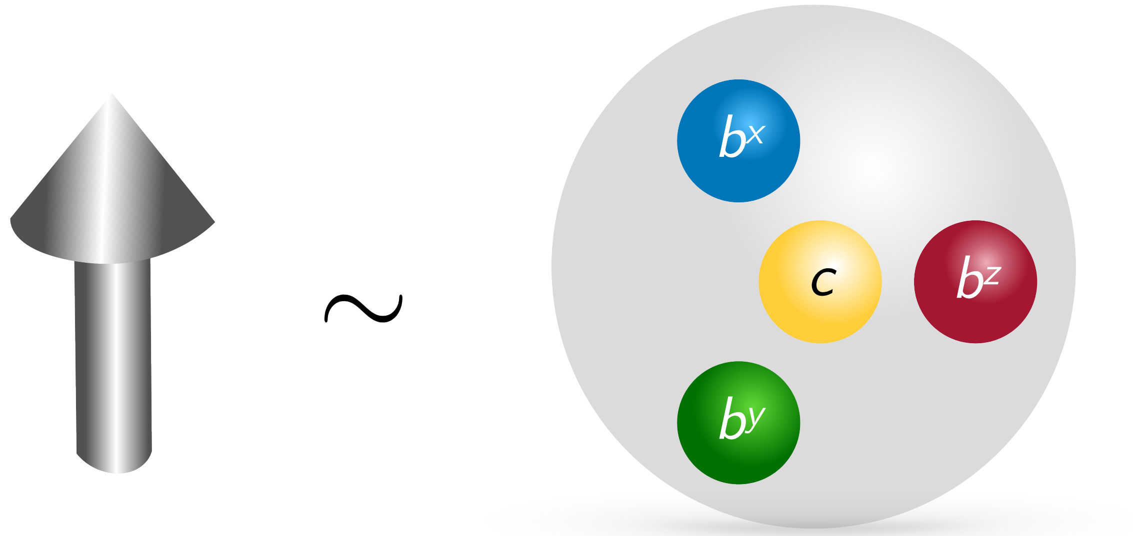


spin

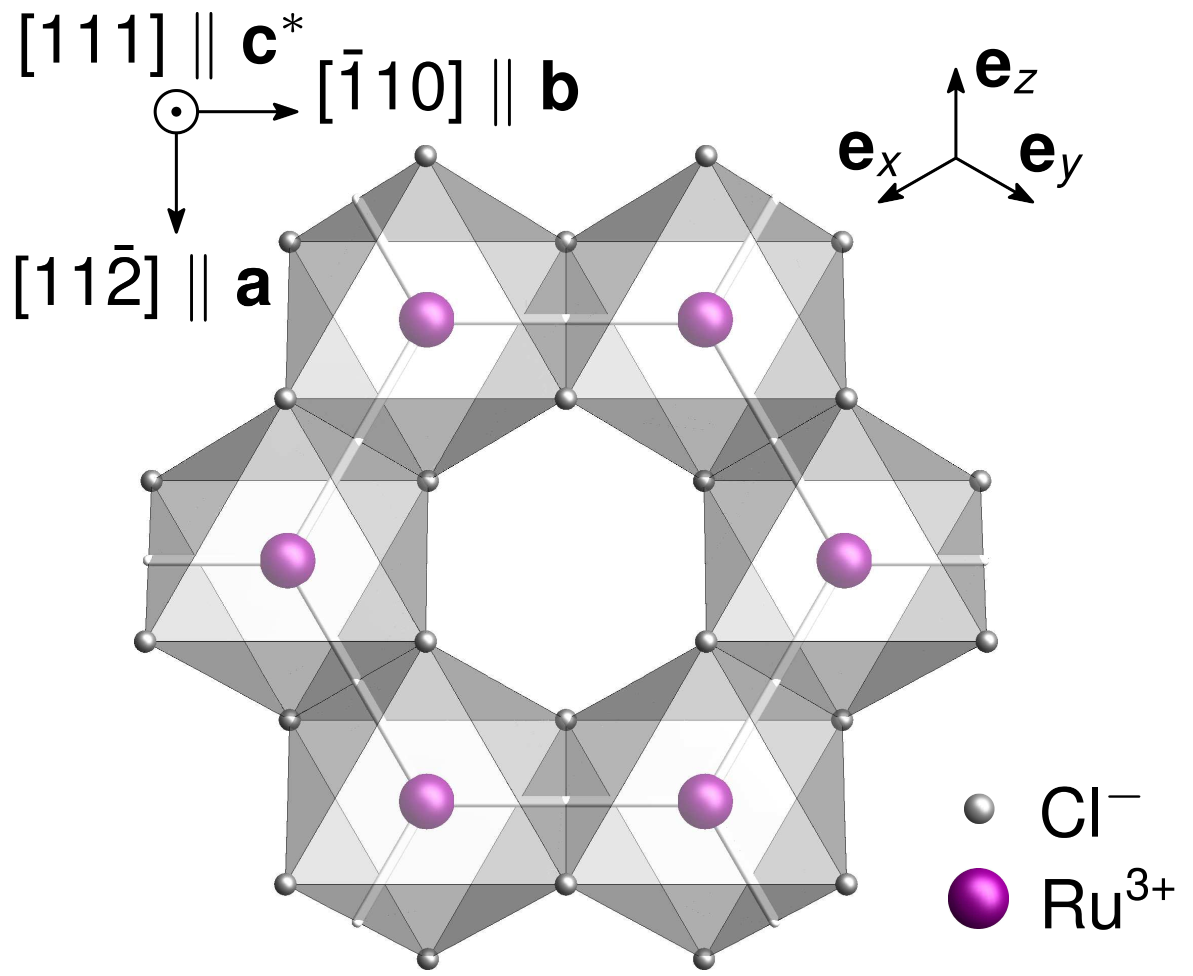
4 Majoranas
with gauge constraint

Fractionalization:

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

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

Kitaev-Heisenberg spin-1/2 model

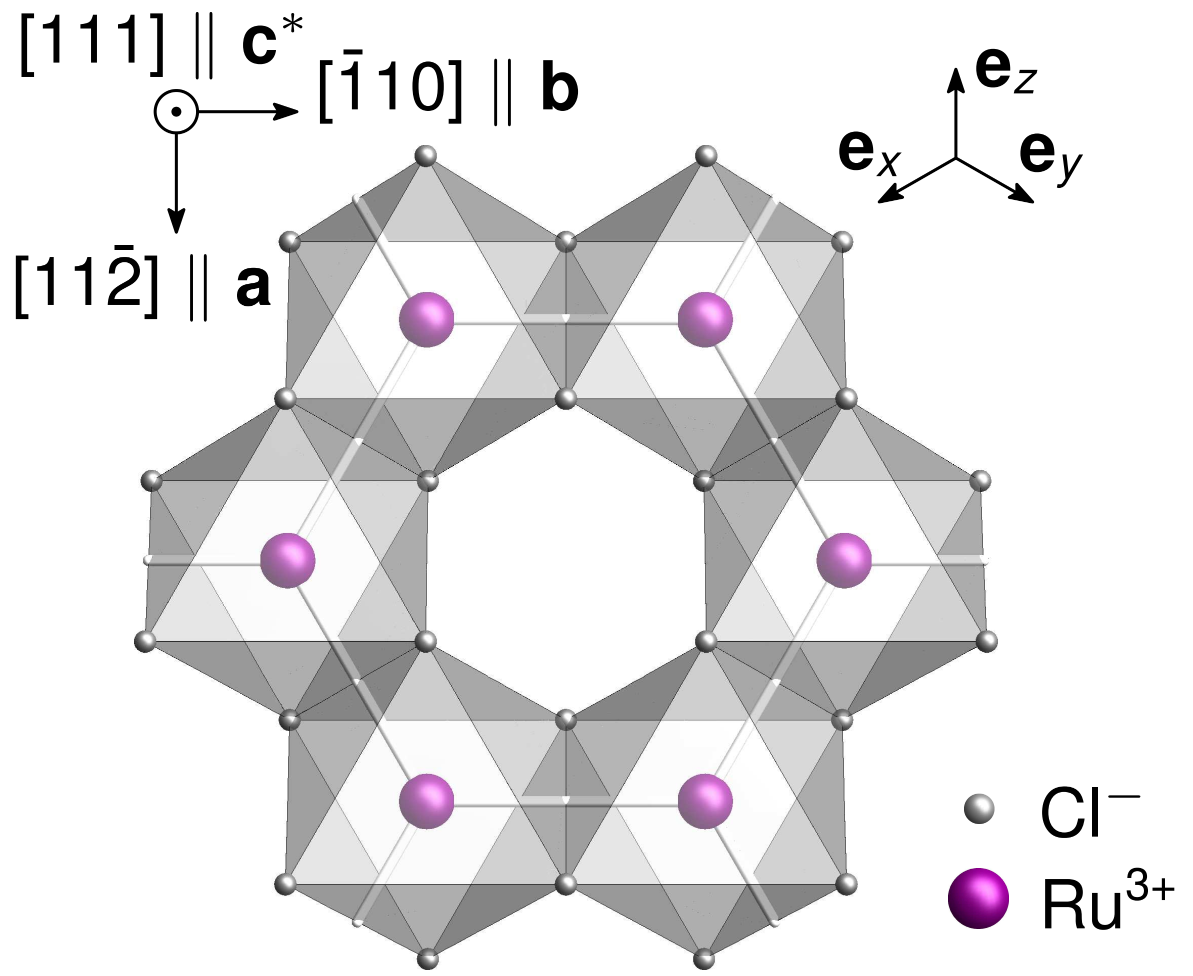


Hamiltonian:

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

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

Kitaev-Heisenberg spin-1/2 model



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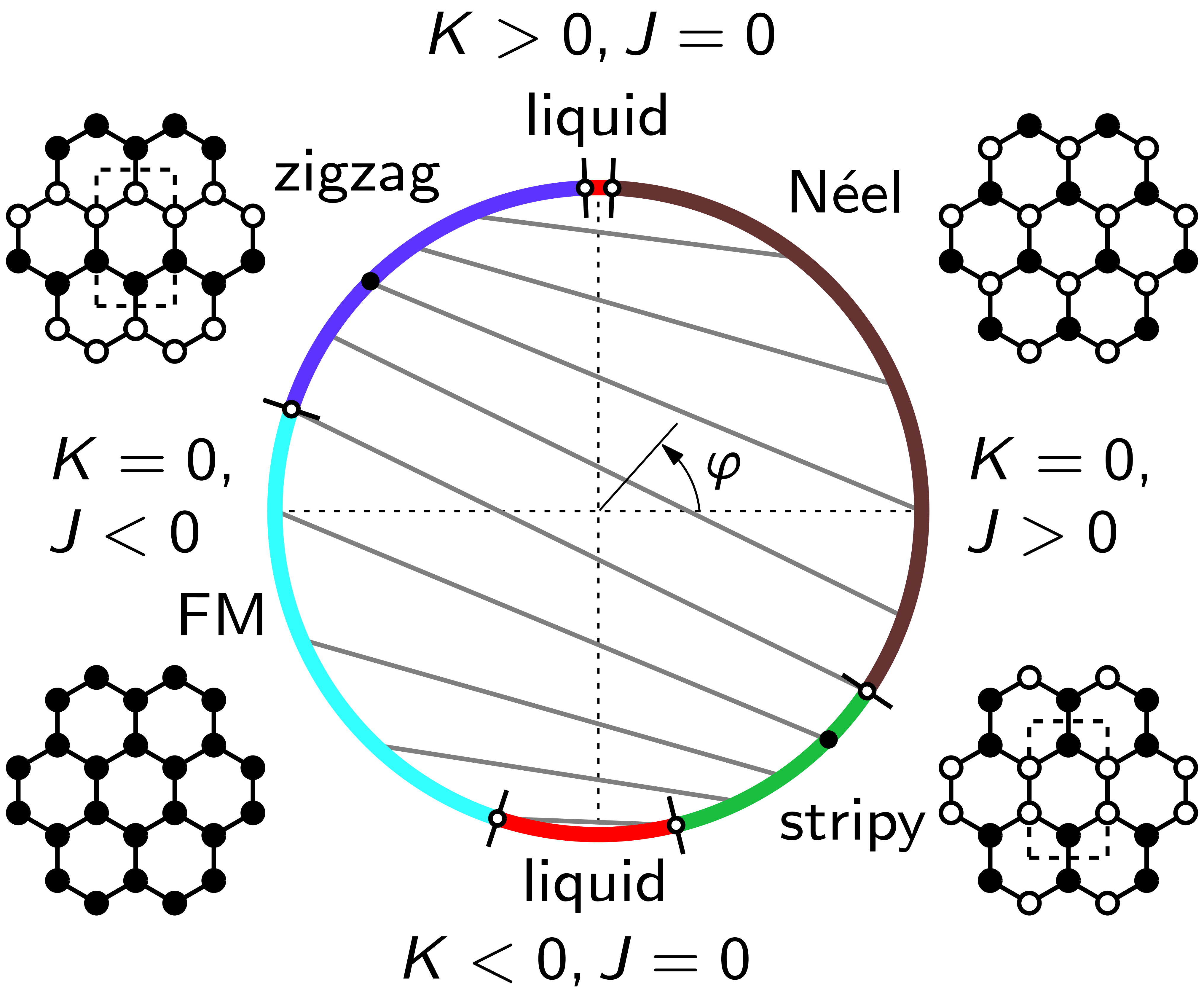
Phase diagram:



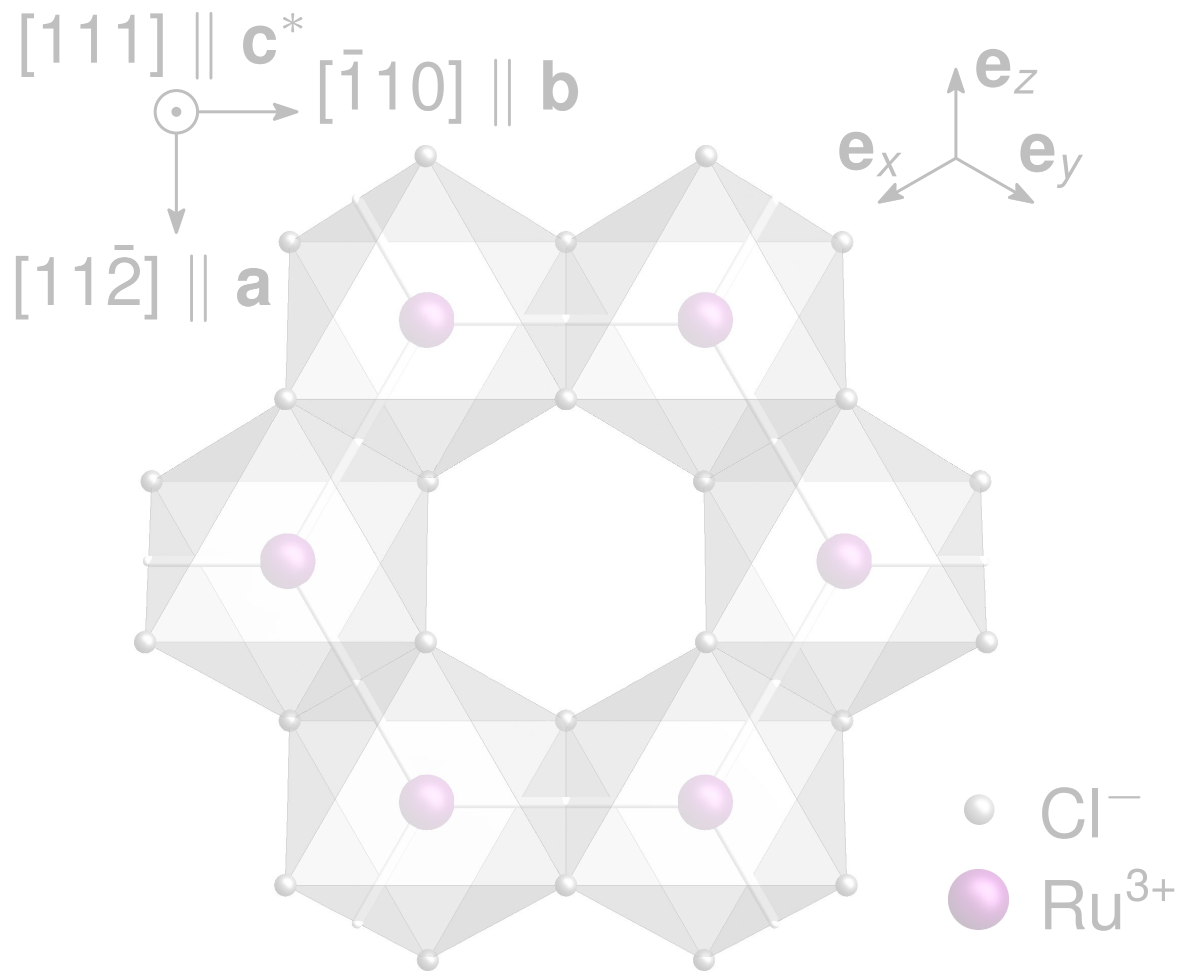
... possible relevance to α-$RuCl_3$, Na_2IrO_3, $Na_2Co_2TeO_6$, ...

$$J = A \cos\varphi$$

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

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

Kitaev-Heisenberg spin-1/2 model



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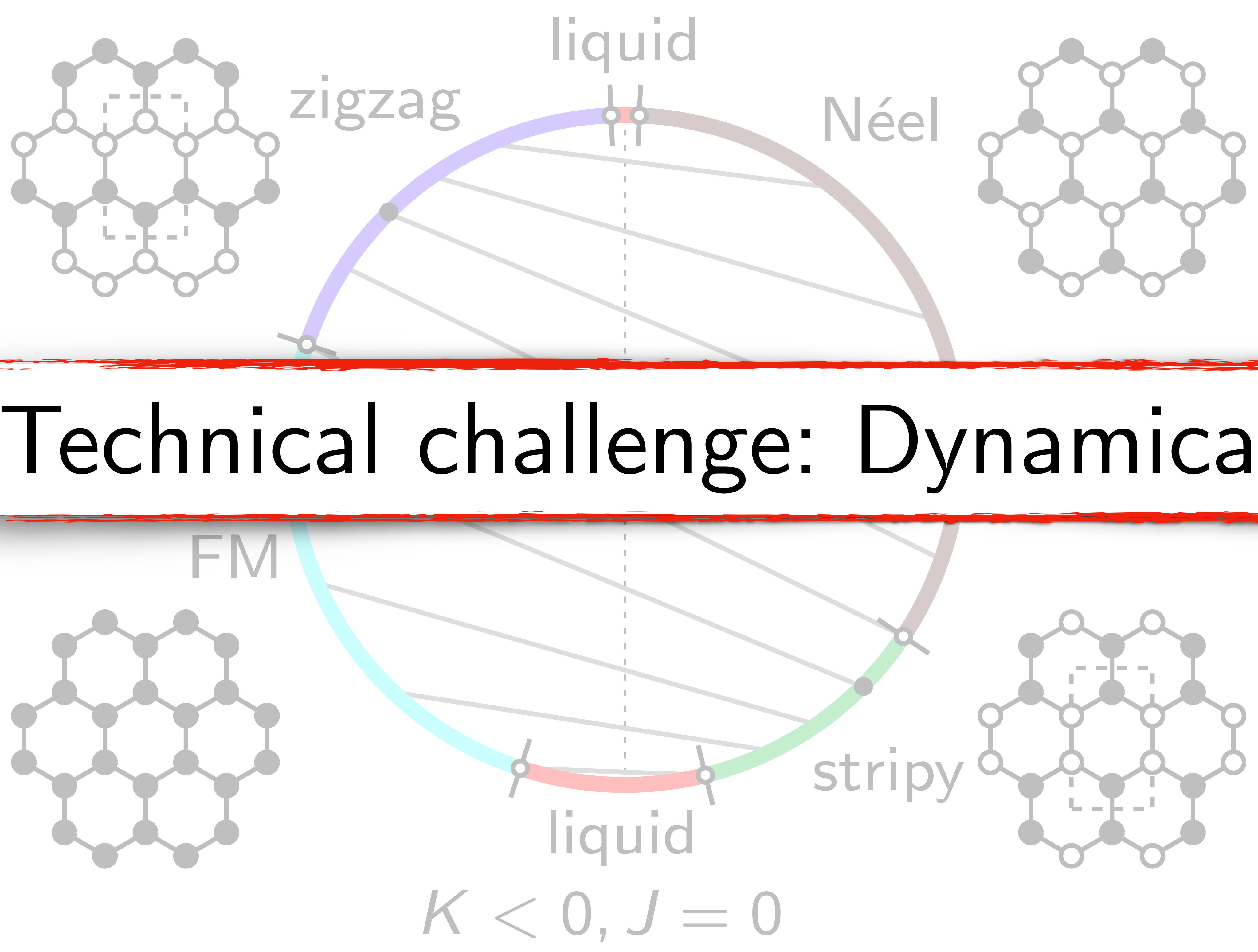
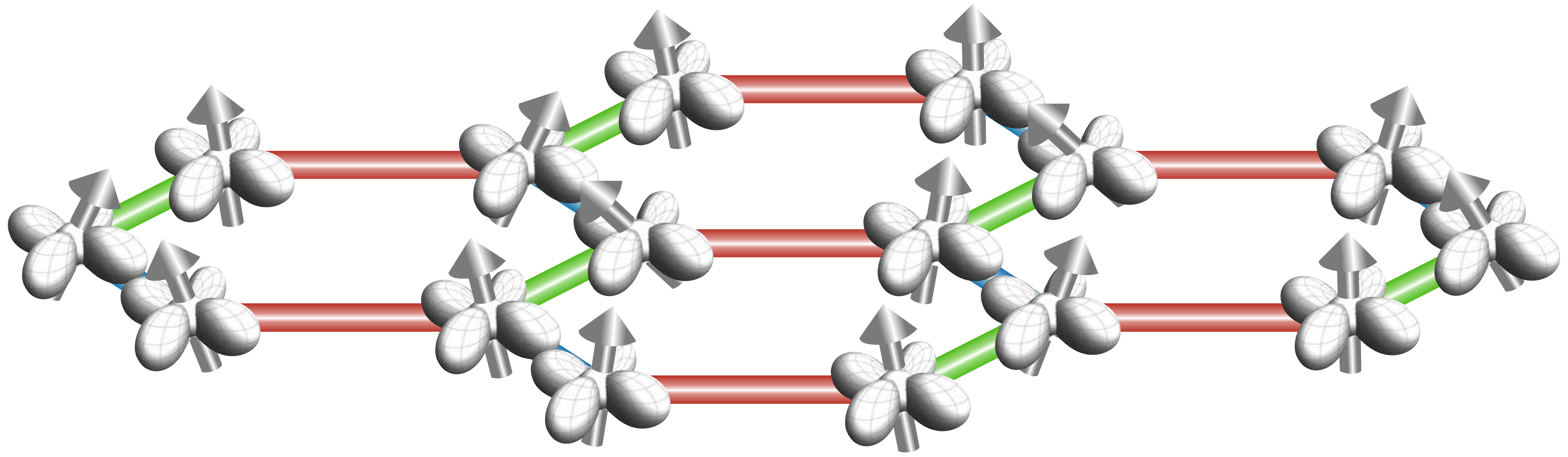


Technical challenge: Dynamical $\mathbb{Z}_2$ gauge field!

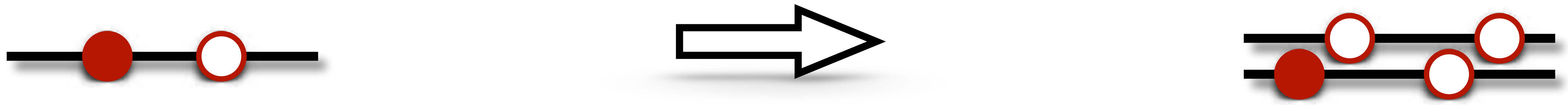
... no sign-problem-free QMC available: [Sato & Assaad, PRB '21]

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

Beyond Kitaev spin-1/2



Spin-orbital generalization:

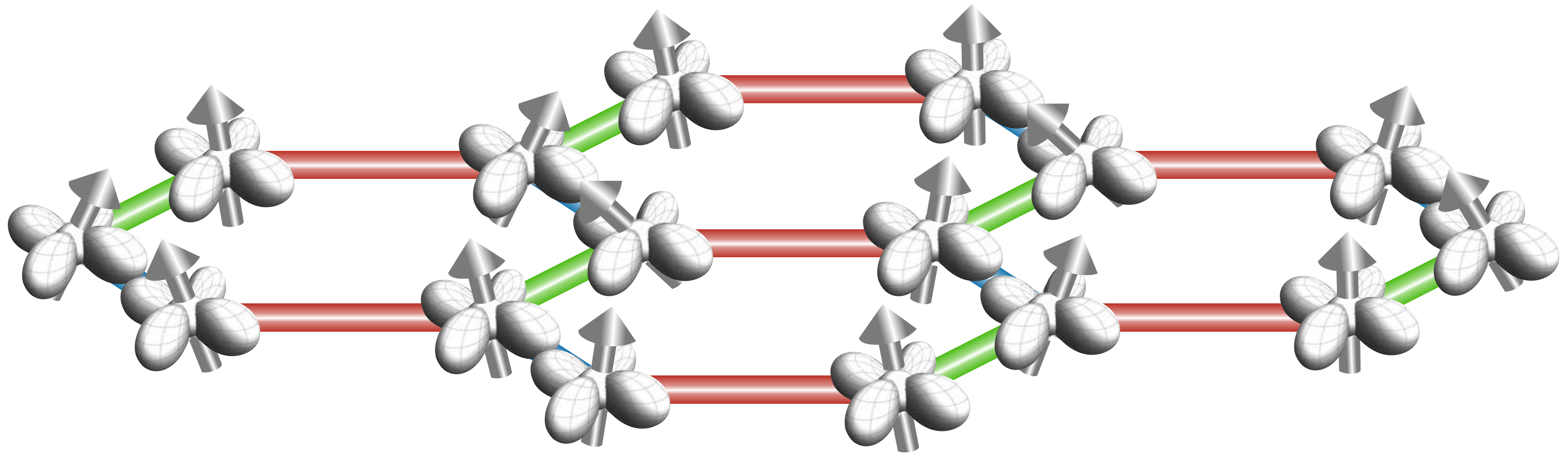


$\sigma^{\alpha} \quad 2 \times 2$

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

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

Beyond Kitaev spin-1/2



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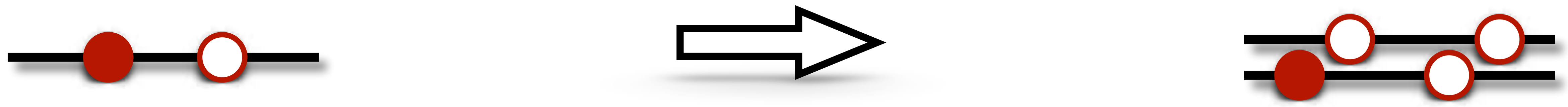

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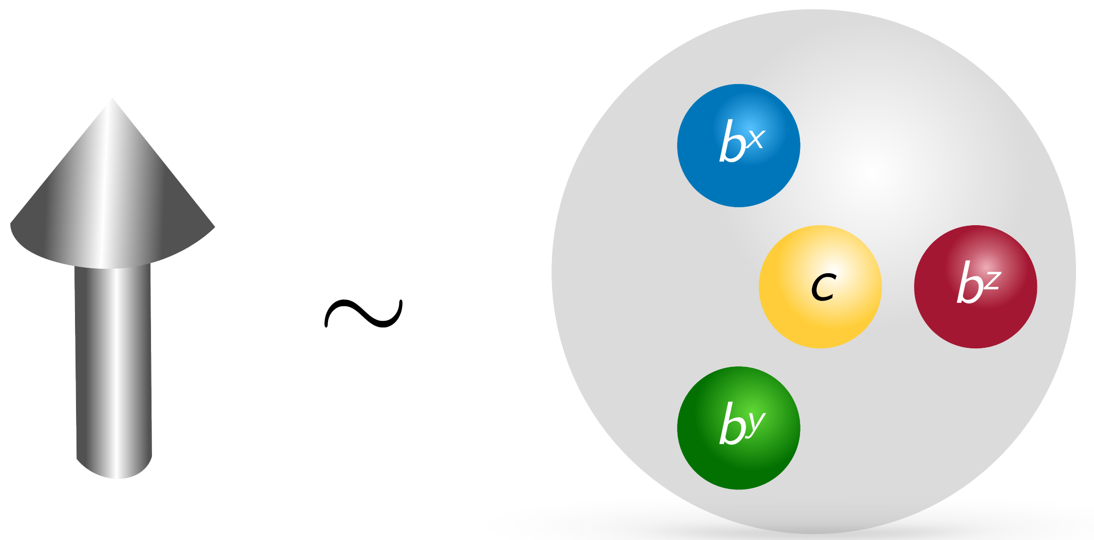
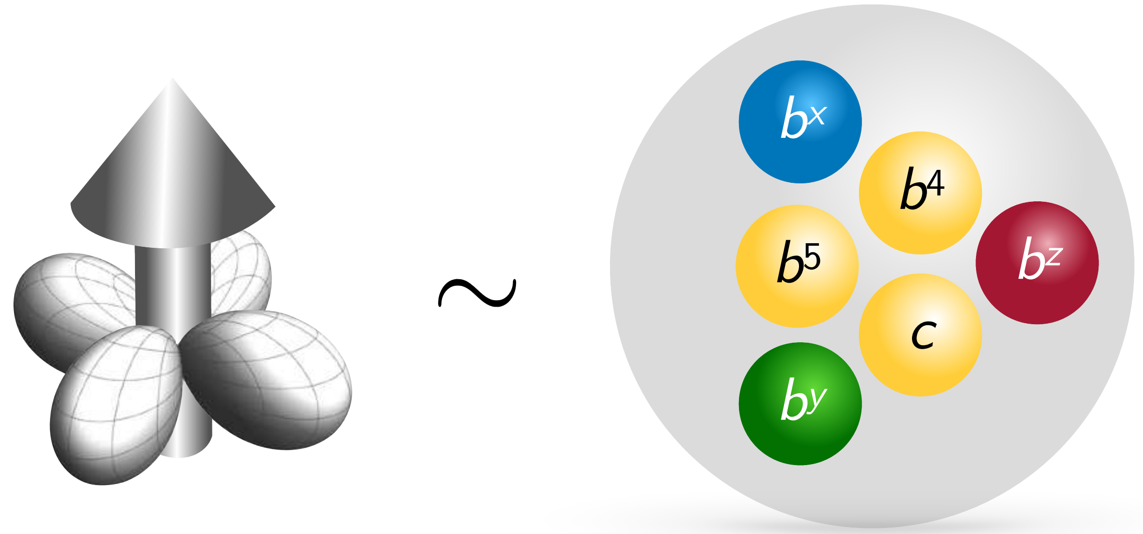


spin

4 Majoranas
with gauge constraint



spin + orbital

6 Majoranas
with gauge constraint

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

Kitaev spin-orbital models

Hamiltonian:

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

Heisenberg spin

Kitaev orbital

Kitaev spin-orbital models

Hamiltonian:

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

Heisenberg spin

Kitaev orbital

$$\mapsto iK \sum_{\langle ij \rangle_\gamma} \hat{u}_{ij} \left(c_i c_j + b_i^4 b_j^4 + b_i^5 b_j^5 \right)$$

Spin-orbital representation:

$$\gamma^1 = \sigma^y \otimes \tau^x \mapsto i b^x c$$
$$\gamma^2 = \sigma^y \otimes \tau^y \mapsto i b^y c$$
$$\gamma^3 = \sigma^y \otimes \tau^z \mapsto i b^z c$$
$$\gamma^4 = \sigma^x \otimes \mathbb{1} \mapsto i b^4 c$$
$$\gamma^5 = \sigma^z \otimes \mathbb{1} \mapsto i b^5 c$$

Kitaev spin-orbital models

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$$\gamma^5 = \sigma^z \otimes \mathbb{1} \mapsto i b^5 c$$

Ground state:

$$\hat{u}_{ij} \mapsto u_{ij} \equiv 1 \quad \Longrightarrow \quad \mathcal{H} \sim \mathrm{i}K \sum_{\langle ij \rangle} \boldsymbol{c}_i^\top \boldsymbol{c}_j$$

[Lieb, PRL '94]

with $\boldsymbol{c}_i \equiv \begin{pmatrix} c_i \\ b_i^4 \\ b_i^5 \end{pmatrix}$

Kitaev spin-orbital models

Hamiltonian:

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Heisenberg spin

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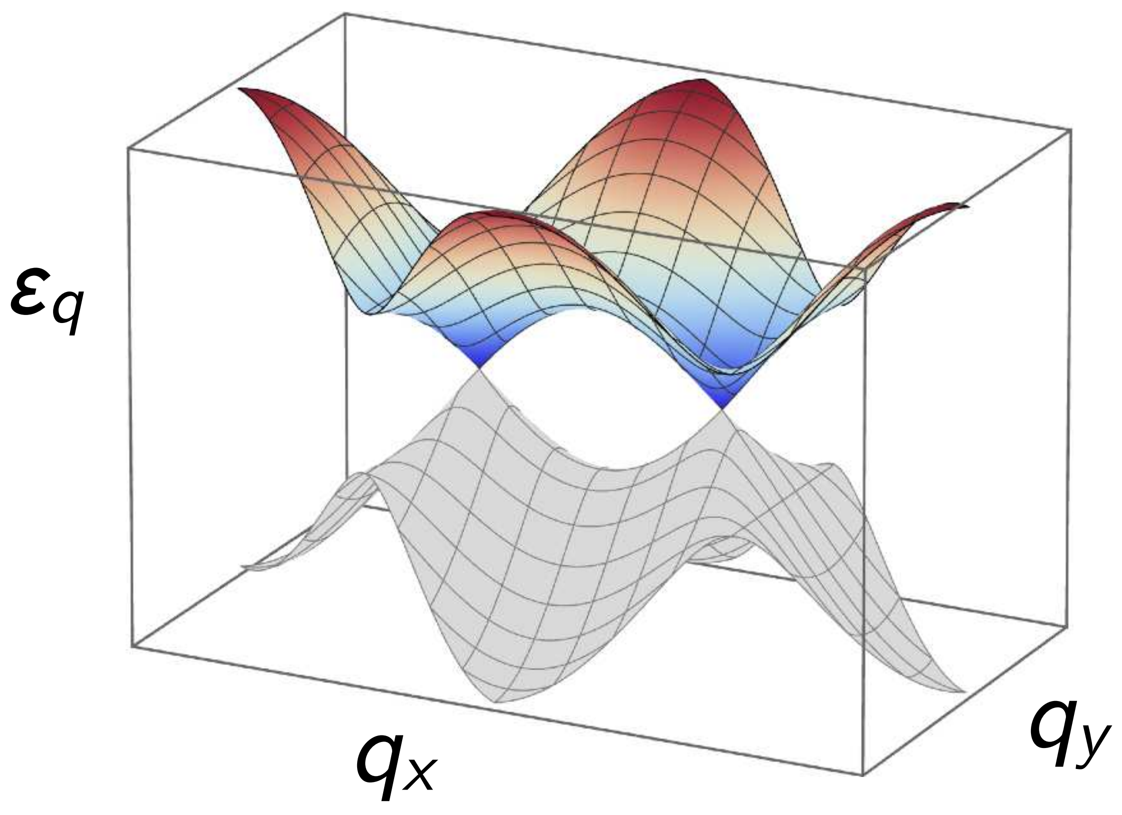
$$\gamma^4 = \sigma^x \otimes \mathbb{1} \mapsto i b^4 c$$
$$\gamma^5 = \sigma^z \otimes \mathbb{1} \mapsto i b^5 c$$

Majorana spectrum:



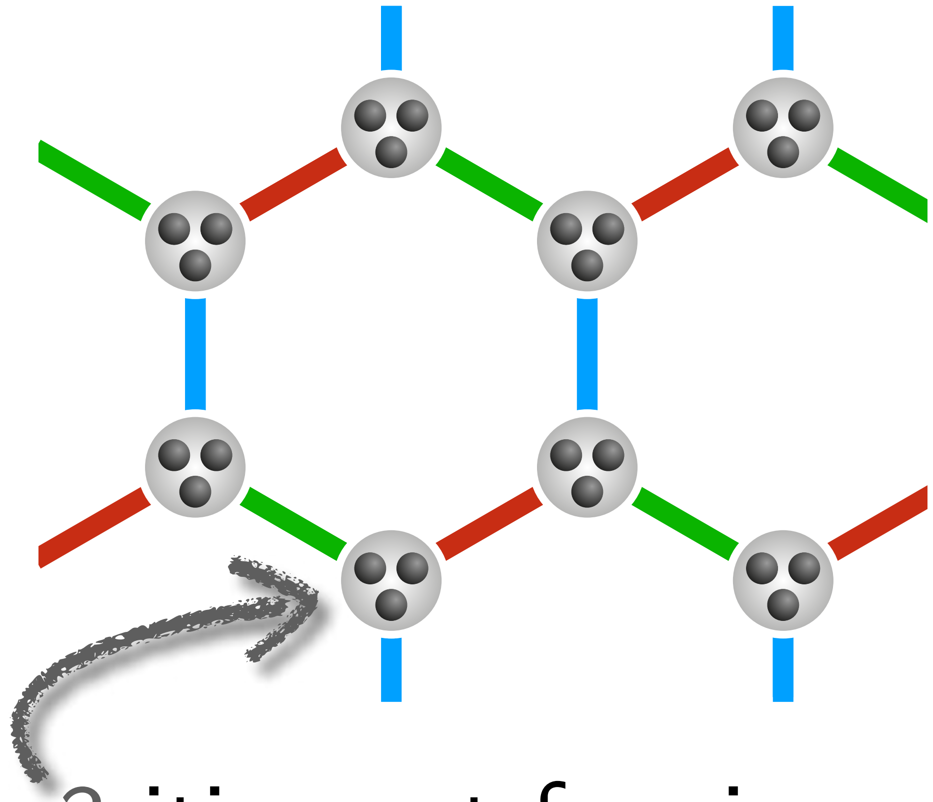
$\times 3$

Kitaev-Heisenberg spin-orbital model

Hamiltonian:

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

Kitaev-Heisenberg spin-orbital model



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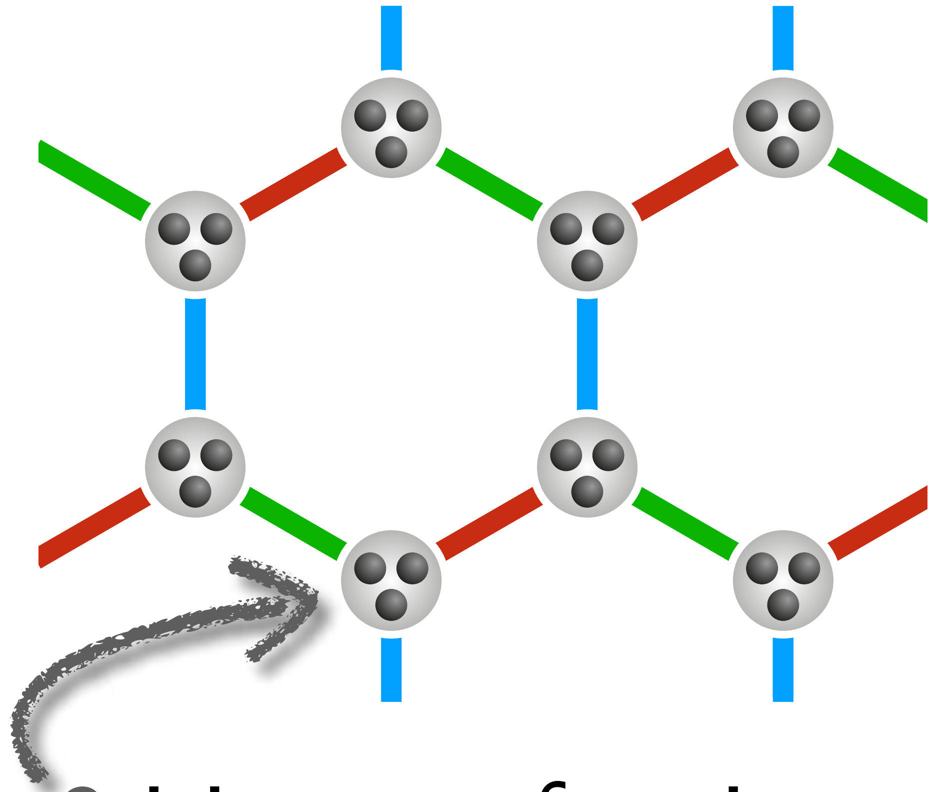
$$\mathcal{H} = K \sum_{\langle ij \rangle_\gamma} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma} + J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j$$

$$\mapsto \quad \hat{u}_{ij} \boldsymbol{c}_i^\top \boldsymbol{c}_j$$

Kitaev-Heisenberg spin-orbital model



3 itinerant fermions

Hamiltonian:

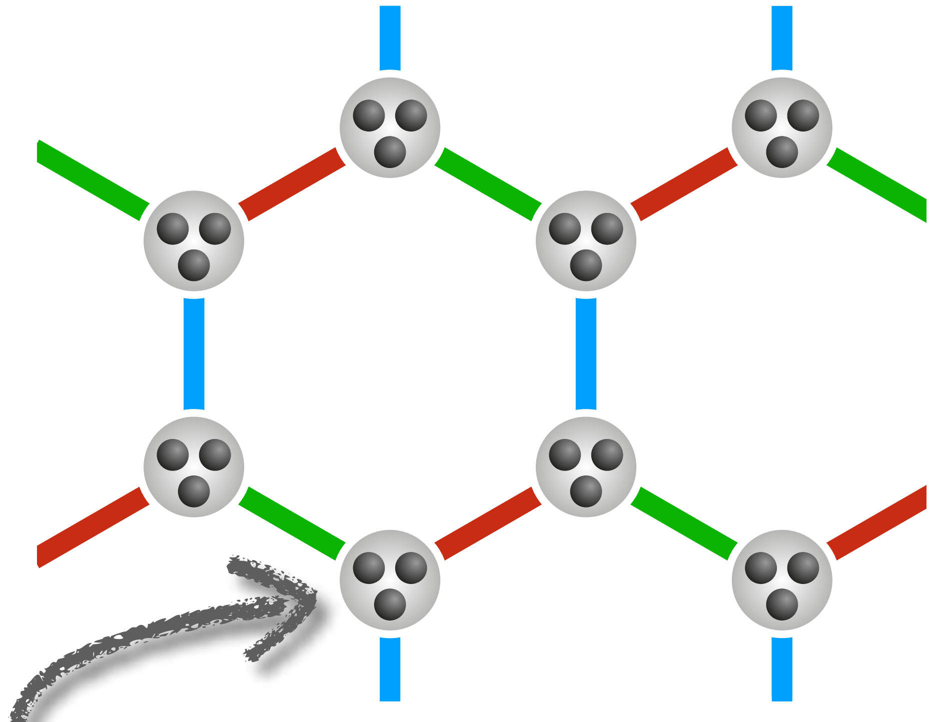
$$\mathcal{H} = K \sum_{\langle ij \rangle_\gamma} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma} + J \sum_{\langle ij \rangle} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j}$$

spin-1 matrices

$$\mapsto \quad \hat{u}_{ij} \boldsymbol{c}_i^\top \boldsymbol{c}_j \qquad\qquad \mapsto \quad \tfrac{1}{4}(\boldsymbol{c}_i^\top \vec{L} \boldsymbol{c}_i) \cdot (\boldsymbol{c}_j \vec{L} \boldsymbol{c}_j)$$

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

Kitaev-Heisenberg spin-orbital model



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spin-1 matrices

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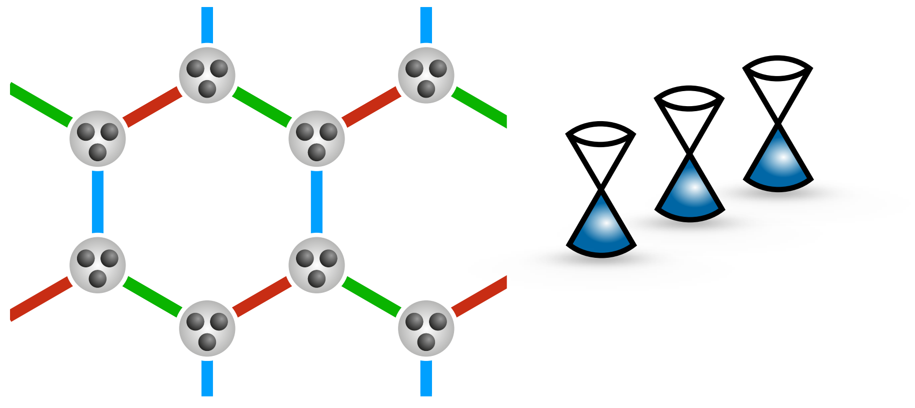
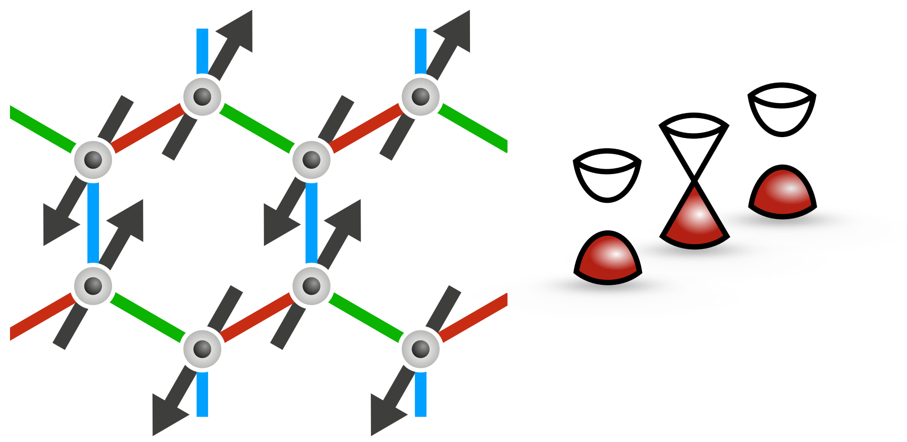
Phase diagram:



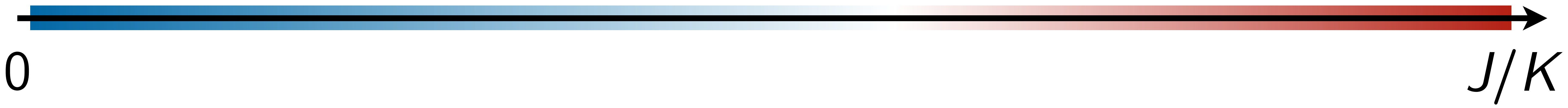
Kitaev spin-orbital liquid



SO(3) Kitaev liquid

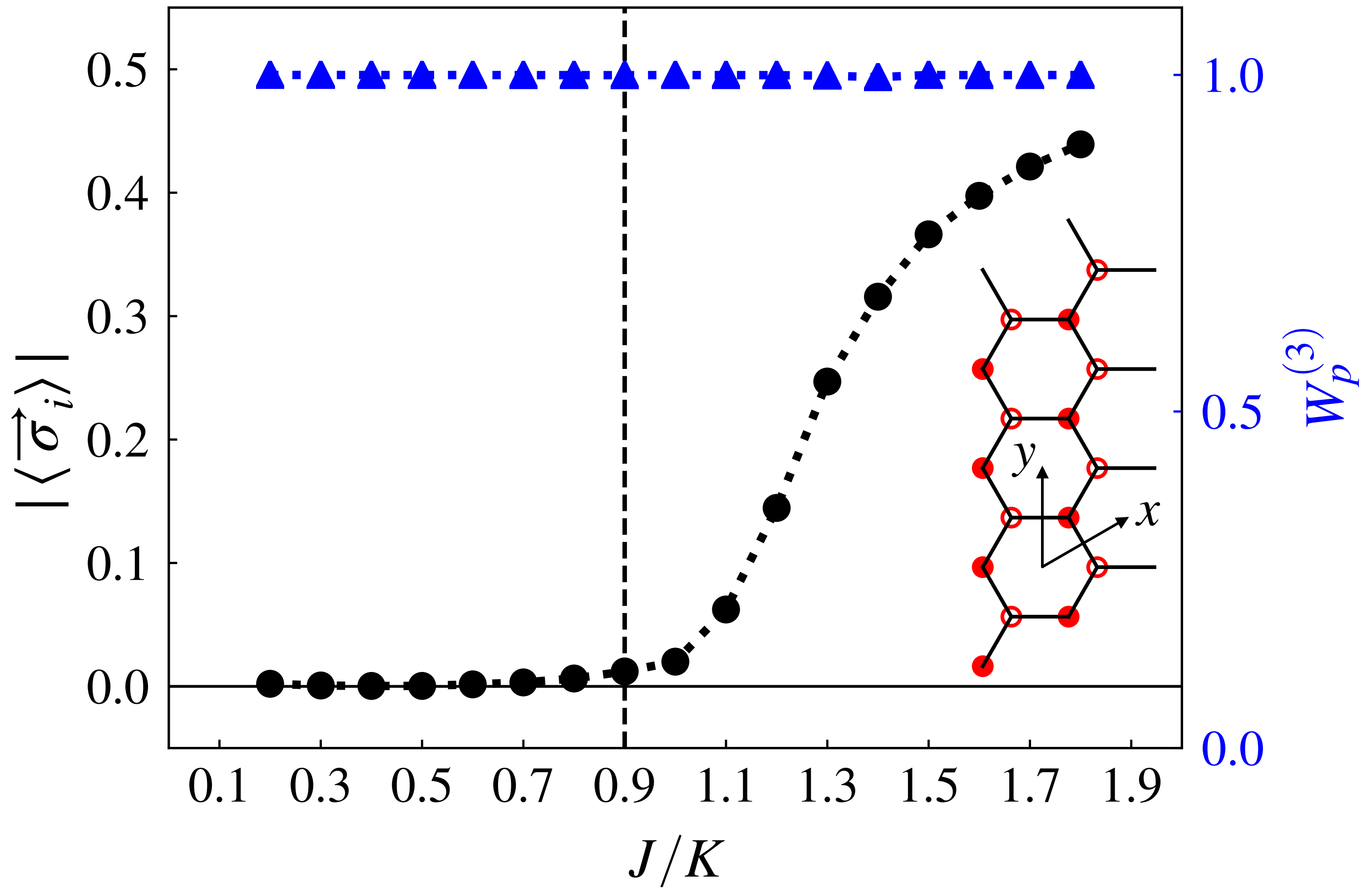
$\langle \boldsymbol{c}_{iA}^\top \vec{L} \boldsymbol{c}_{iA} \rangle \neq \langle \boldsymbol{c}_{jB}^\top \vec{L} \boldsymbol{c}_{jB} \rangle$

"spin density wave"



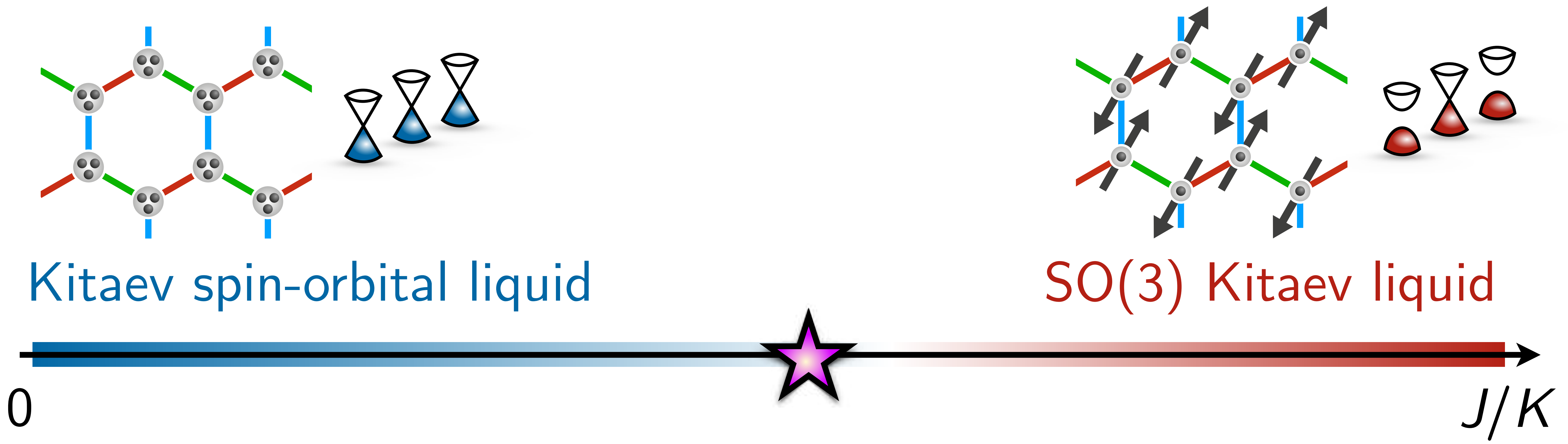
Fractionalized fermionic quantum criticality

iDMRG:



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

Phase diagram:



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

"Fractionalized fermionic quantum critical point"

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

Effective field theory

Gradient expansion:

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

"Gross-Neveu-SO(3)"

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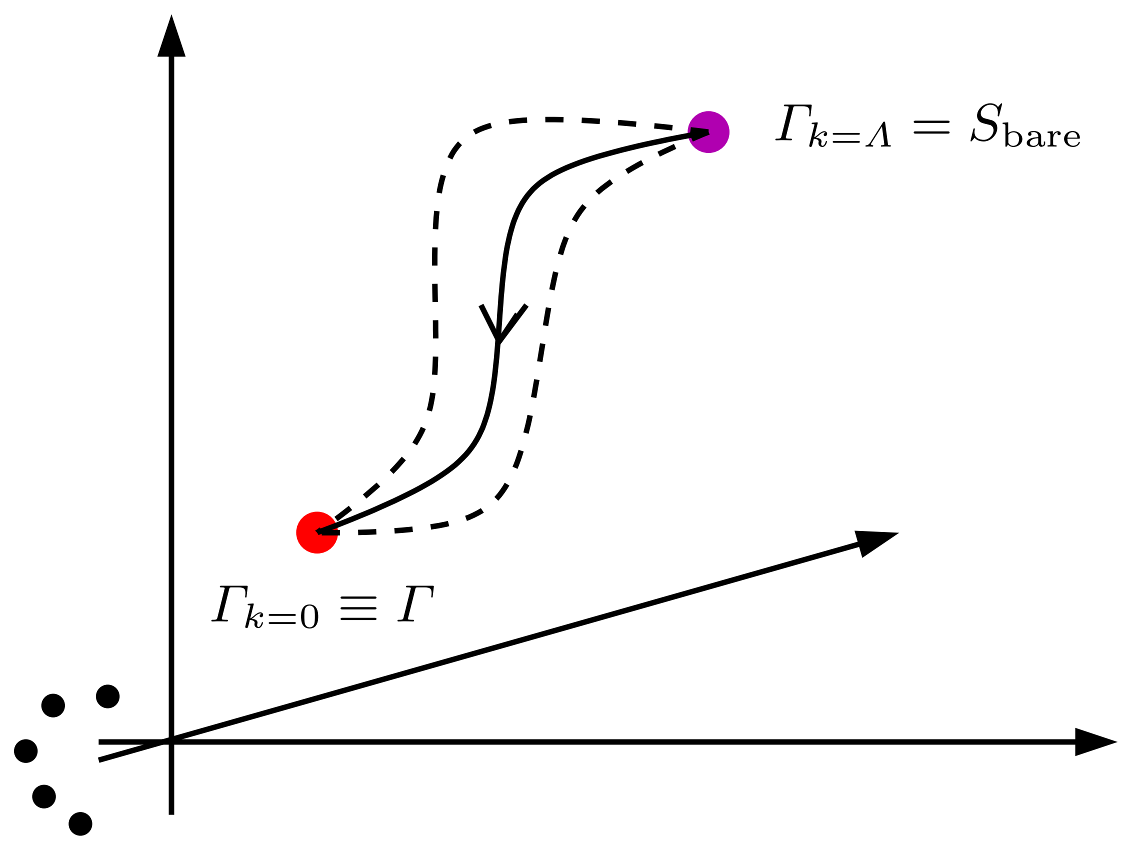
Wetterich equation:

$$\partial_k\Gamma_k = \frac{1}{2}\,\mathrm{STr}\,\frac{\partial_k R_k}{\Gamma_k^{(2)} + R_k}$$



[Gies, Lect. Notes Phys. '12]

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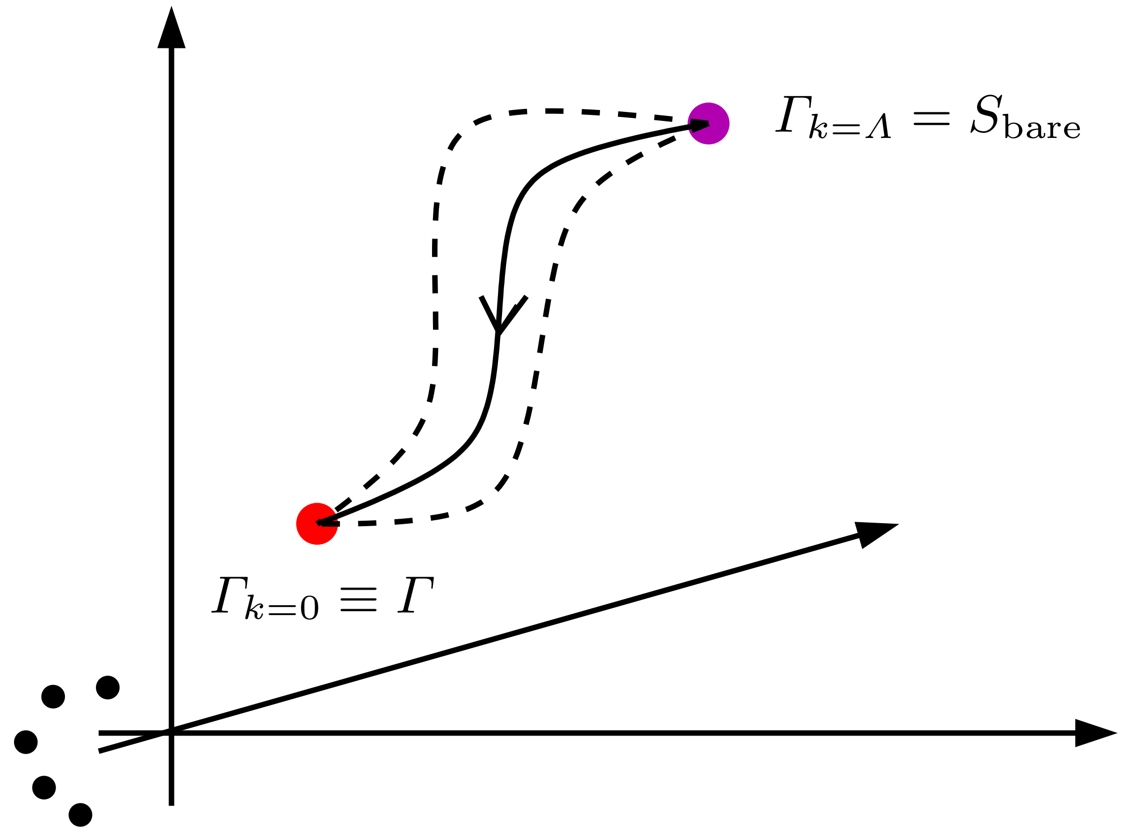


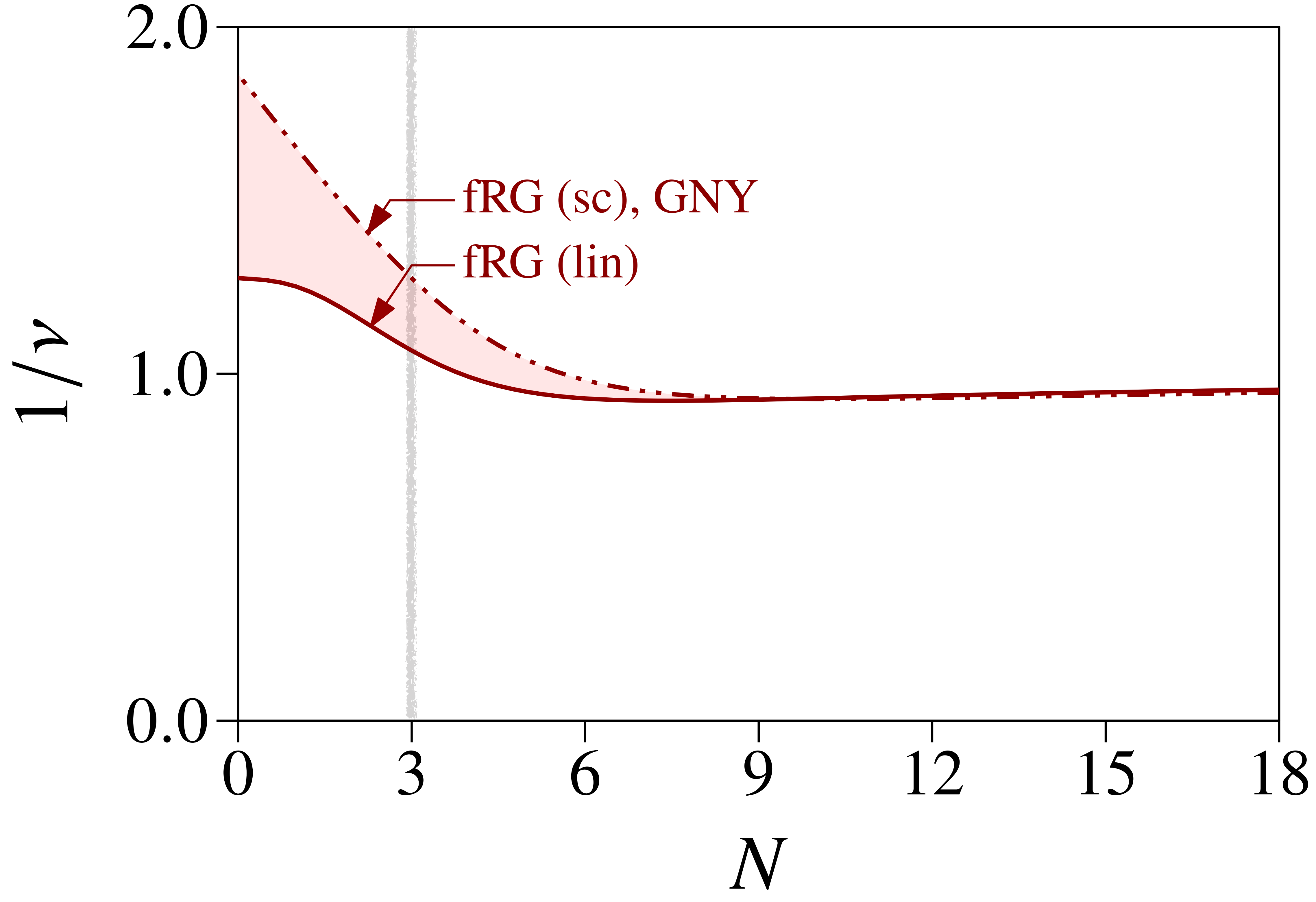
[Gies, Lect. Notes Phys. '12]

Effective action (LPA'):

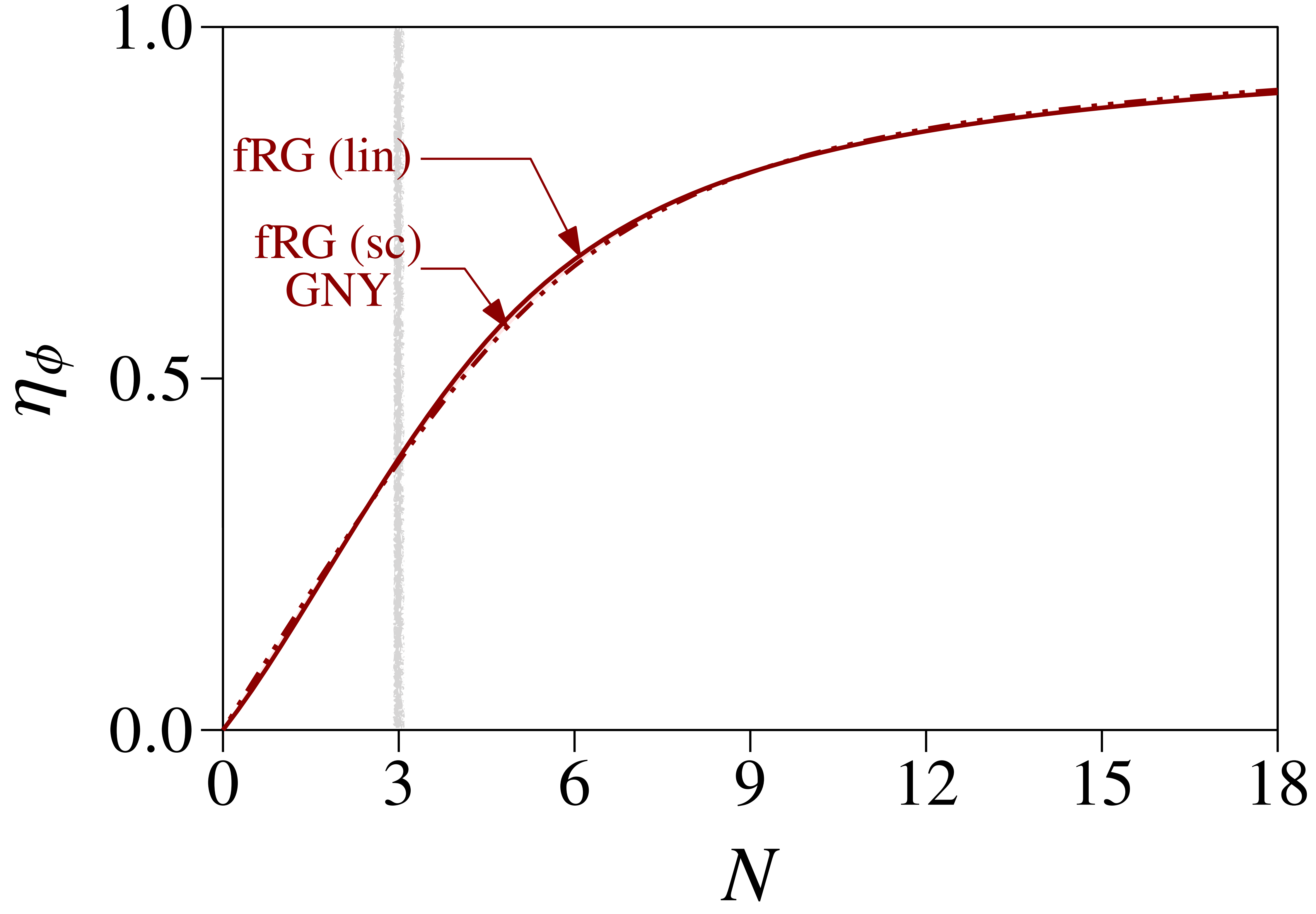
$$\Gamma_k = \int d^{2+1}x \left[Z_{\psi,k}\bar{\psi}\gamma^\mu\partial_\mu\psi + \frac{1}{2}Z_{\varphi,k}(\partial_\mu\vec{\varphi})^2 - g_k\vec{\varphi}\cdot\bar{\psi}\vec{L}\psi + U_k(\varrho)\right]$$

Fractionalized Gross-Neveu-SO(3) criticality

Correlation length exponent:



Anomalous dimension:



Levels of approximation:

- Functional RG @ LPA'

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

Fractionalized Gross-Neveu-SO(3) criticality

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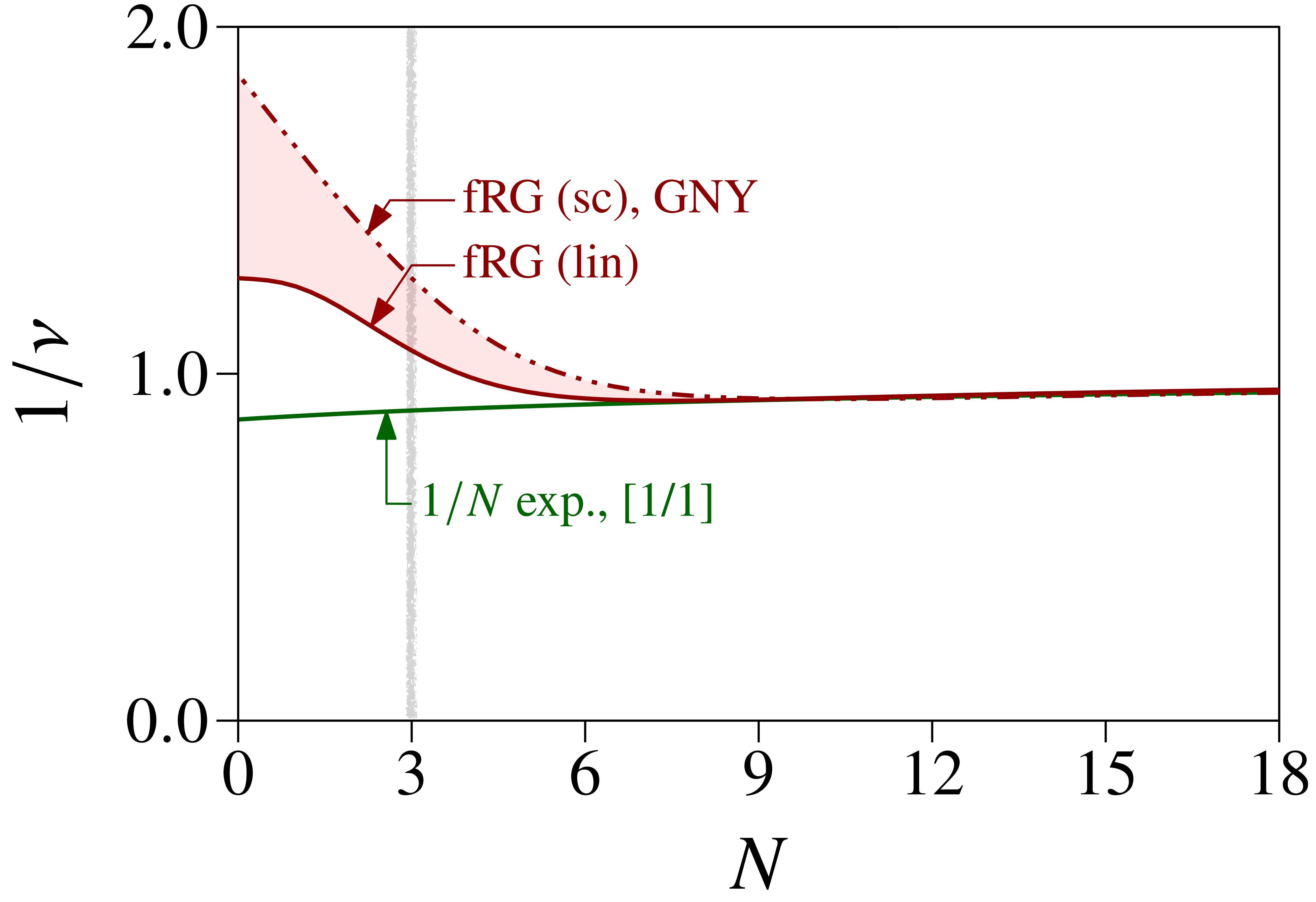

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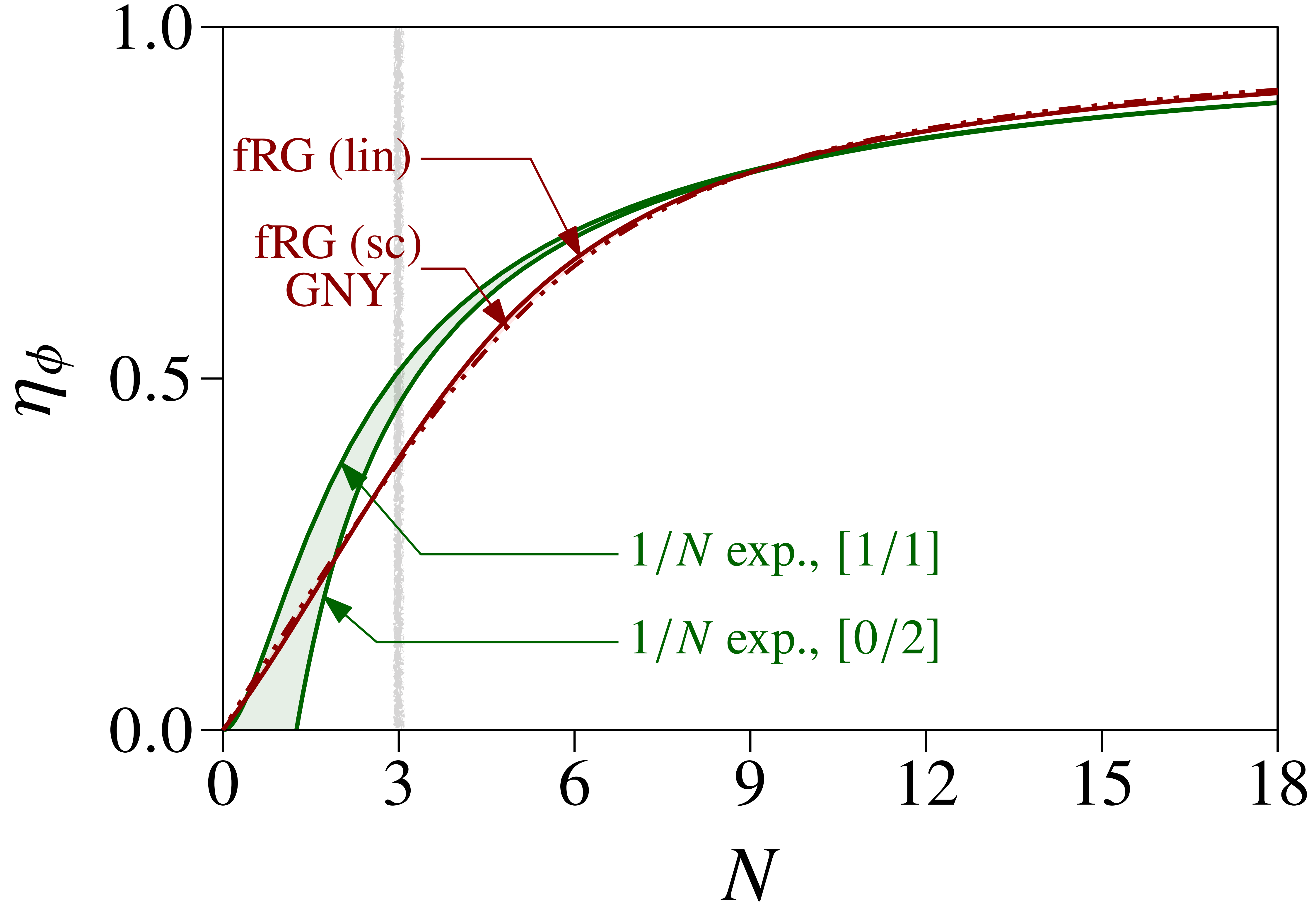

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[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

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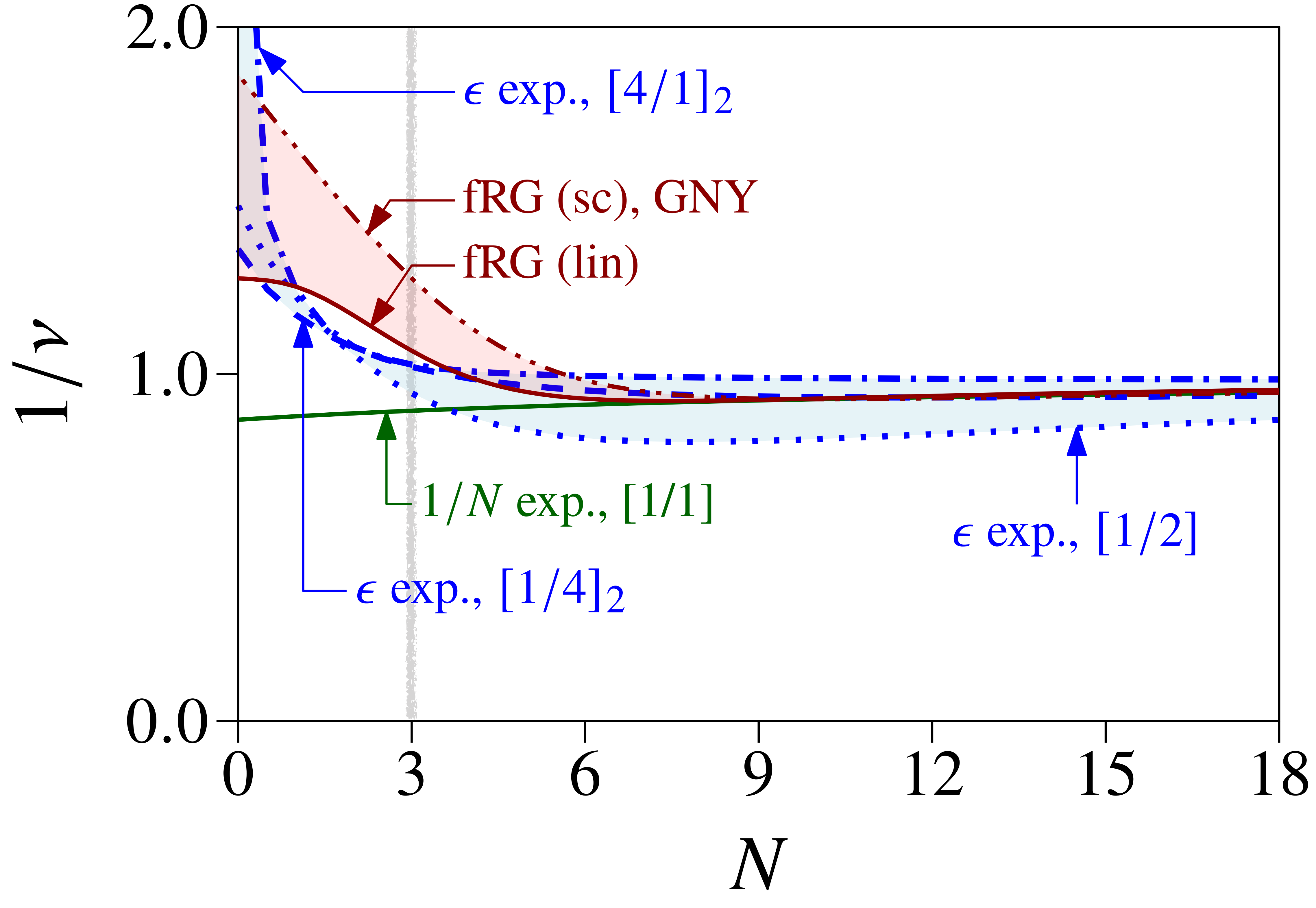

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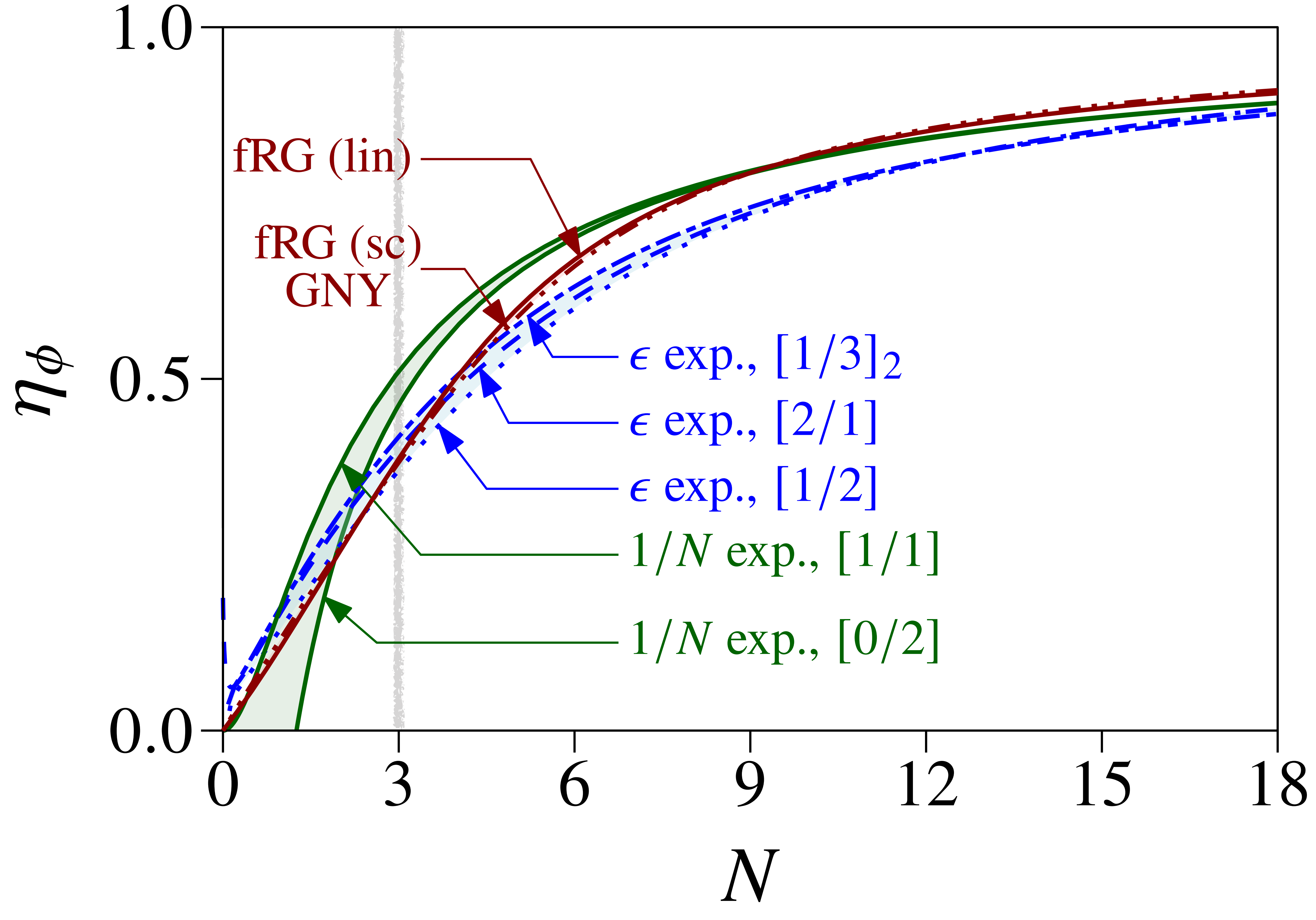

Levels of approximation:

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

Fractionalized Gross-Neveu-SO(3) criticality

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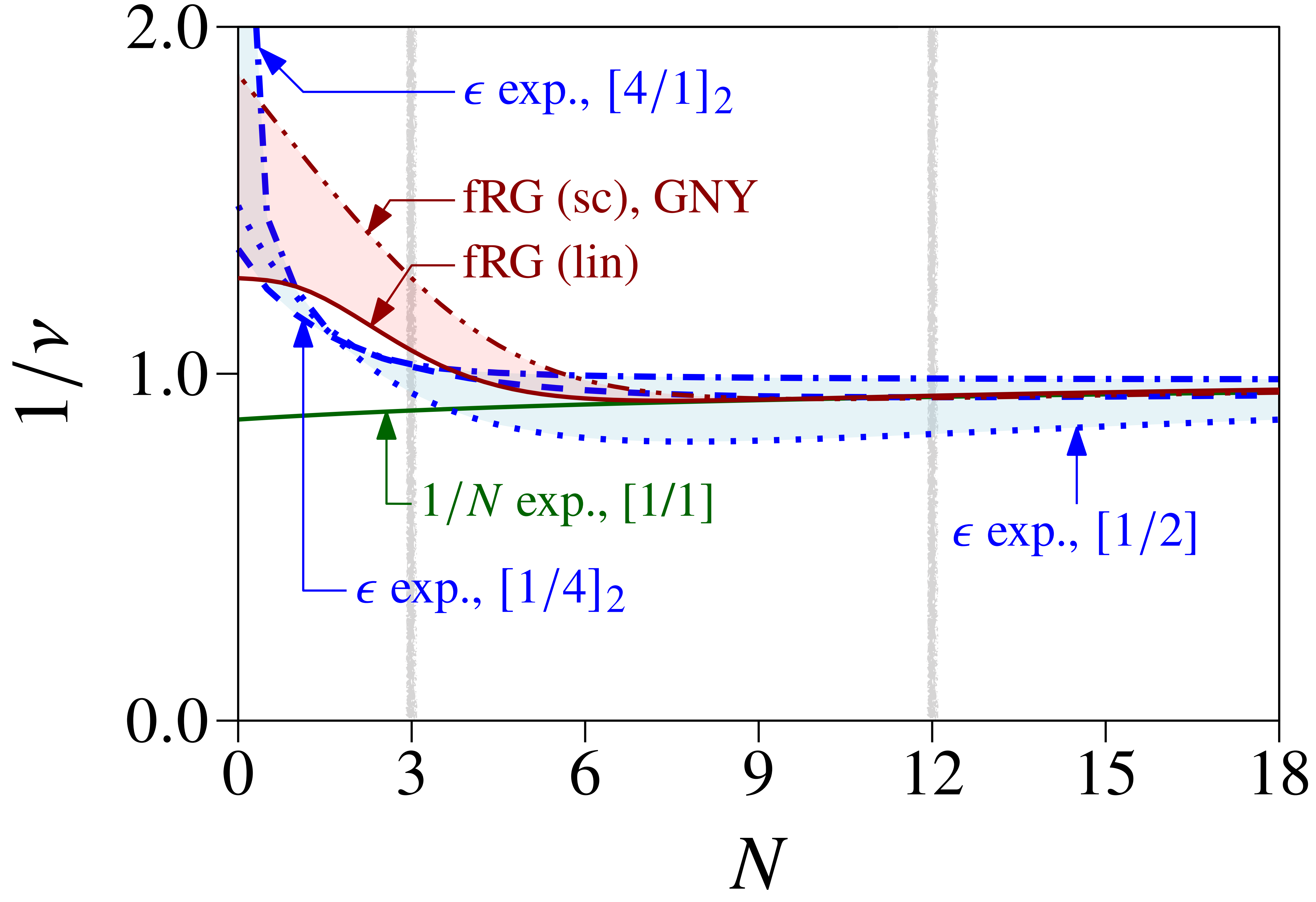

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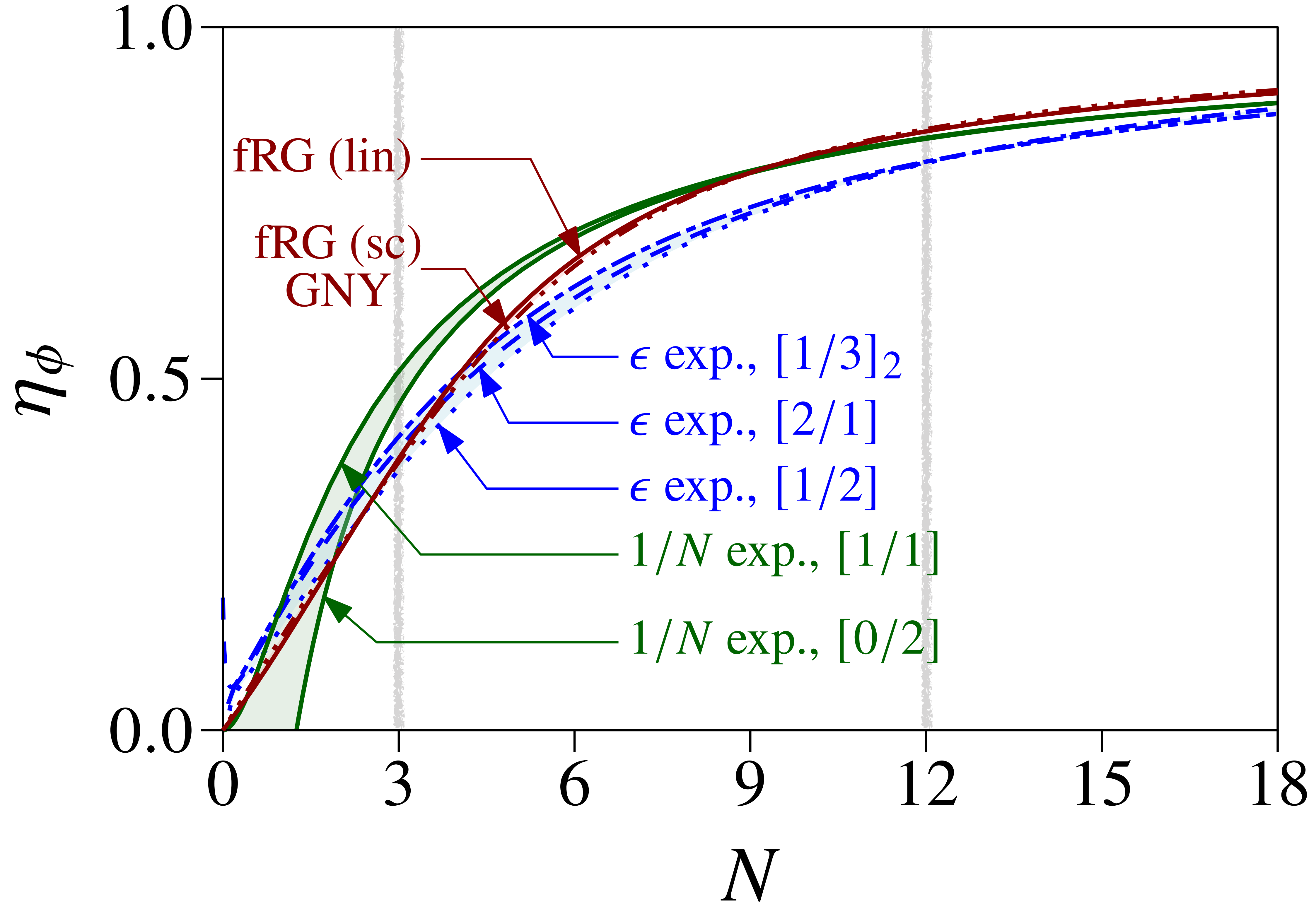

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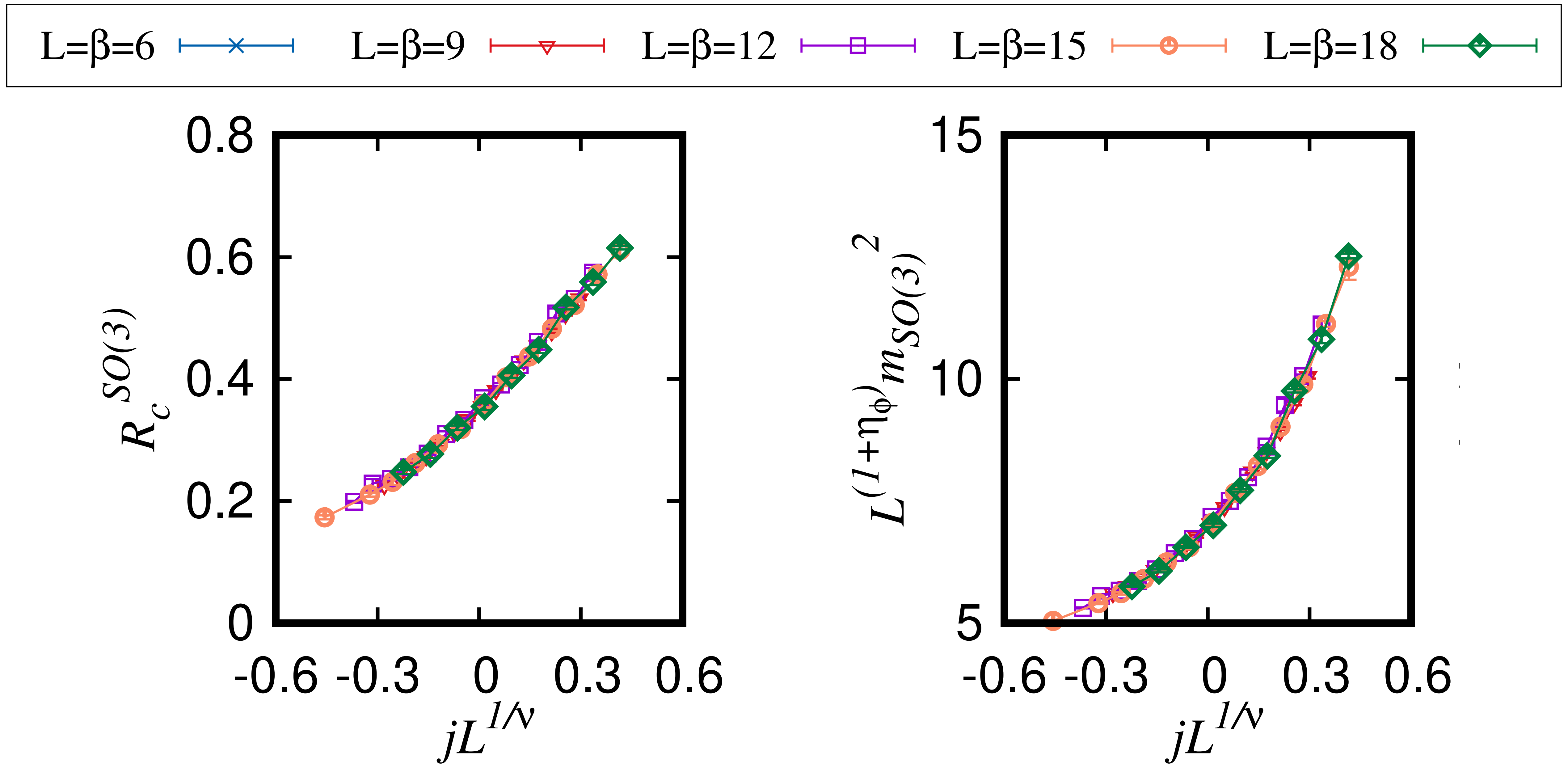
[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

QMC simulations ($N = 12$)

Scaling collapse:



Zihong Liu

[Liu, Vojta, Assaad, LJ, PRL '22]
[Liu, Vojta, Assaad, LJ, *in preparation*]

QMC simulations (*N* = 12)

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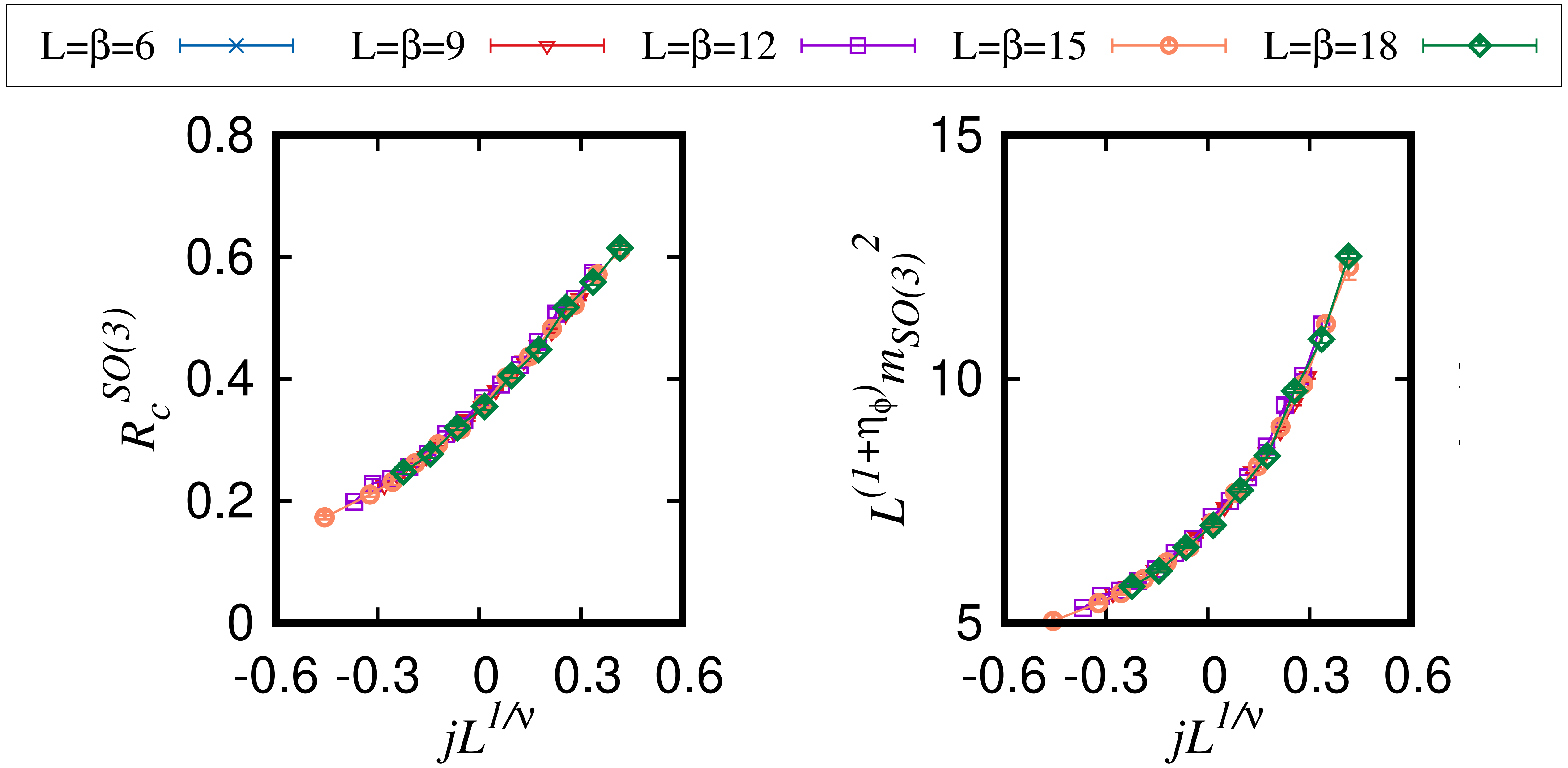
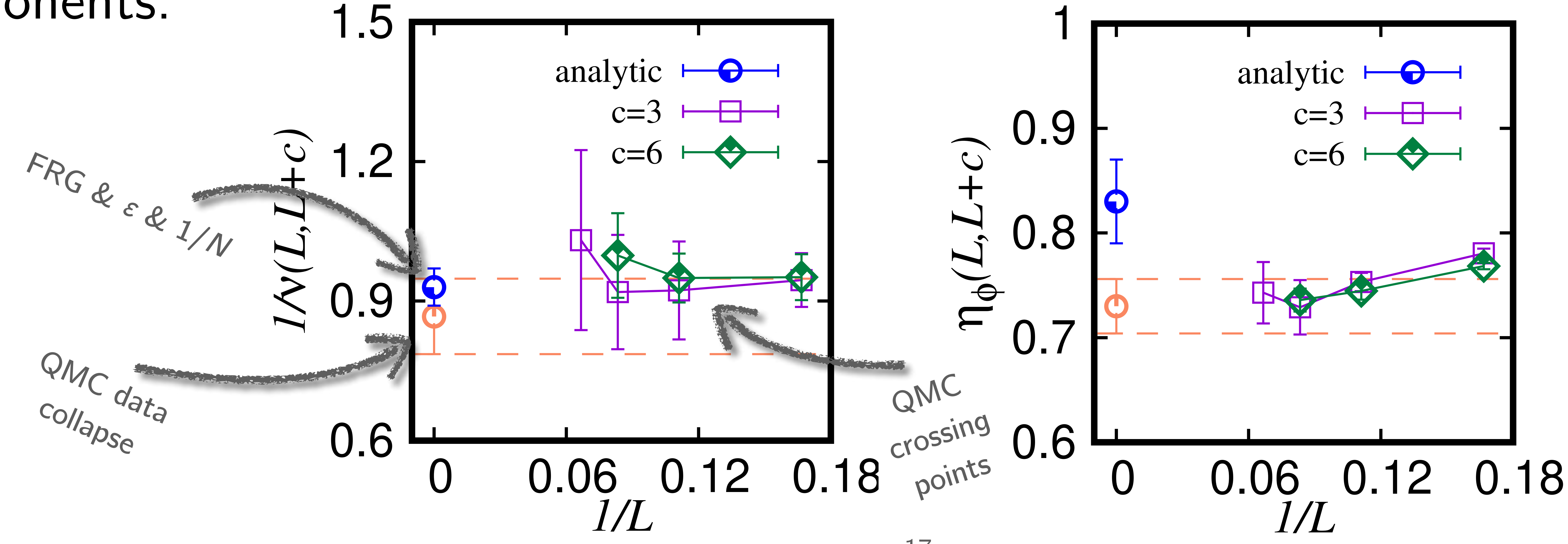
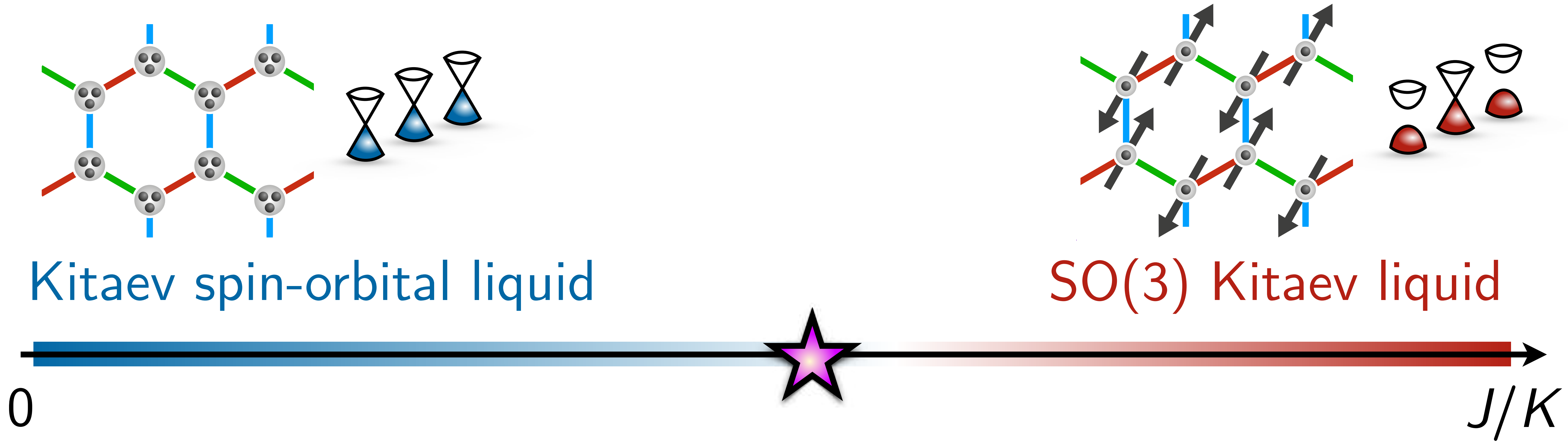


Critical exponents:



[Liu, Vojta, Assaad, LJ, PRL '22]
[Liu, Vojta, Assaad, LJ, *in preparation*]

Conclusions



"Fractionalized fermionic quantum critical point"

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