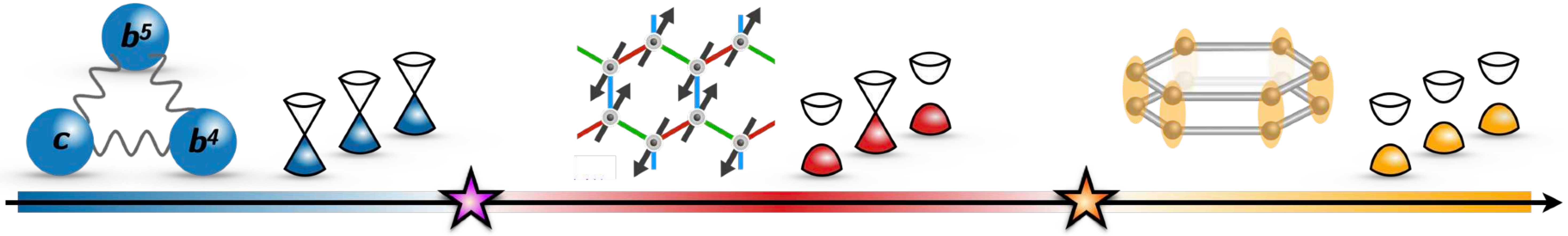
TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Gross-Neveu criticality in quantum magnets

Lukas Janssen



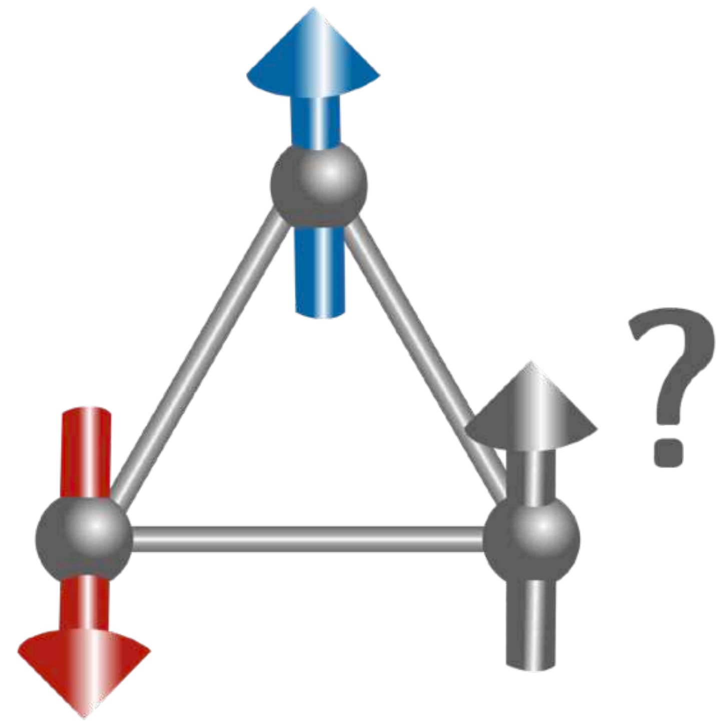
Emmy Noether-Programm
DFG Deutsche Forschungsgemeinschaft
JA 2306/4-1

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

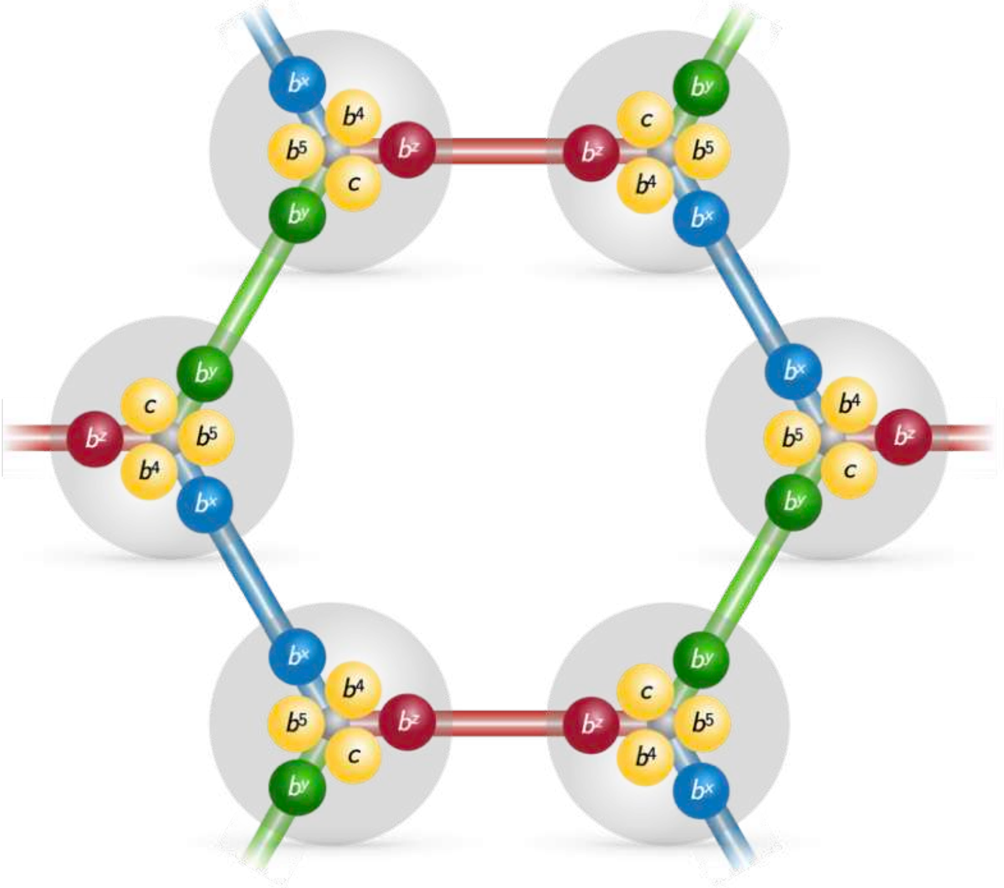
SFB 1143

Outline

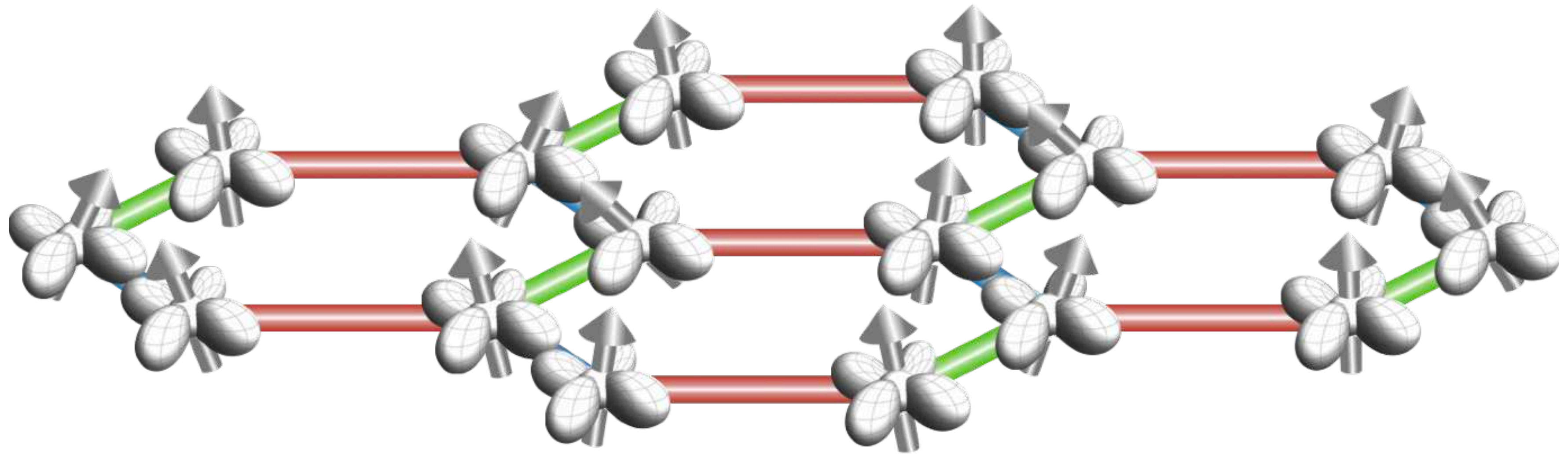
(1) Introduction



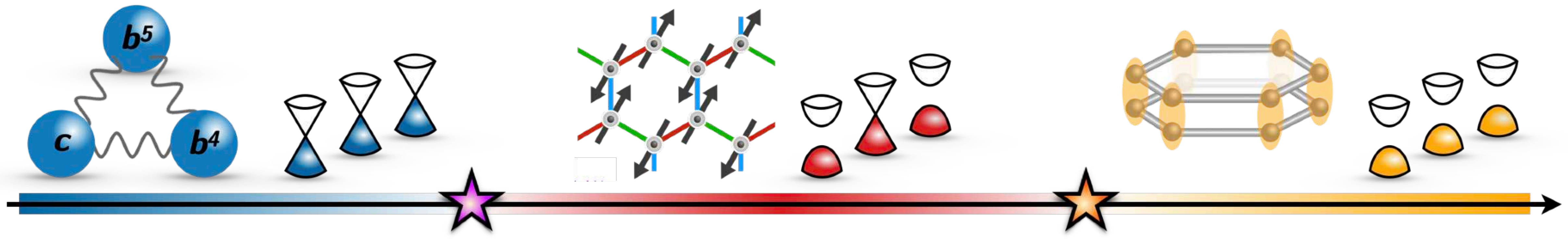
(2) Kitaev honeycomb model



(3) Kitaev-Heisenberg spin-orbital model



(4) Conclusions



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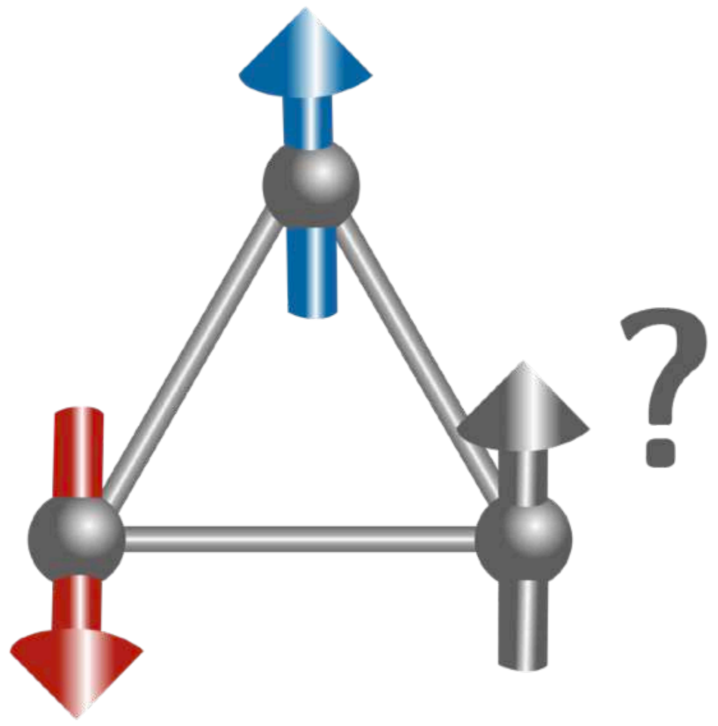

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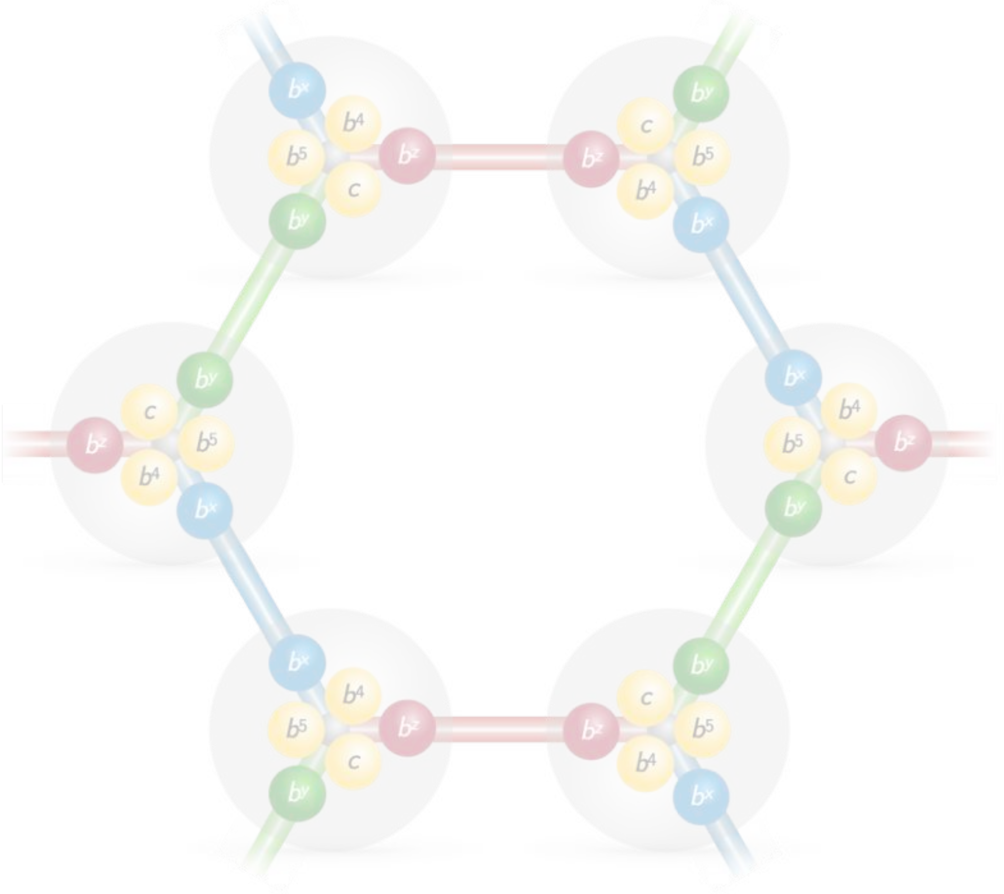
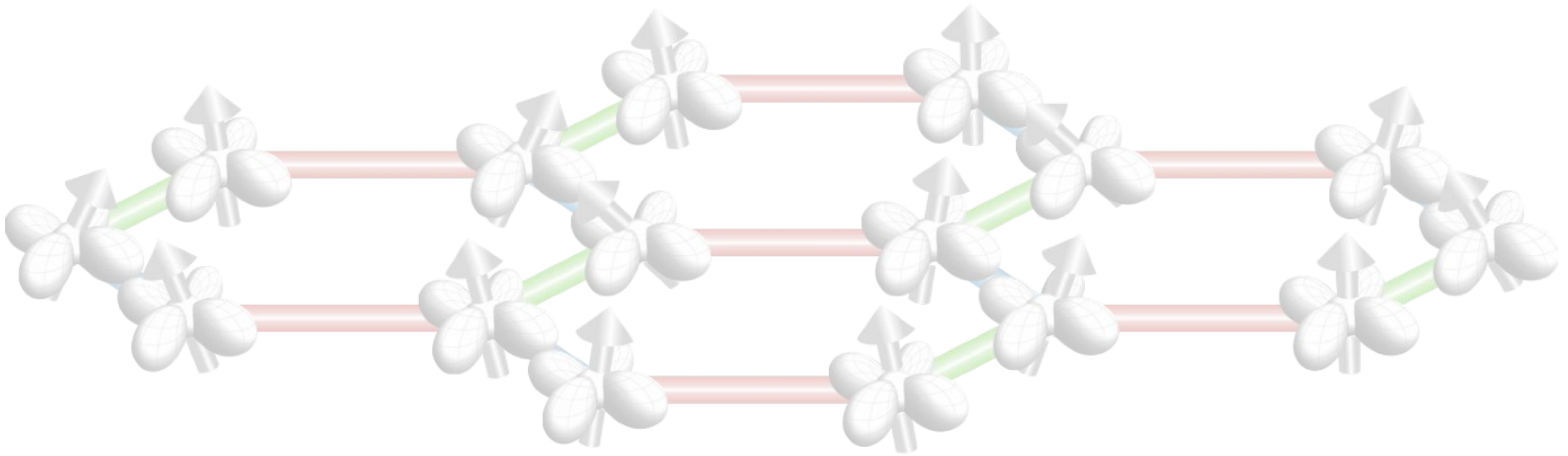


(2) Kitaev spin-1/2 model



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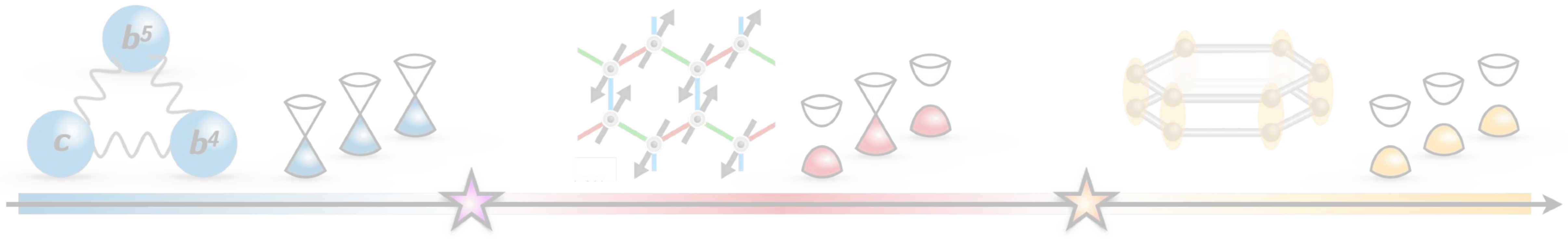
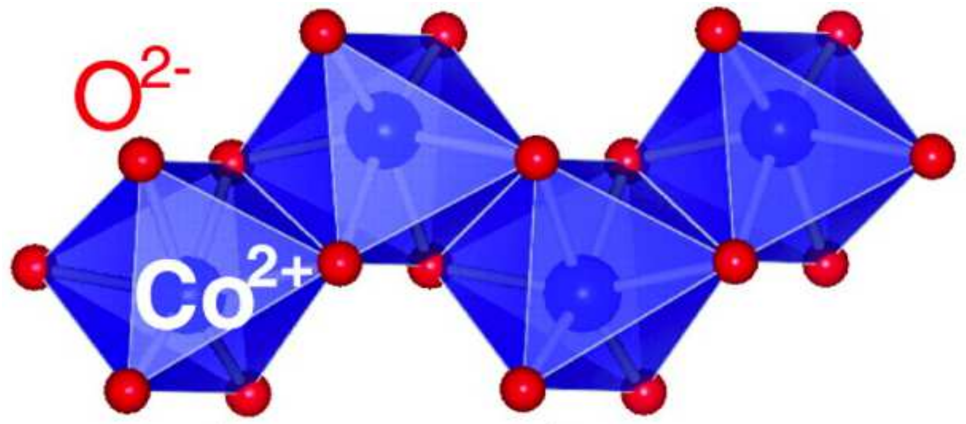
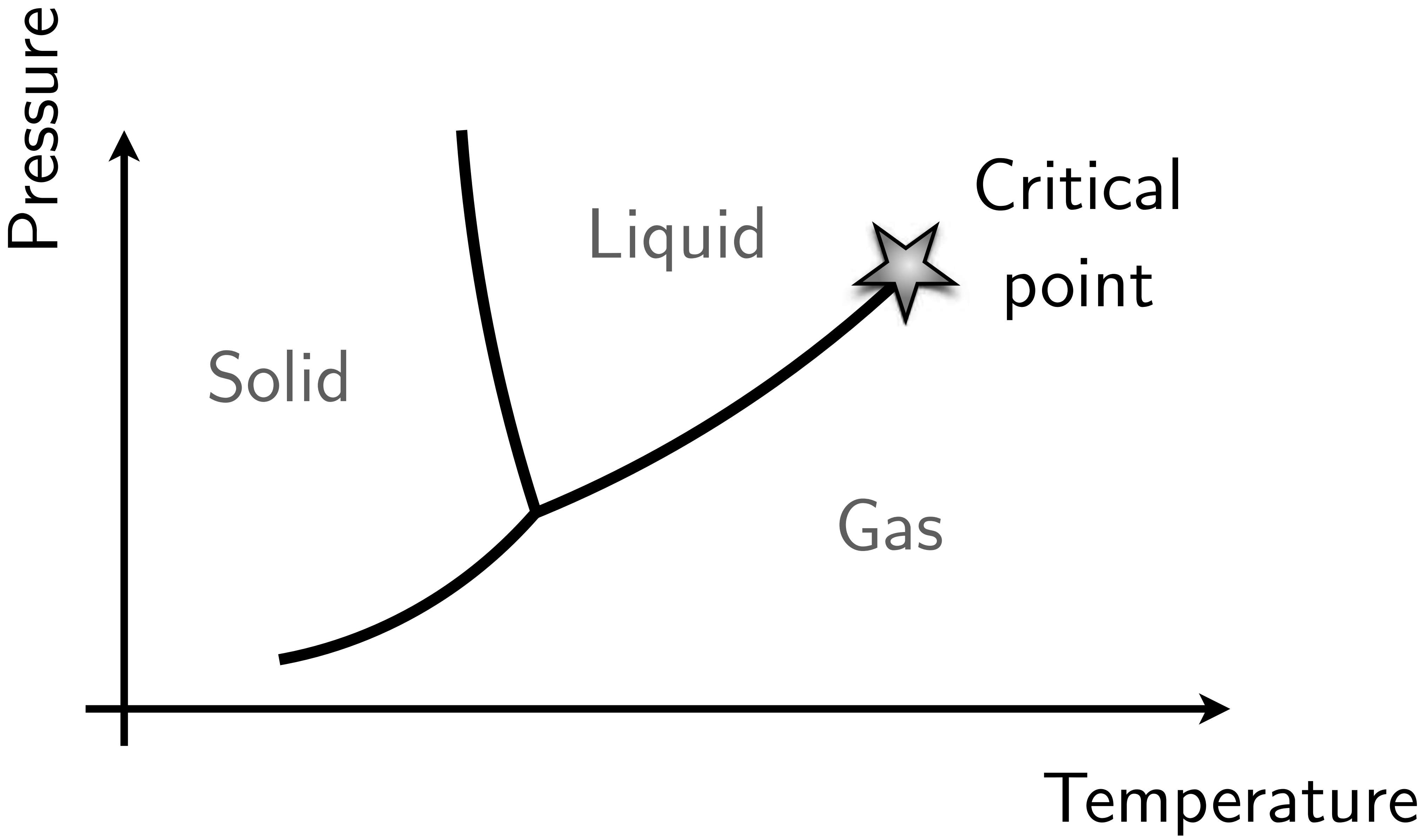


(4) Conclusions

Classical vs quantum criticality



H_2O $\quad$ $T > 0$



Pressure

Liquid

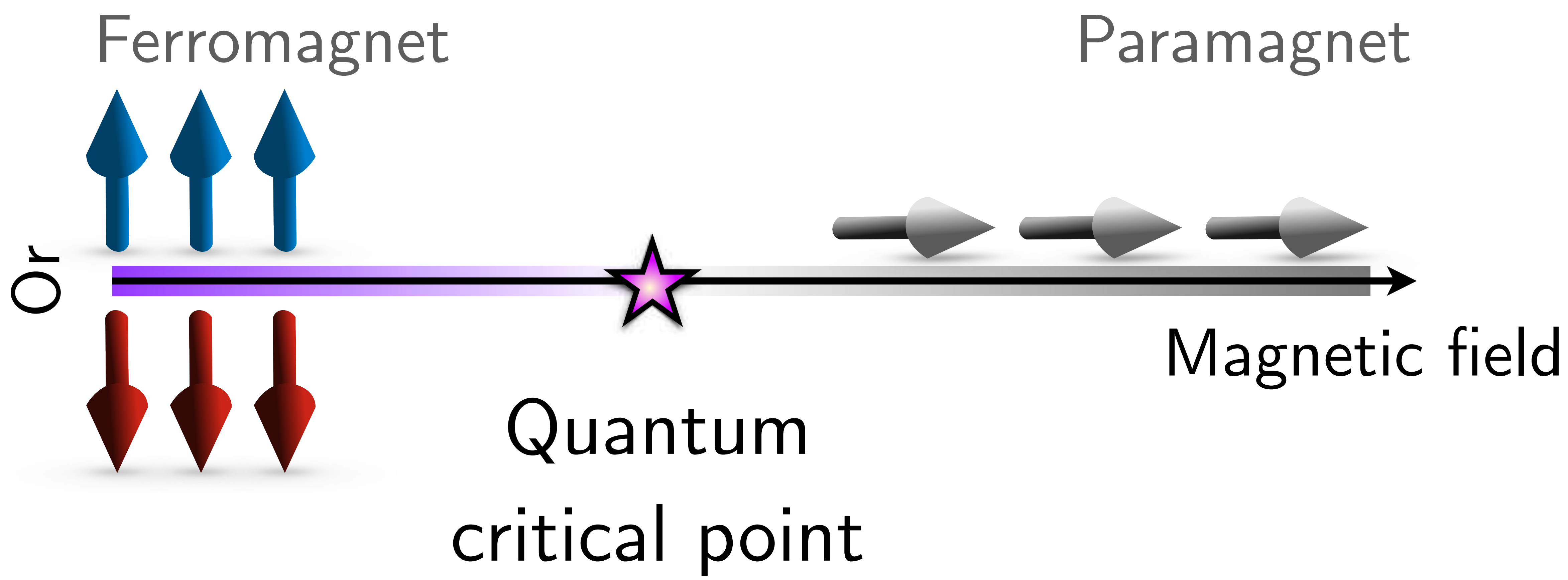
Critical point

Solid

Gas

Temperature

$CoNb_2O_6$ $\quad$ $T \to 0$



Ferromagnet

Paramagnet

Or

Magnetic field

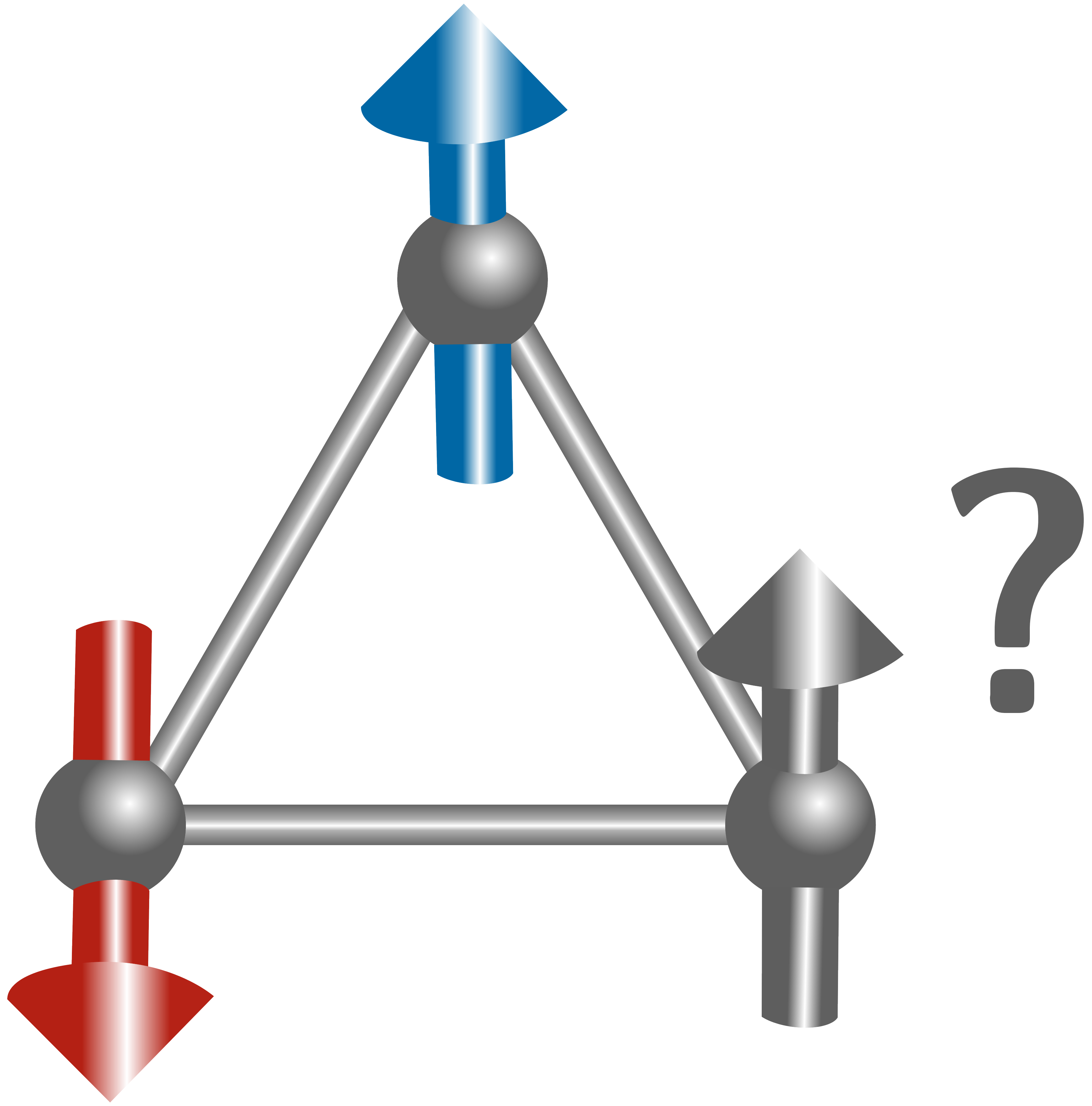
Quantum critical point

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

Magnetic frustration

Antiferromagnetic interaction:

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



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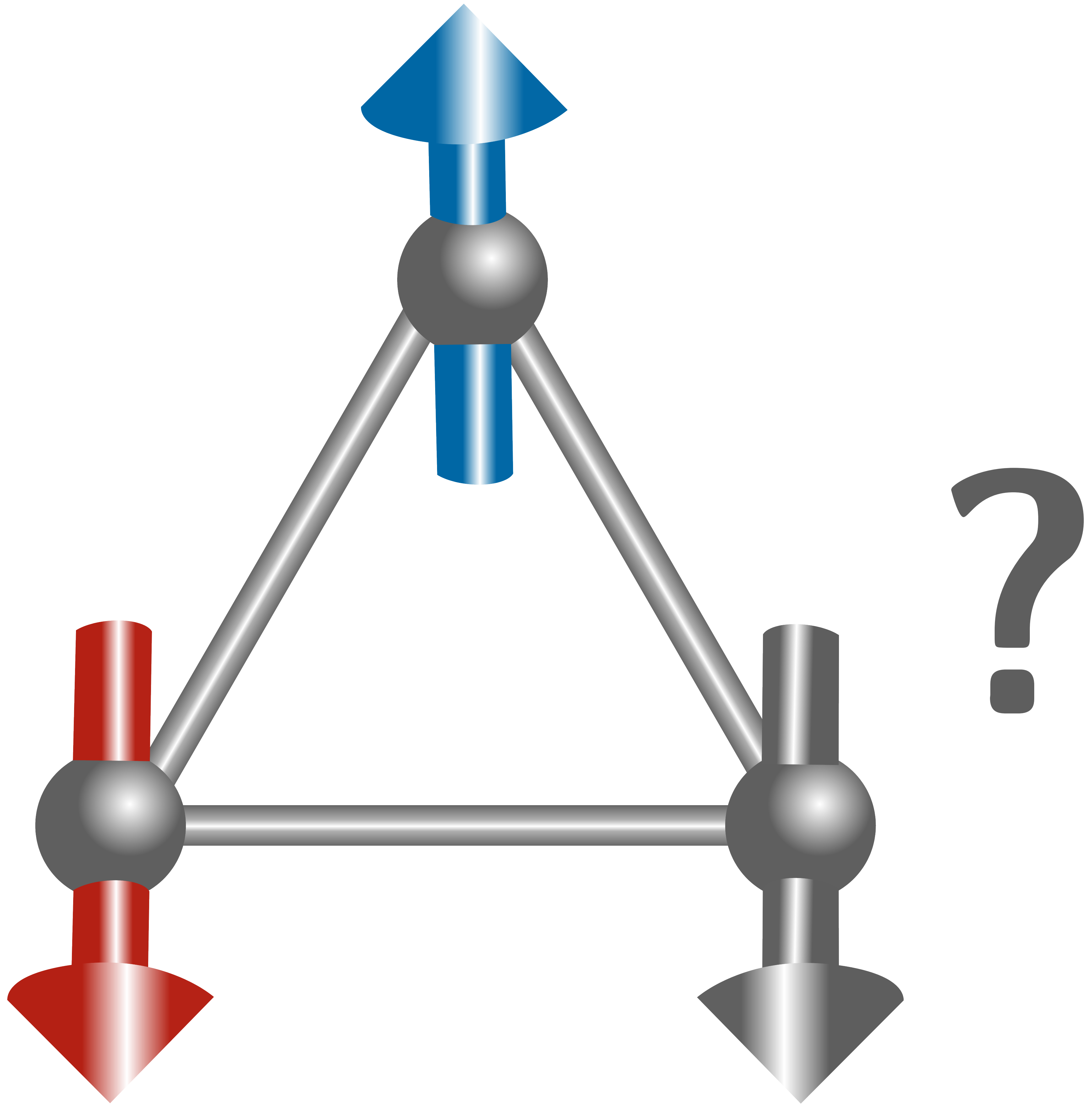

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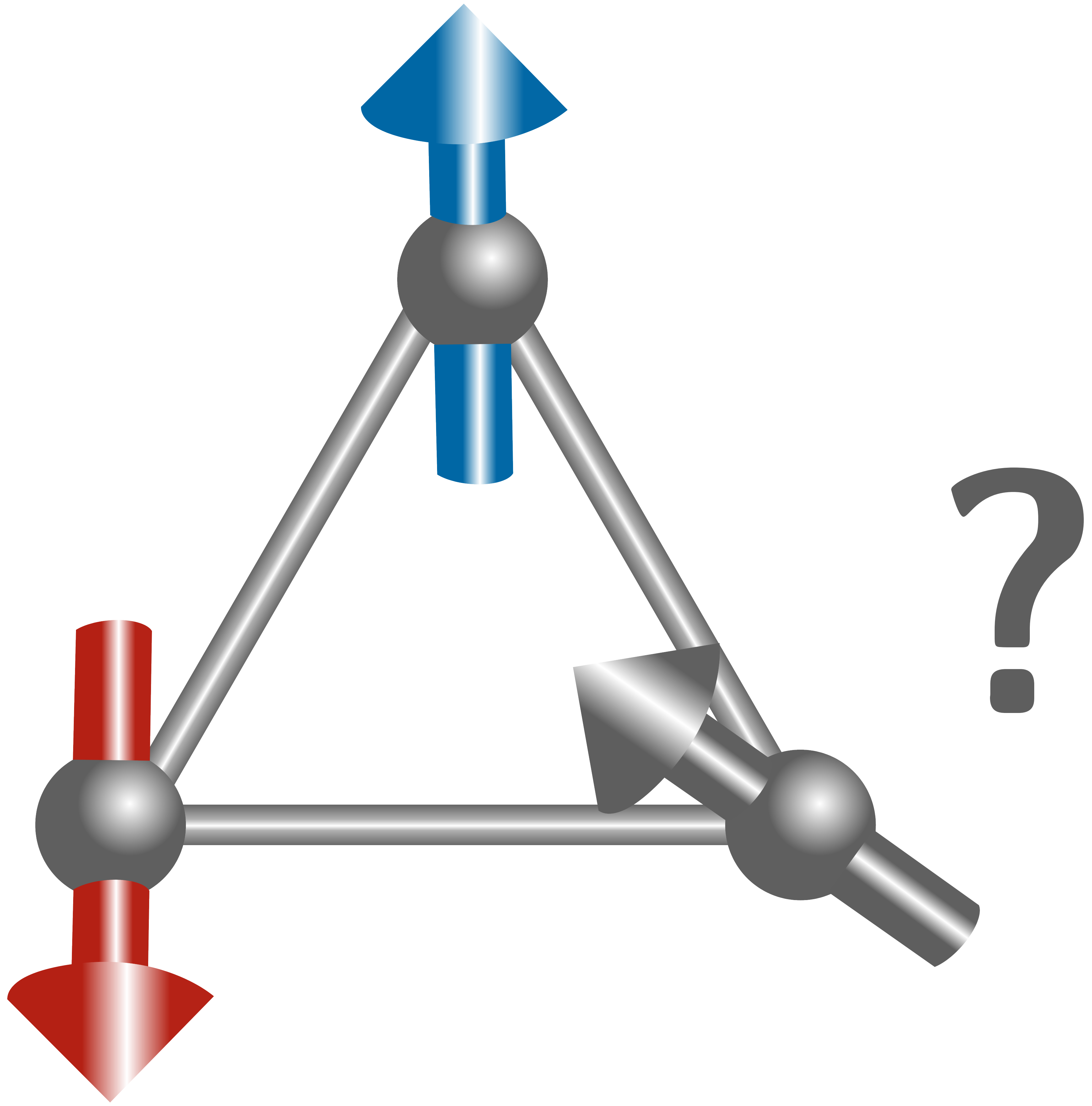

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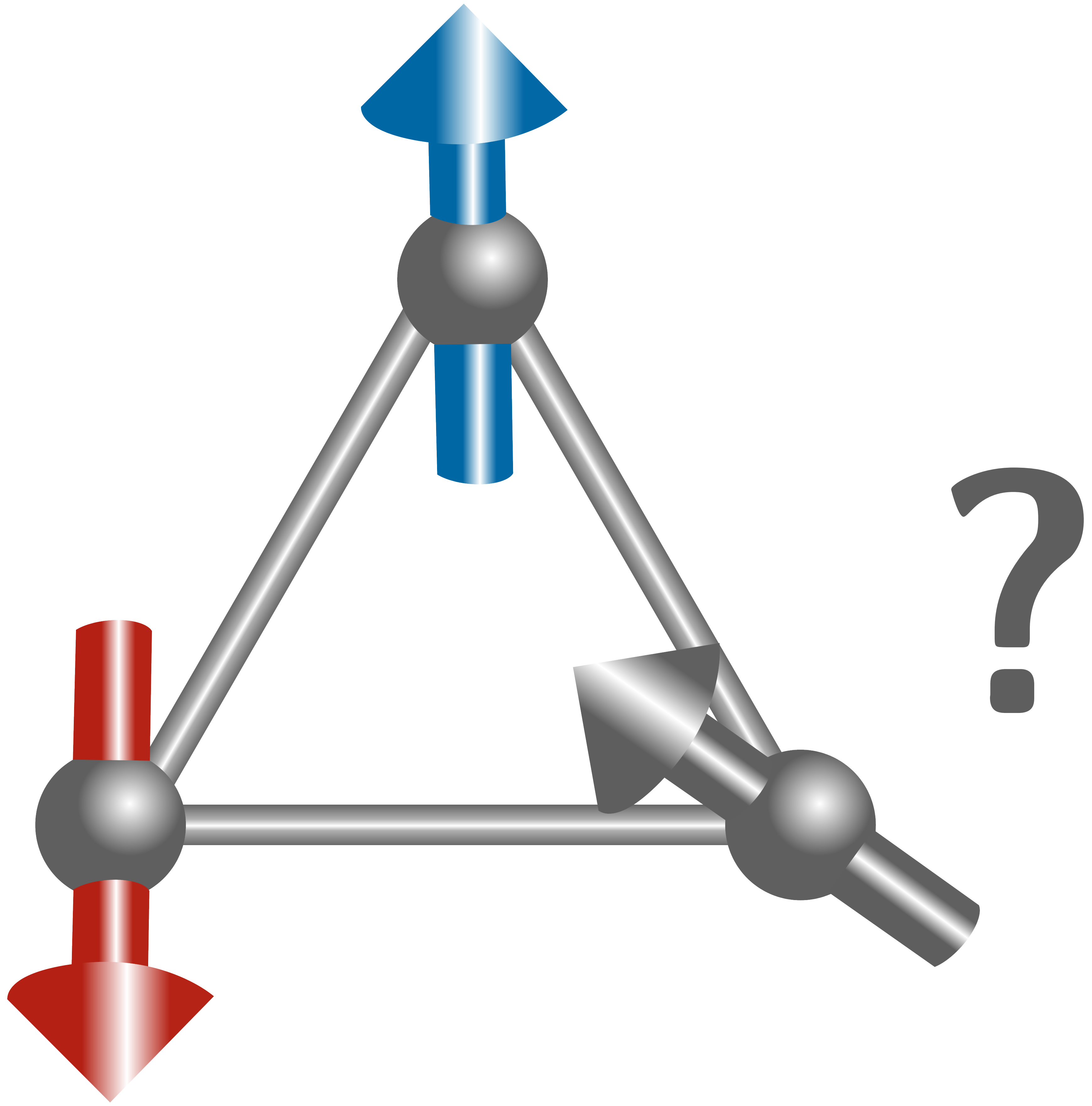
Frustration:

Incompatible interactions



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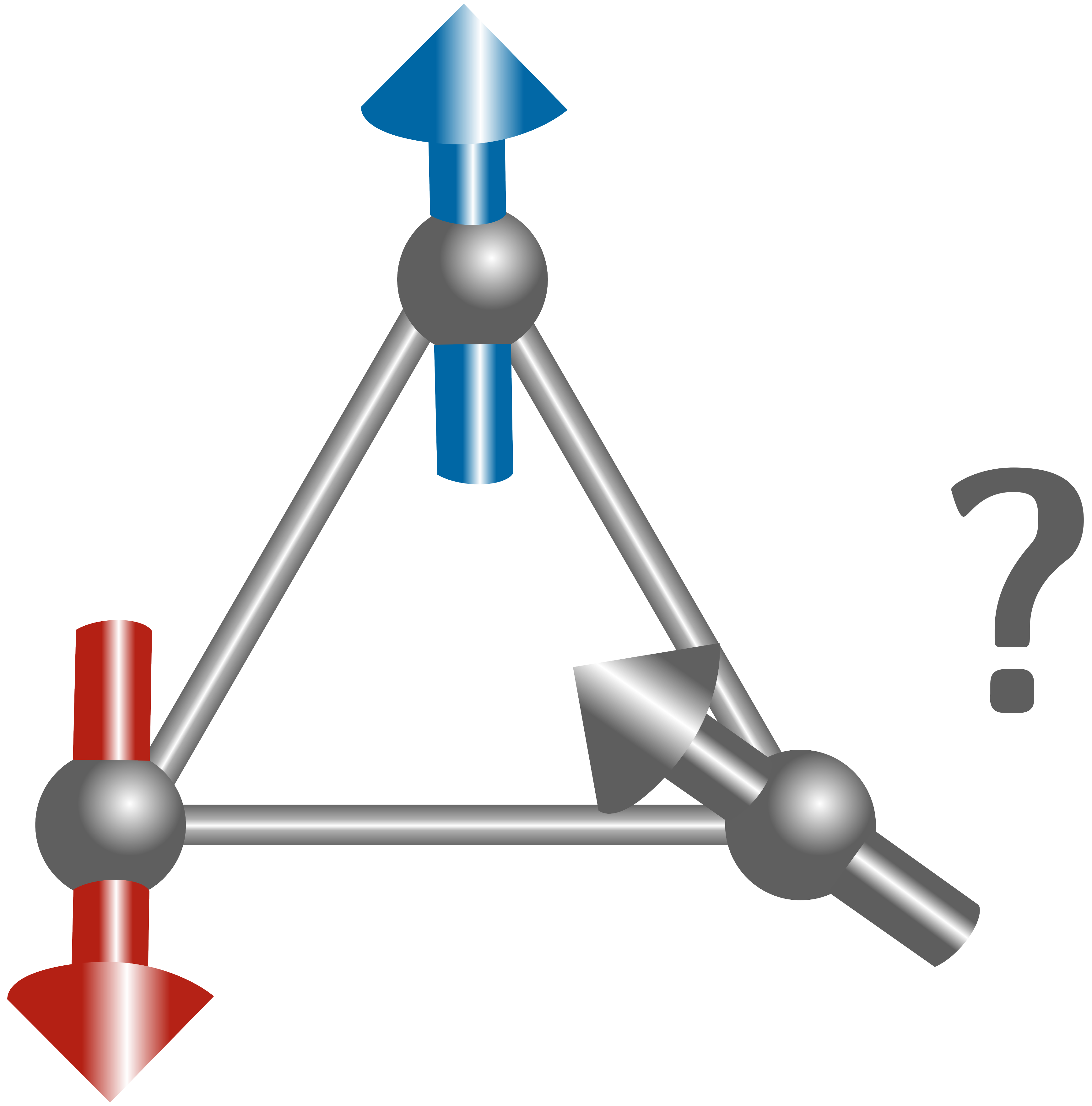
⇓

New states of matter
with exotic excitations?

illustrationsource.com



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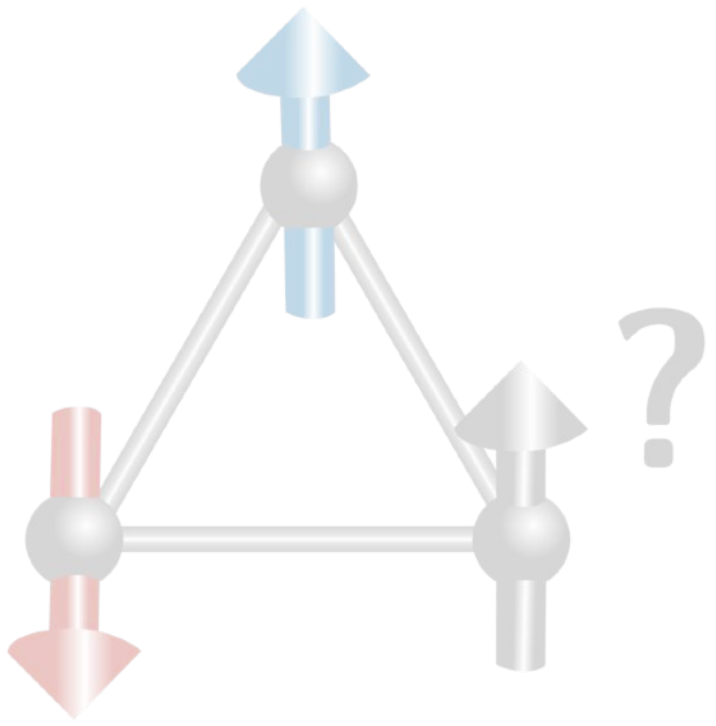

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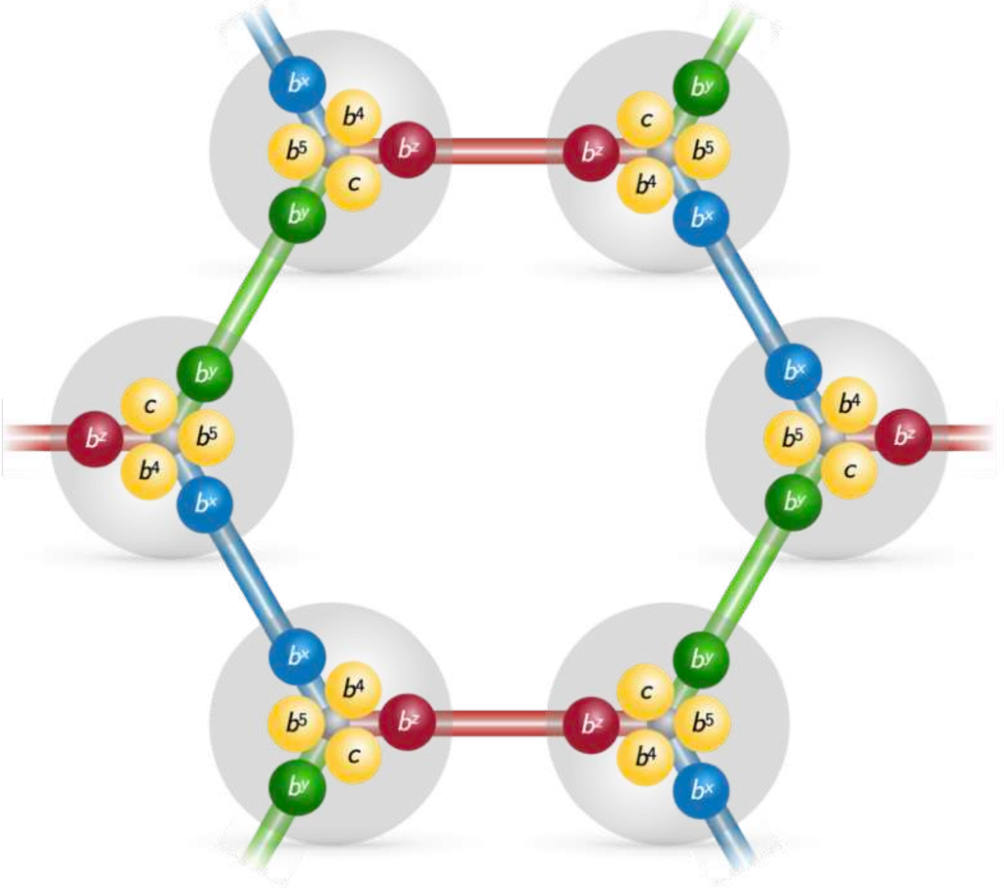

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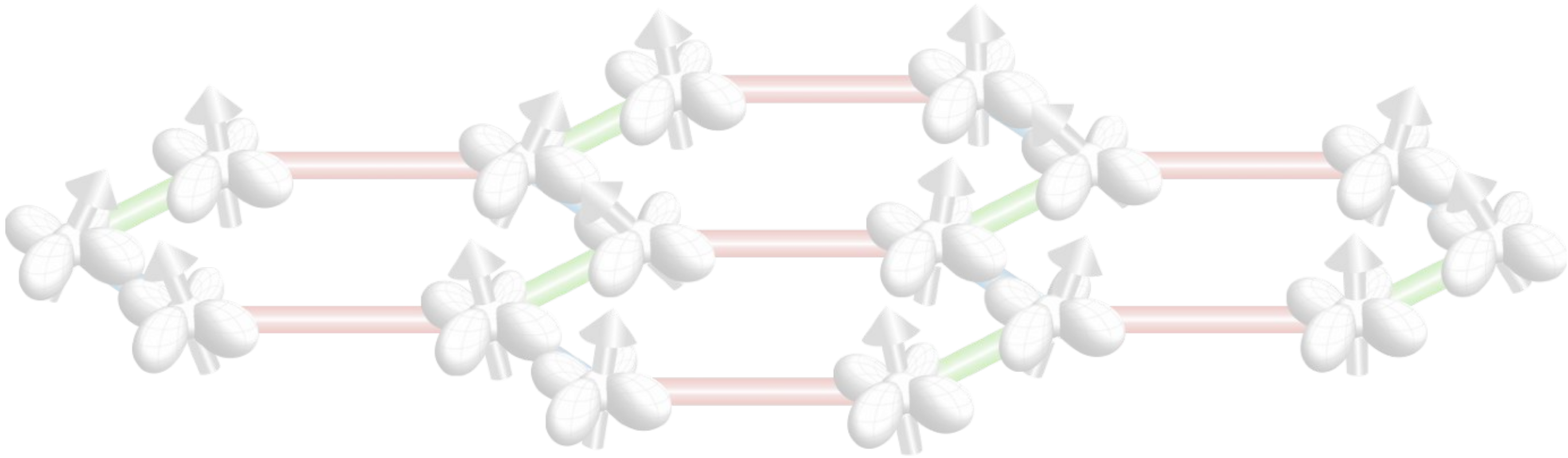

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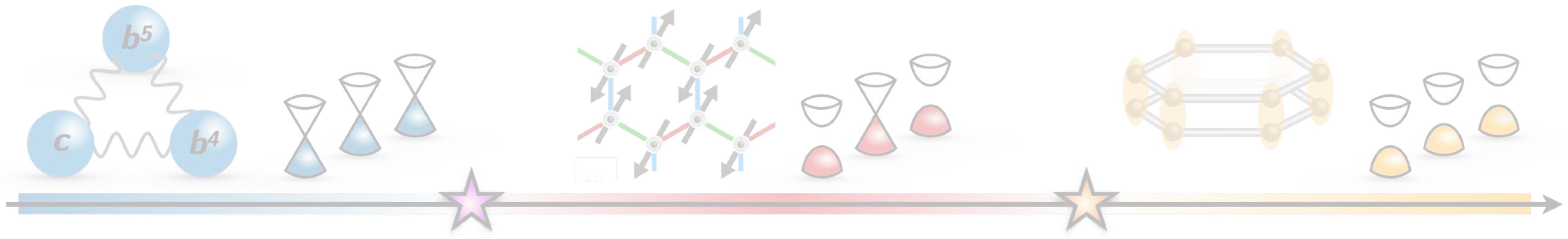

(4) Conclusions

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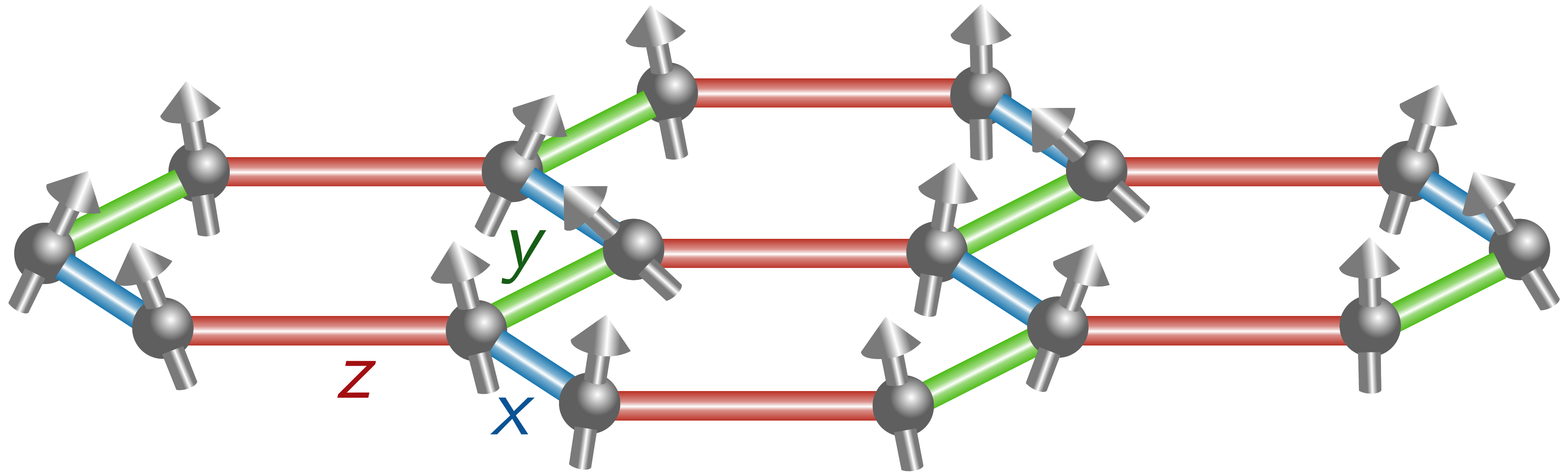

[Kitaev, Ann. Phys. '06]

... can arise in material with strong spin-orbit coupling

Hamiltonian:

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

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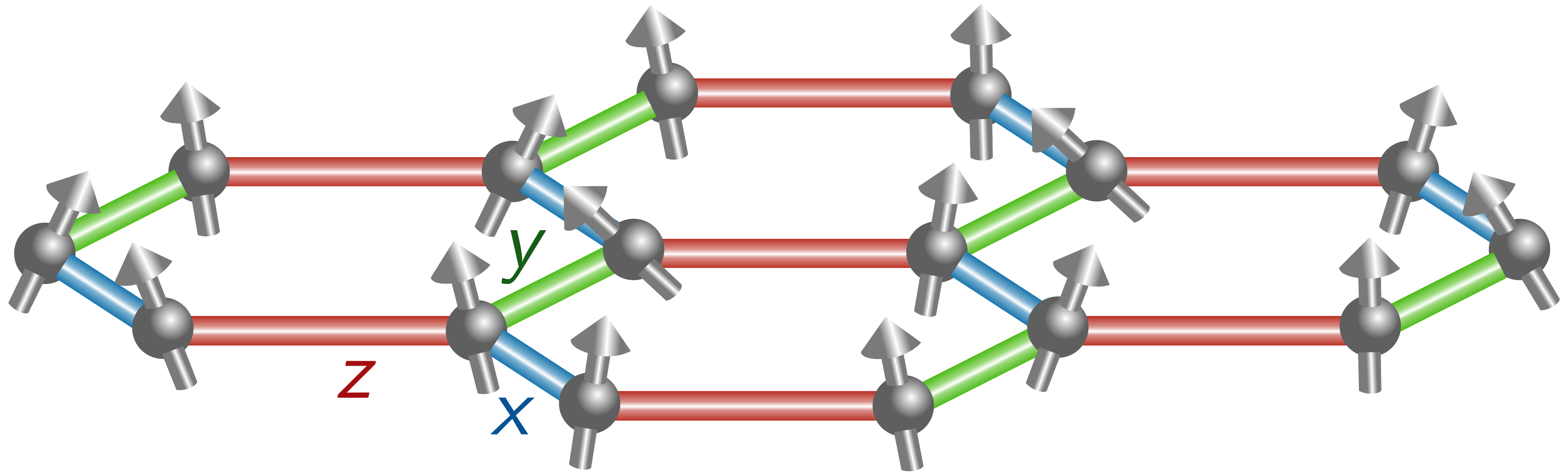

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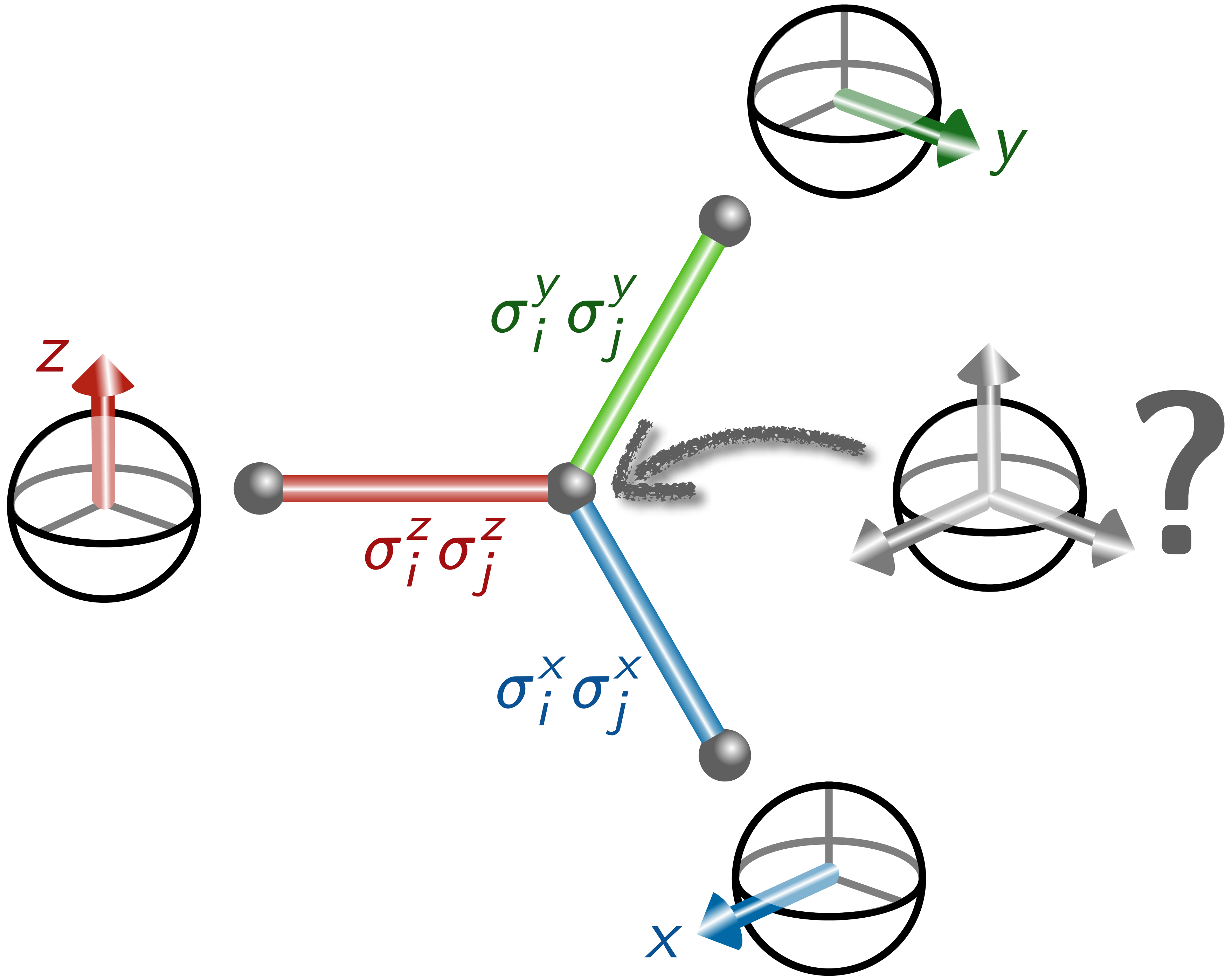

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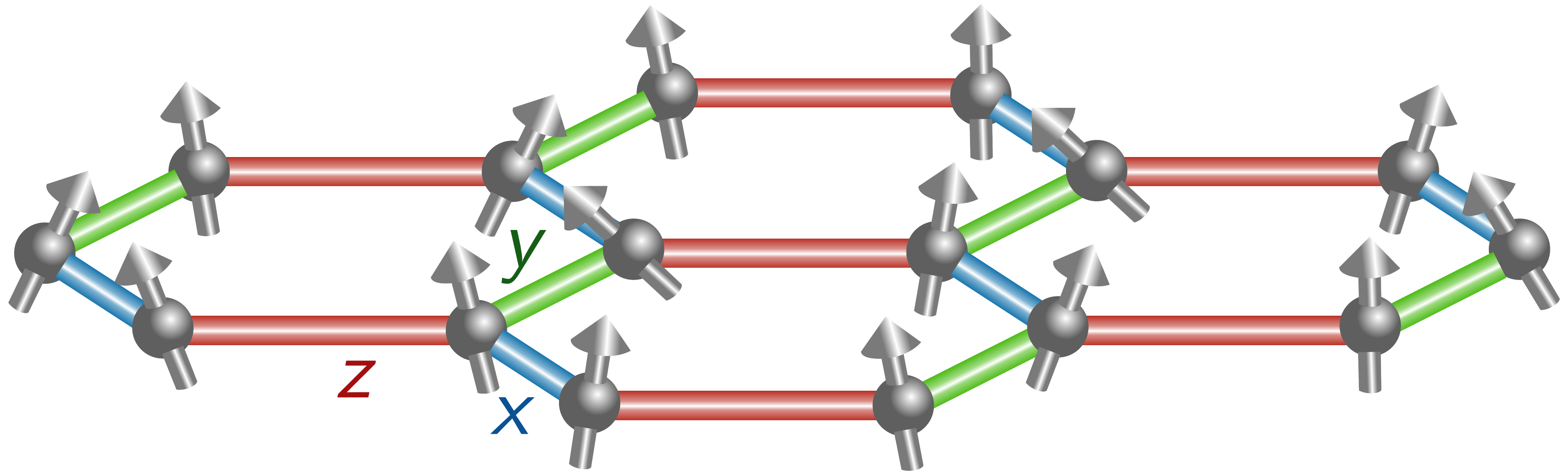

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Majorana fermions:

$$c_1 := a + a^\dagger,$$

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... "real" fermions

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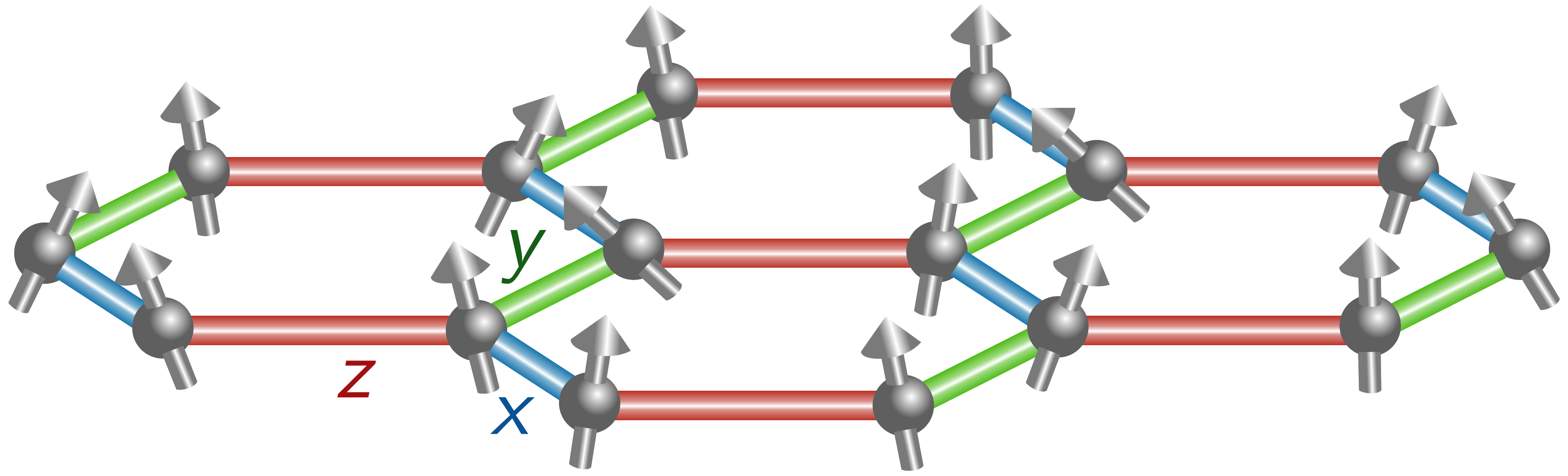

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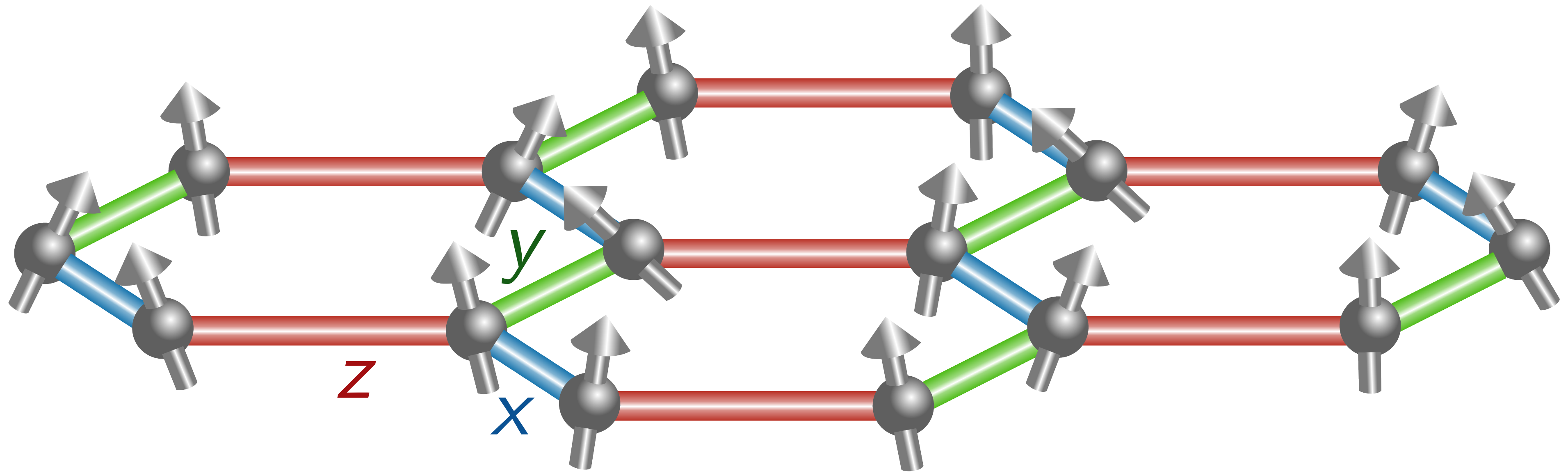

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Representation of single spin:

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

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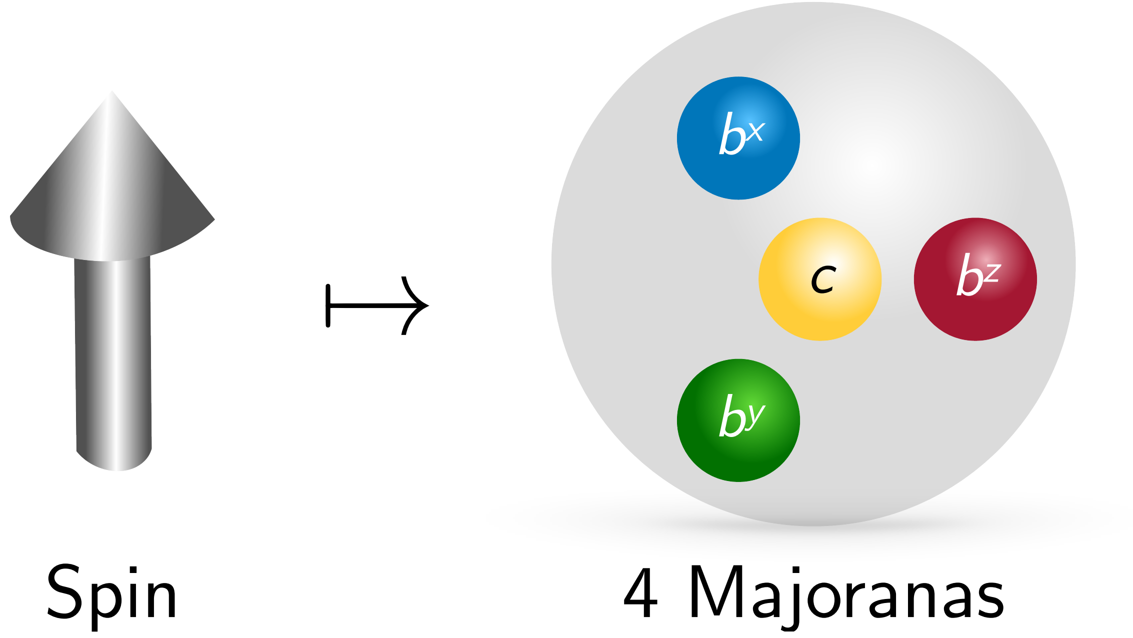

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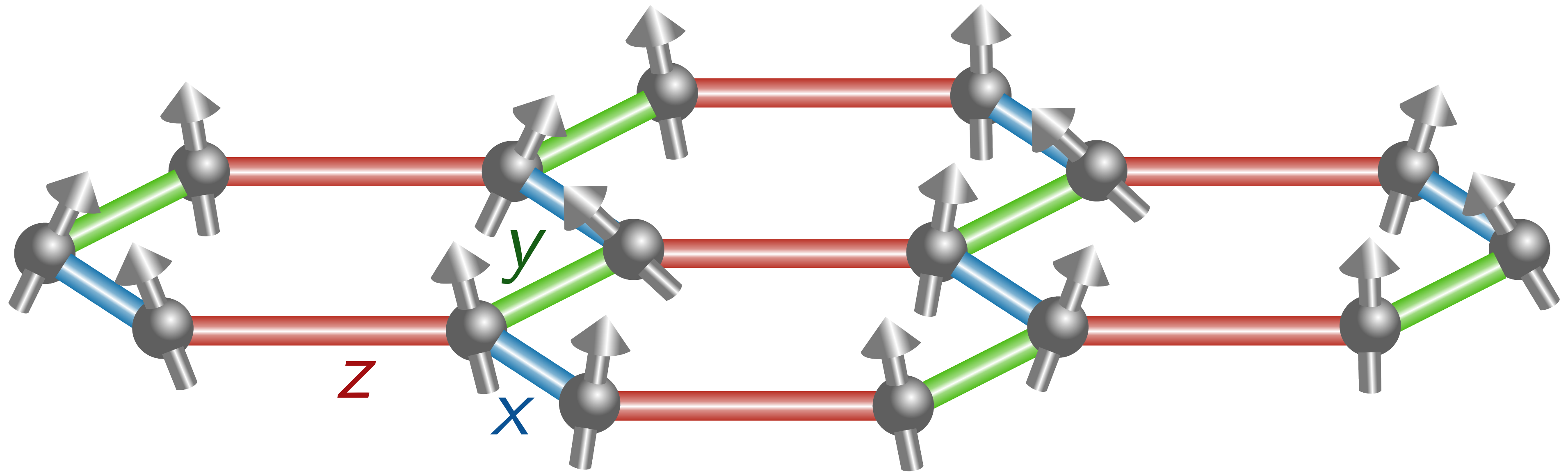

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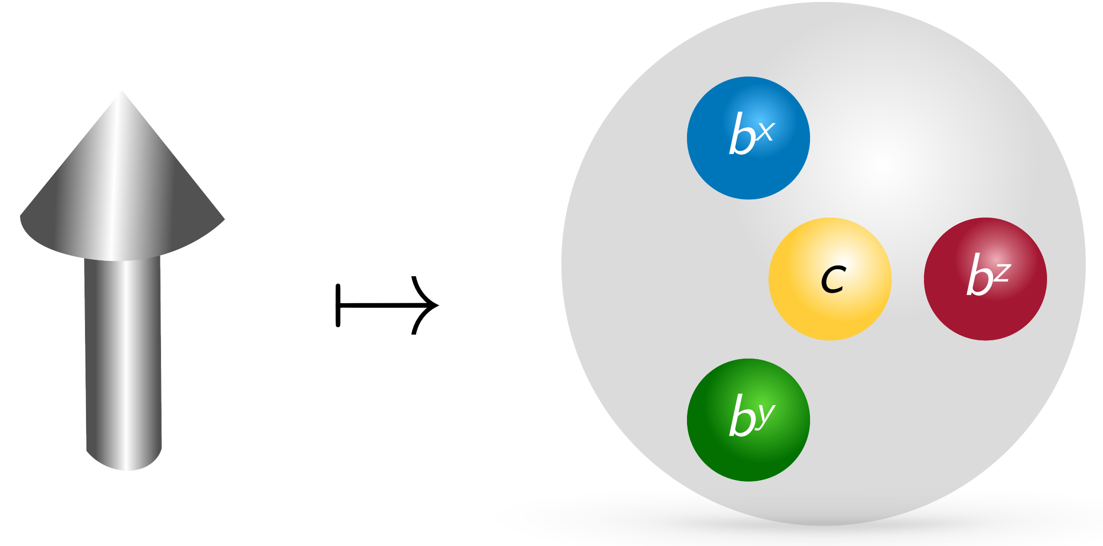
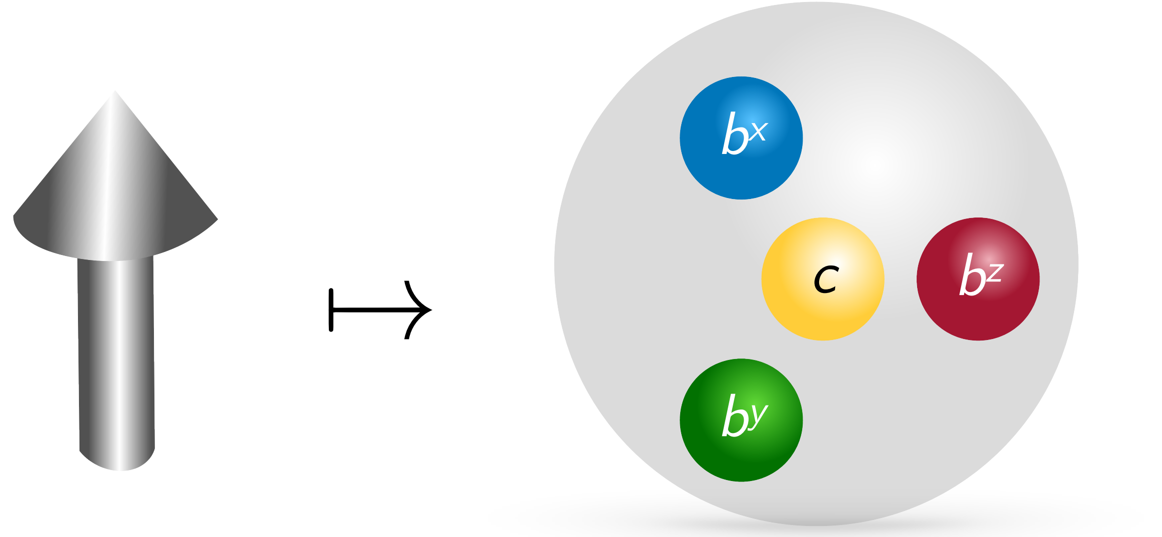
... with $\dim\mathcal{H} = 2$ and $\dim\tilde{\mathcal{H}} = 4$



Spin

4 Majoranas

$\mathbb{Z}_2$ gauge constraint



Spin

4 Majoranas
with gauge constraint

Projection:

$$|\xi\rangle \in \mathcal{H} \subset \tilde{\mathcal{H}} \qquad \Leftrightarrow \qquad D|\xi\rangle = |\xi\rangle, \qquad D = b^x b^y b^z c$$

$\mathbb{Z}_2$ gauge transformation

... with $D^\dagger = D$ and $D^2 = \mathbb{1}$

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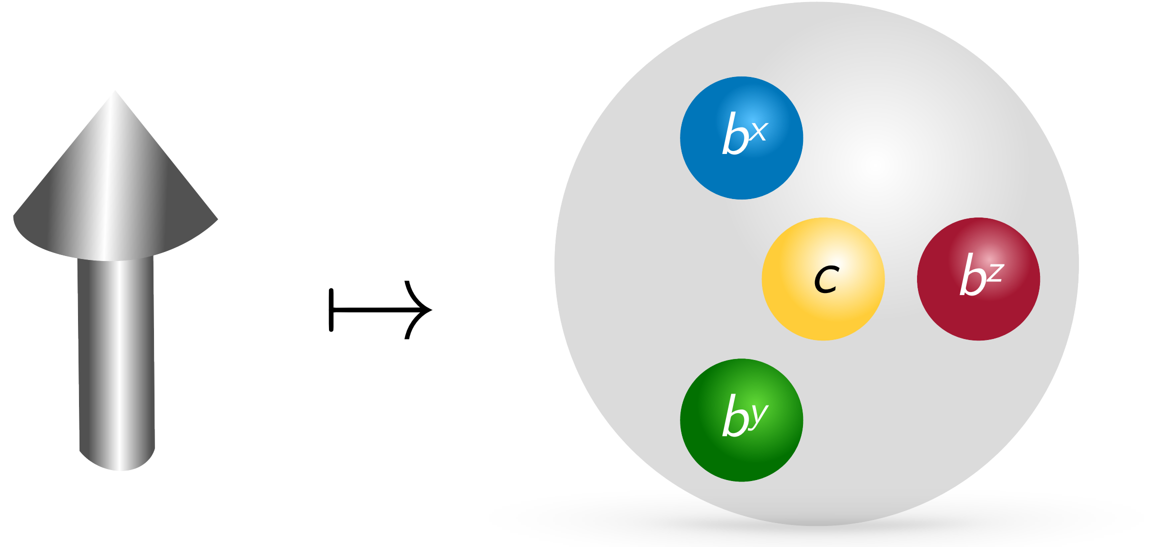

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Spin algebra:

$$[\tilde{\sigma}^\alpha, D] = 0$$

... spin is gauge invariant

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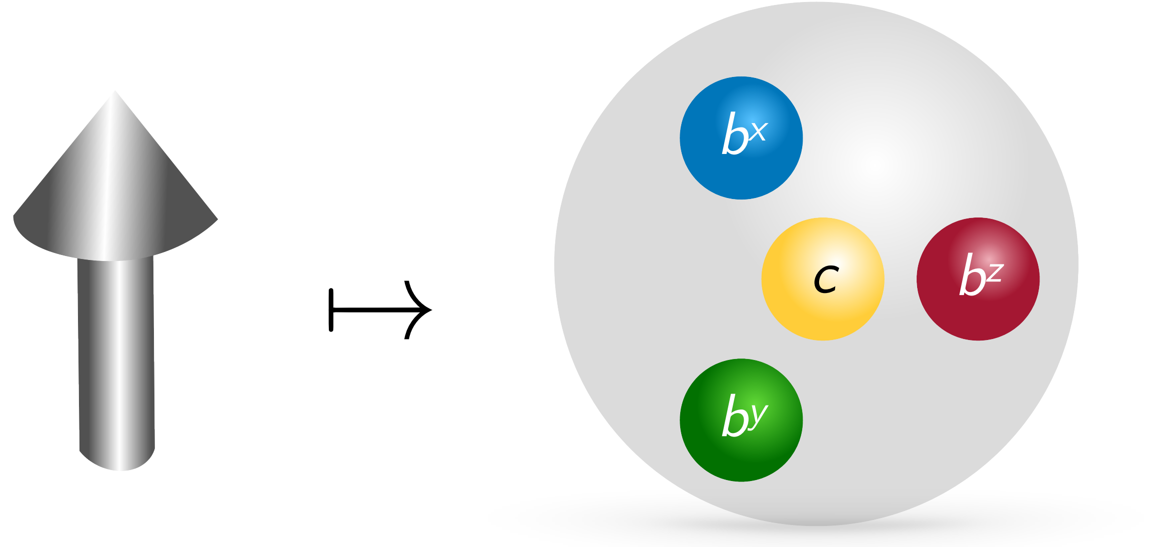

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$$(\tilde{\sigma}^\alpha)^\dagger = (\mathrm{i}b^\alpha c)^\dagger = \tilde{\sigma}^\alpha, \qquad \alpha = x, y, z$$

$$(\tilde{\sigma}^\alpha)^2 = \mathrm{i}^2 b^\alpha c b^\alpha c = \mathbb{1}$$

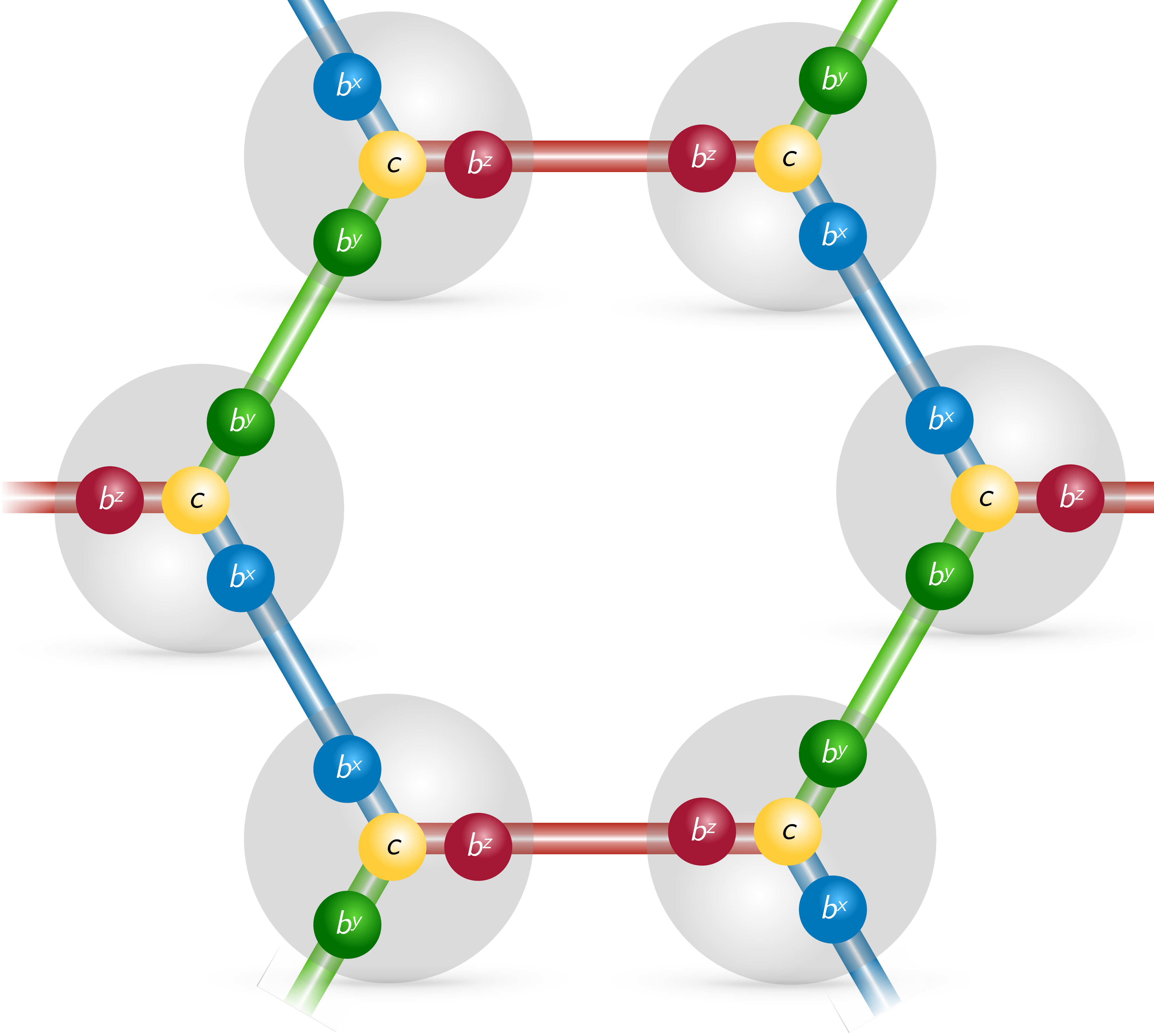
$$\tilde{\sigma}^x \tilde{\sigma}^y \tilde{\sigma}^z = \mathrm{i}^3 b^x c b^y c b^z c = \mathrm{i} b^x b^y b^z c = \mathrm{i}D$$

... spin algebra preserved on gauge-invariant states

Gauge-theory representation

Representation of lattice model:

$$\sigma_i^\alpha \mapsto \tilde{\sigma}_i^\alpha = \mathrm{i} b_i^\alpha c_i, \qquad D_i = b_i^x b_i^y b_i^z c_i$$



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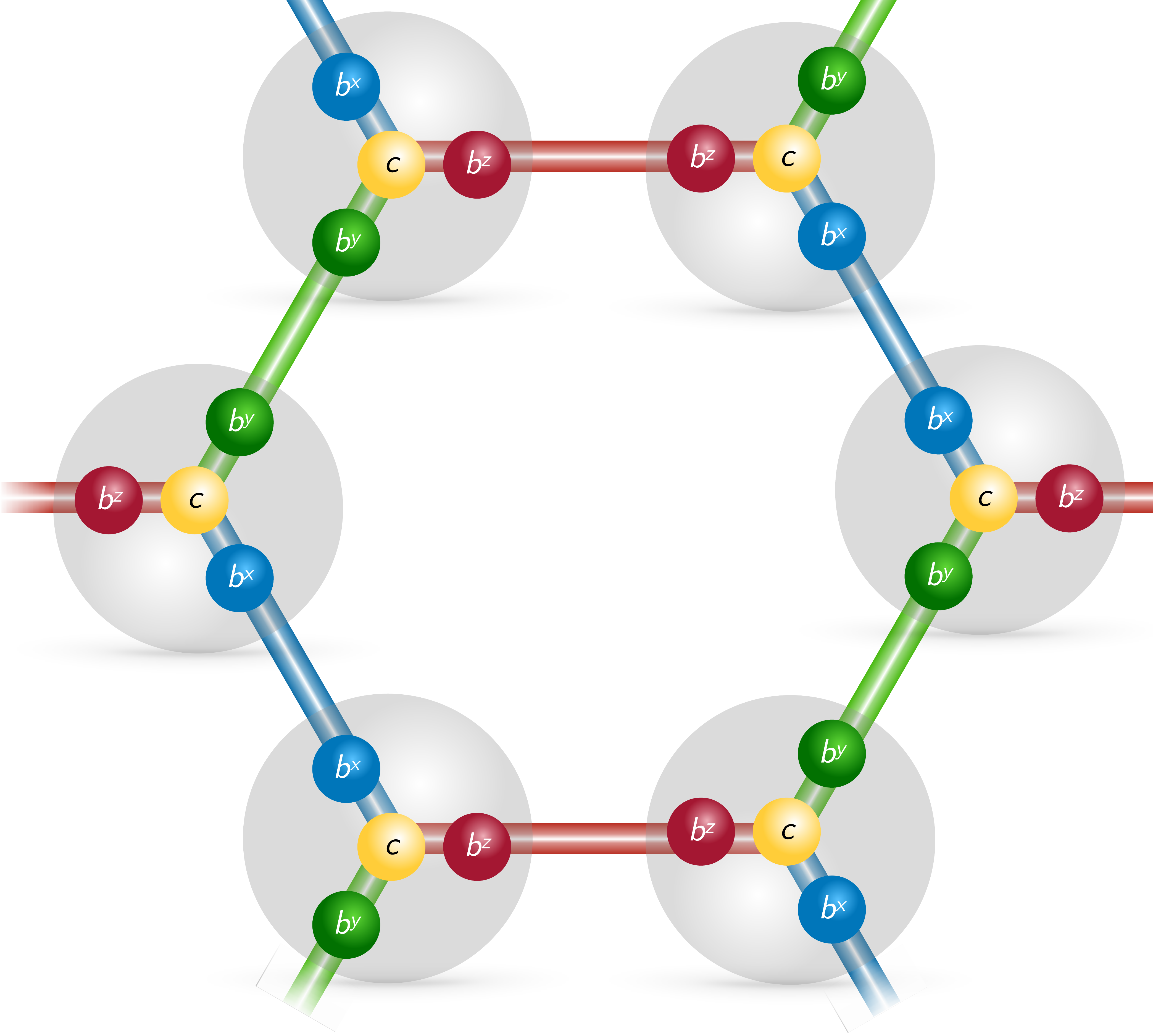

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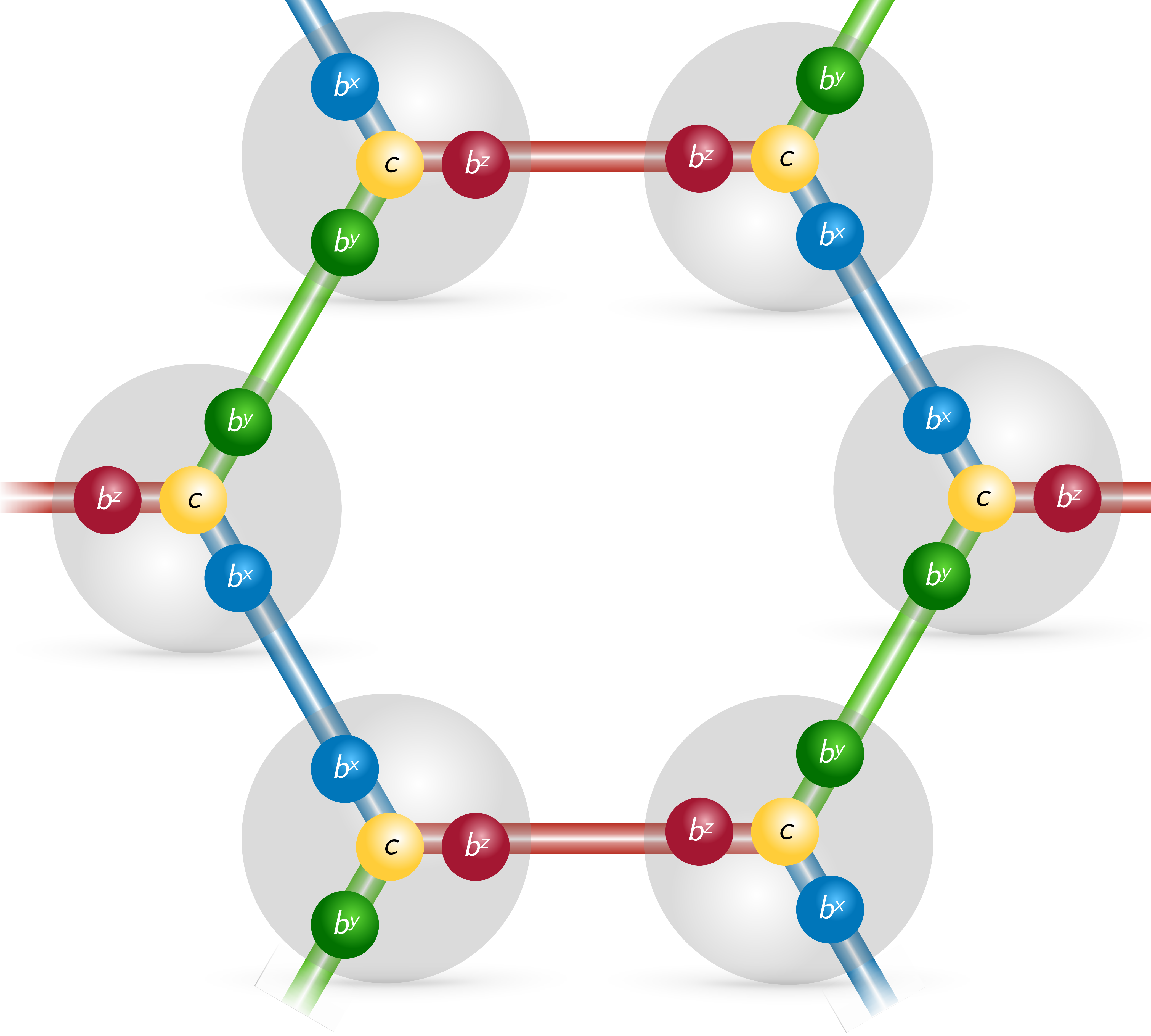

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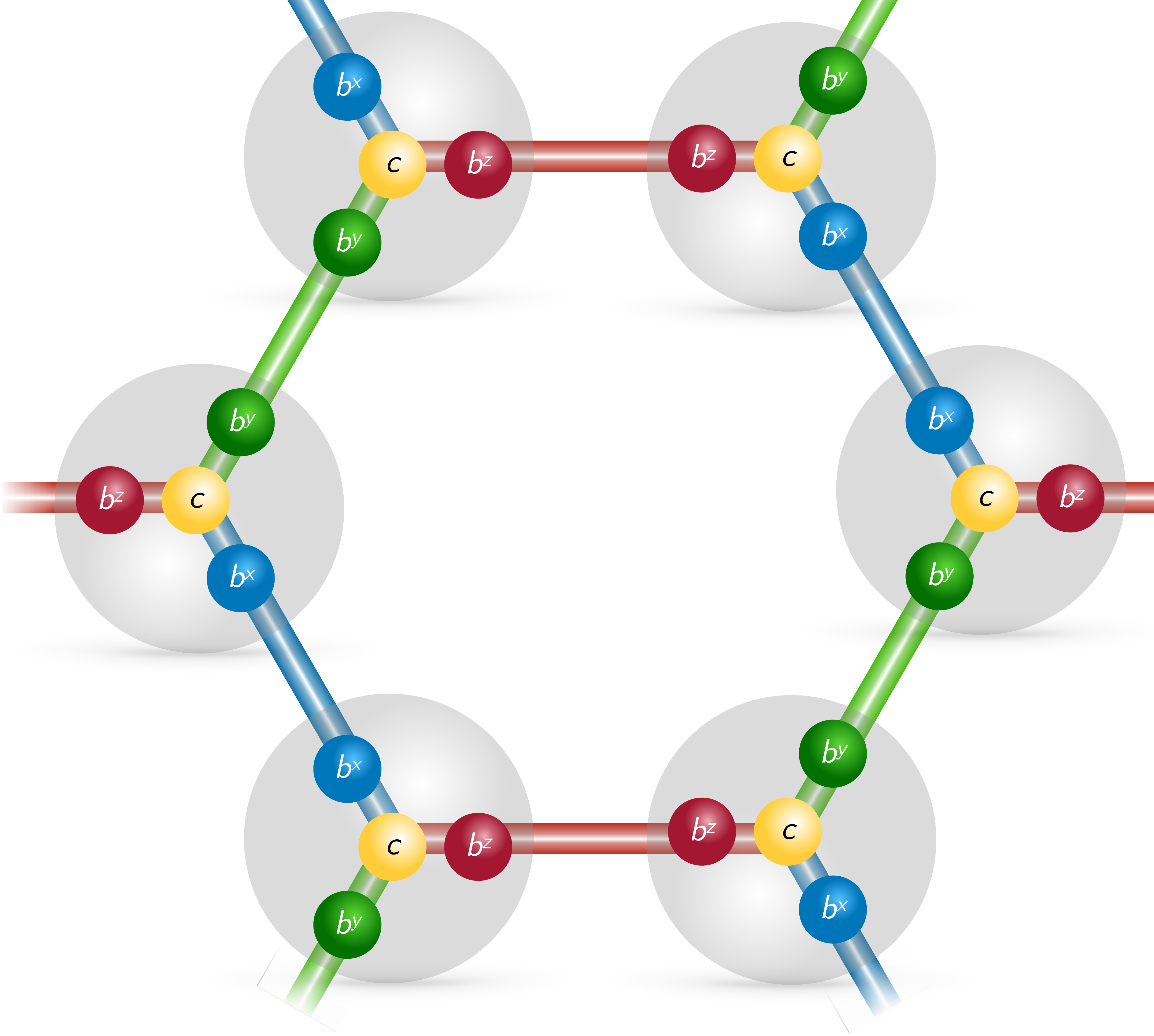

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$$\tilde{H} = -\mathrm{i} K \sum_{\langle ij \rangle_\alpha} \hat{u}_{ij} c_i c_j$$

“$\mathbb{Z}_2$ gauge theory with Majorana fermions”

Static gauge field

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$u_{ij} = \pm 1$ eigenvalues

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$$[\hat{u}_{ij}, \hat{u}_{i'j'}] = [\mathrm{i}b_i^\alpha b_j^\alpha, \mathrm{i}b_{i'}^\beta b_{j'}^\beta] = 0$$

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... static gauge field, u_{jk} good quantum numbers

Majorana spectrum

Simultaneous diagonalization:

$$\tilde{H}_u = \mathrm{i}K \sum_{\langle ij \rangle_\alpha} u_{ij} c_i c_j \qquad \text{with } u_{ij} = \pm 1$$

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[Lieb, PRL '94]

$$u_{ij} = +1 \quad \forall (i,j) \quad \Rightarrow \quad \text{translation invariance}$$

... up to gauge redundancy

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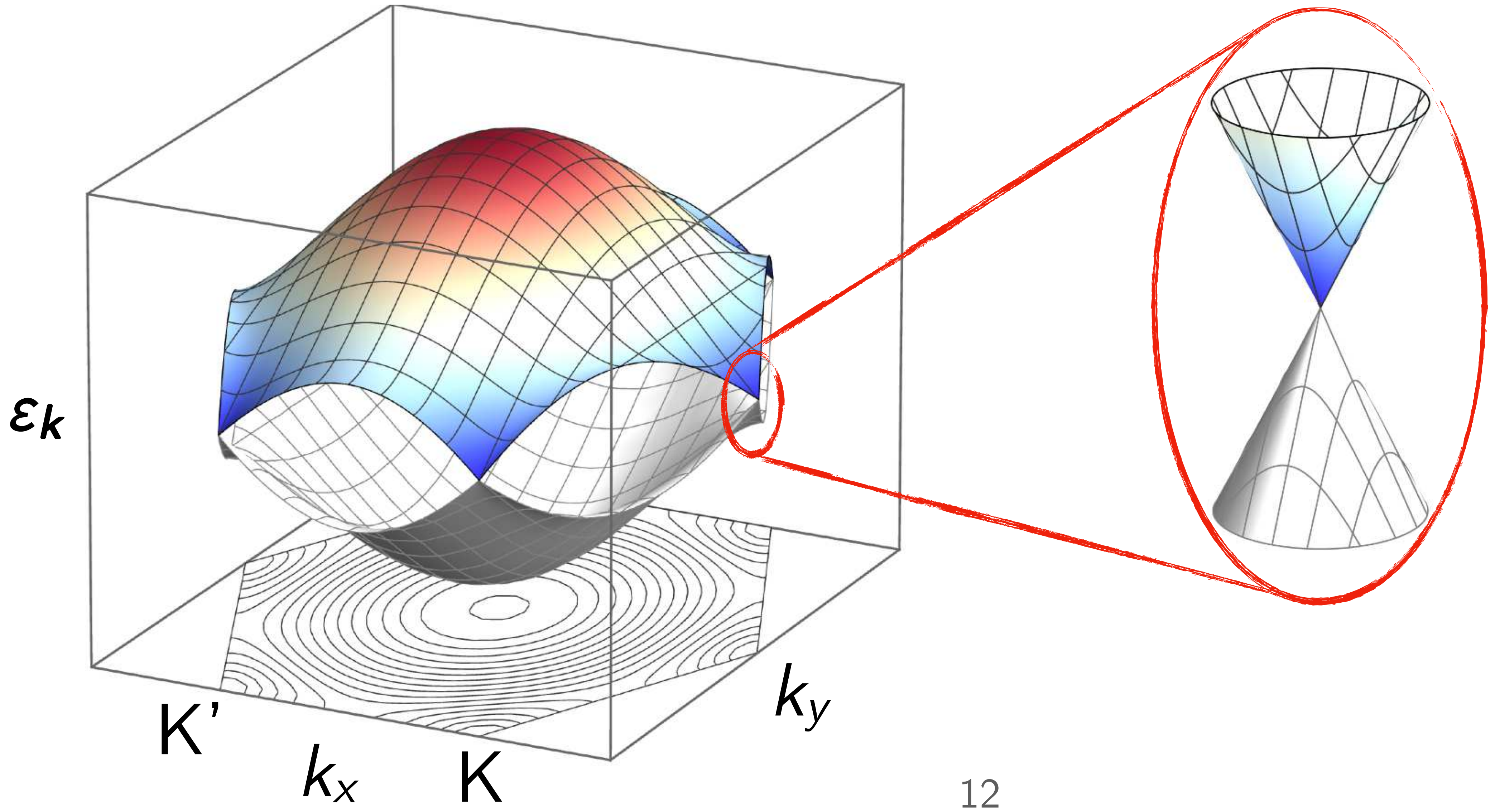
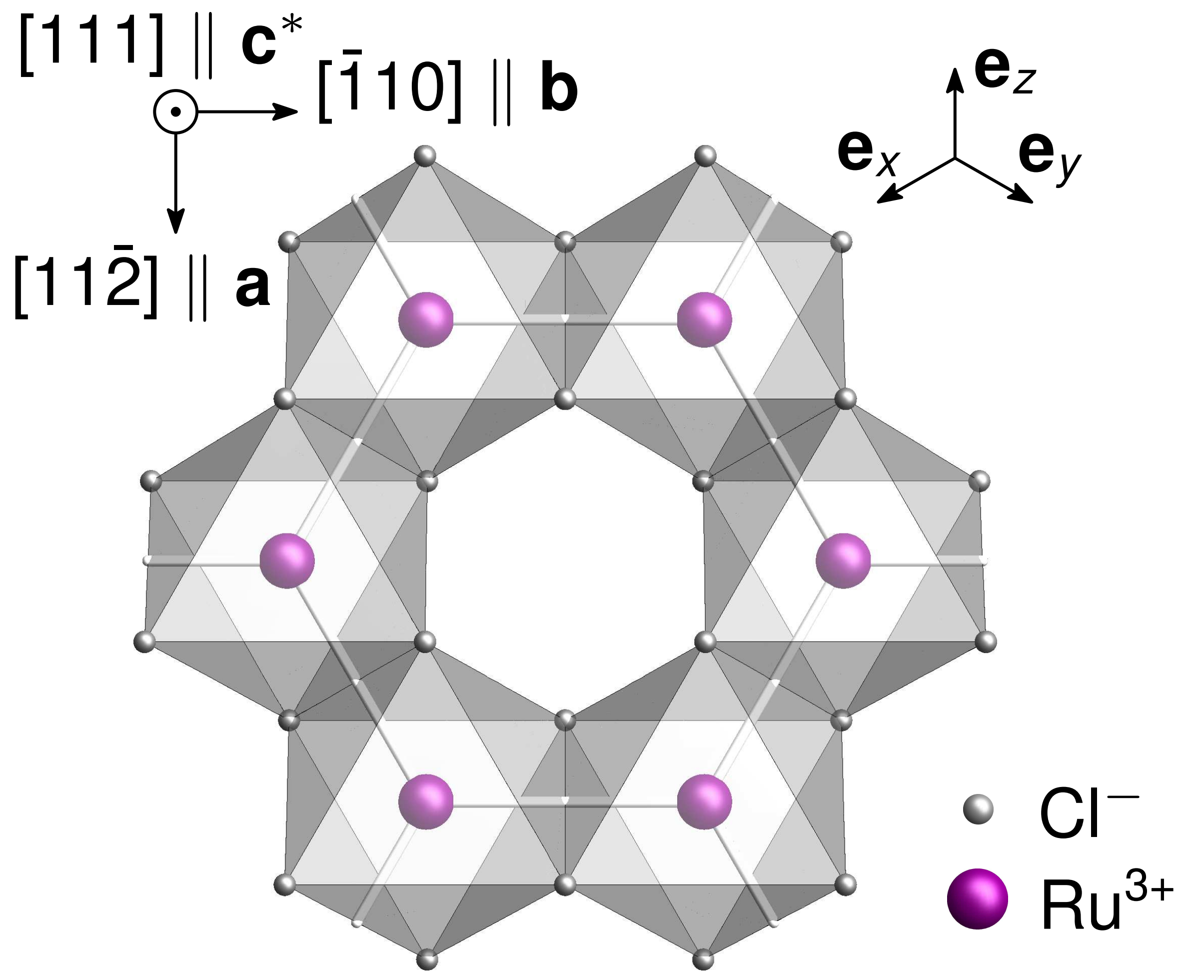


"1/2" of graphene!

Kitaev-Heisenberg spin-1/2 model

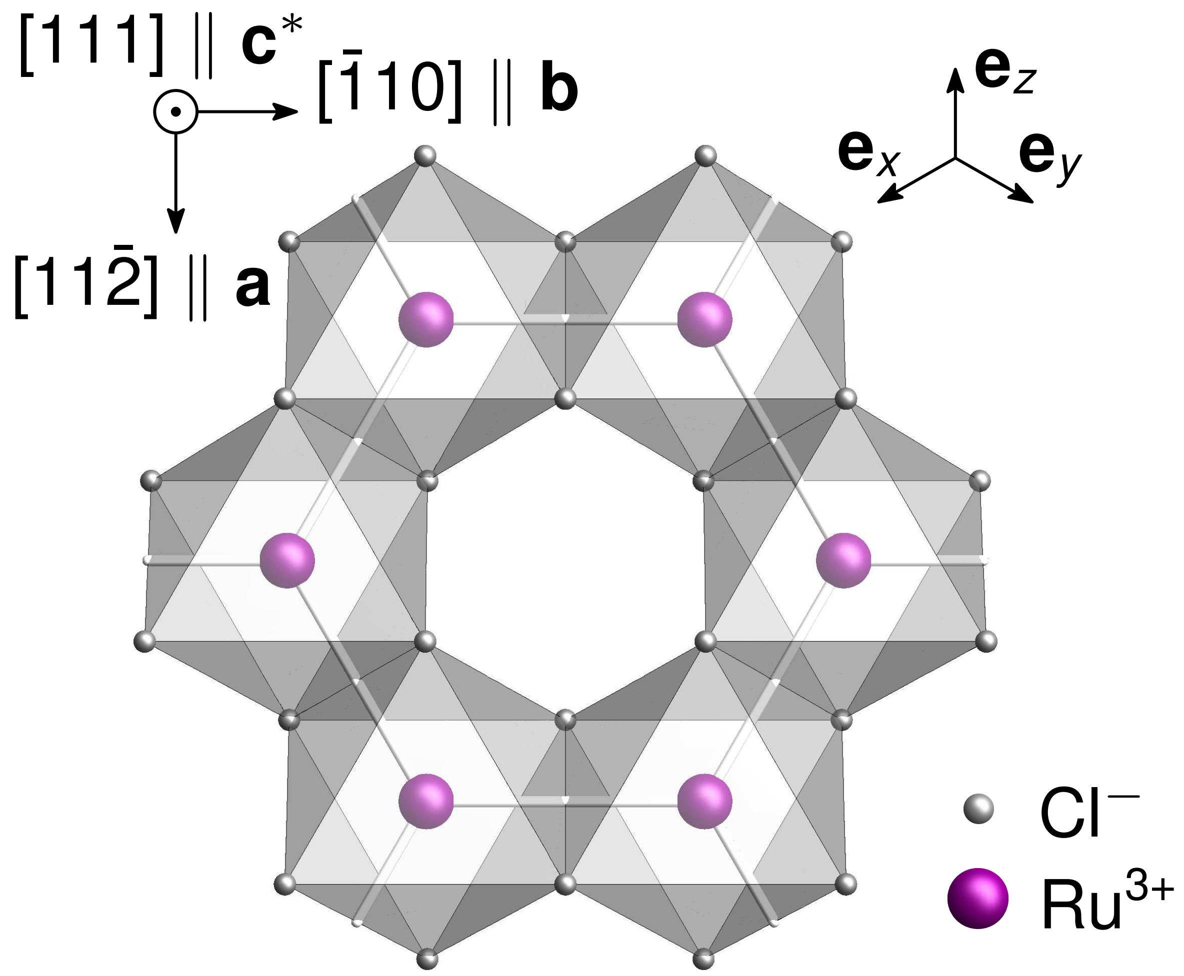


... possible relevance to α-RuCl$_3$, Na$_2$IrO$_3$, Na$_2$Co$_2$TeO$_6$, ...

Hamiltonian:

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

Kitaev-Heisenberg spin-1/2 model



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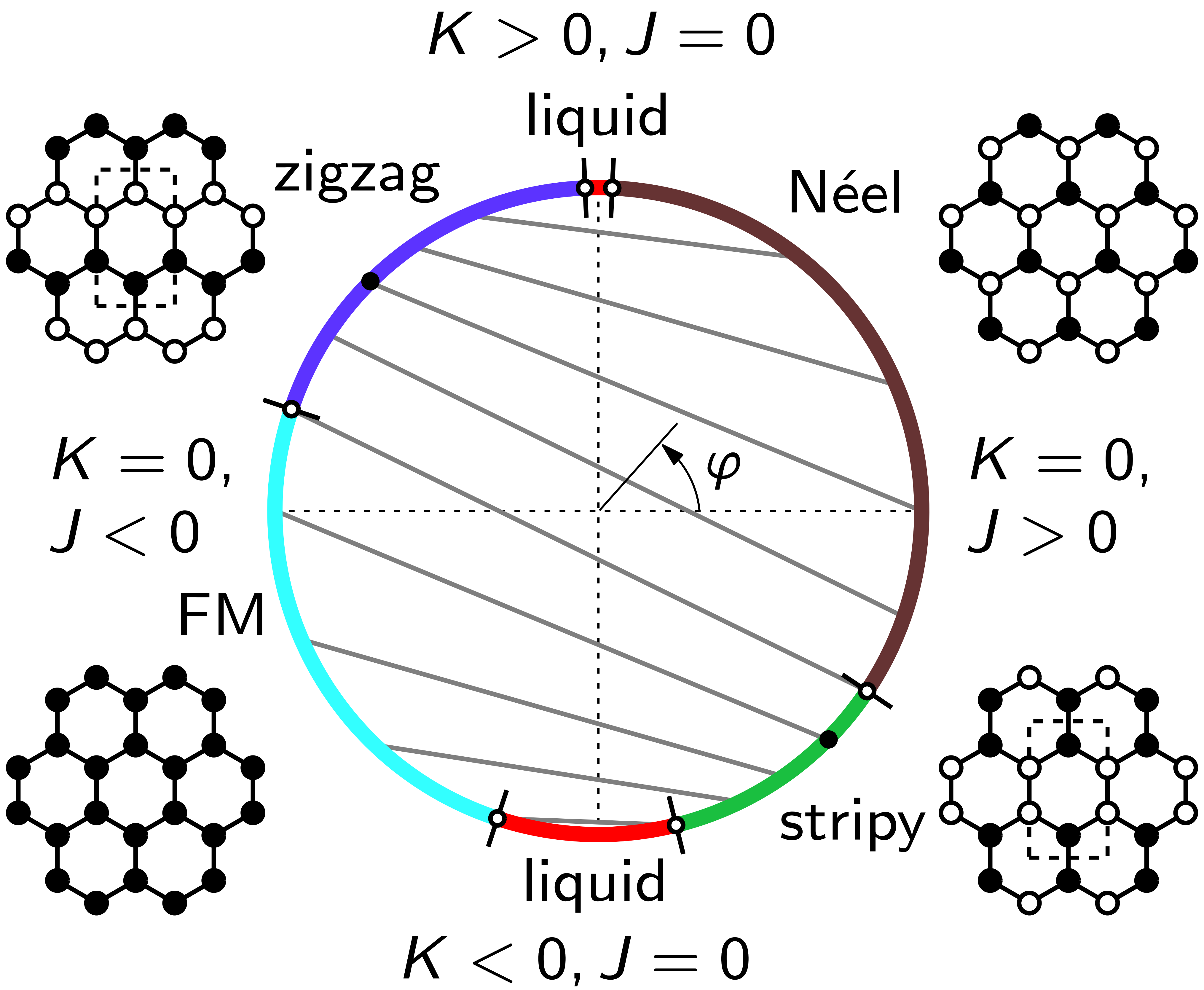
Phase diagram:

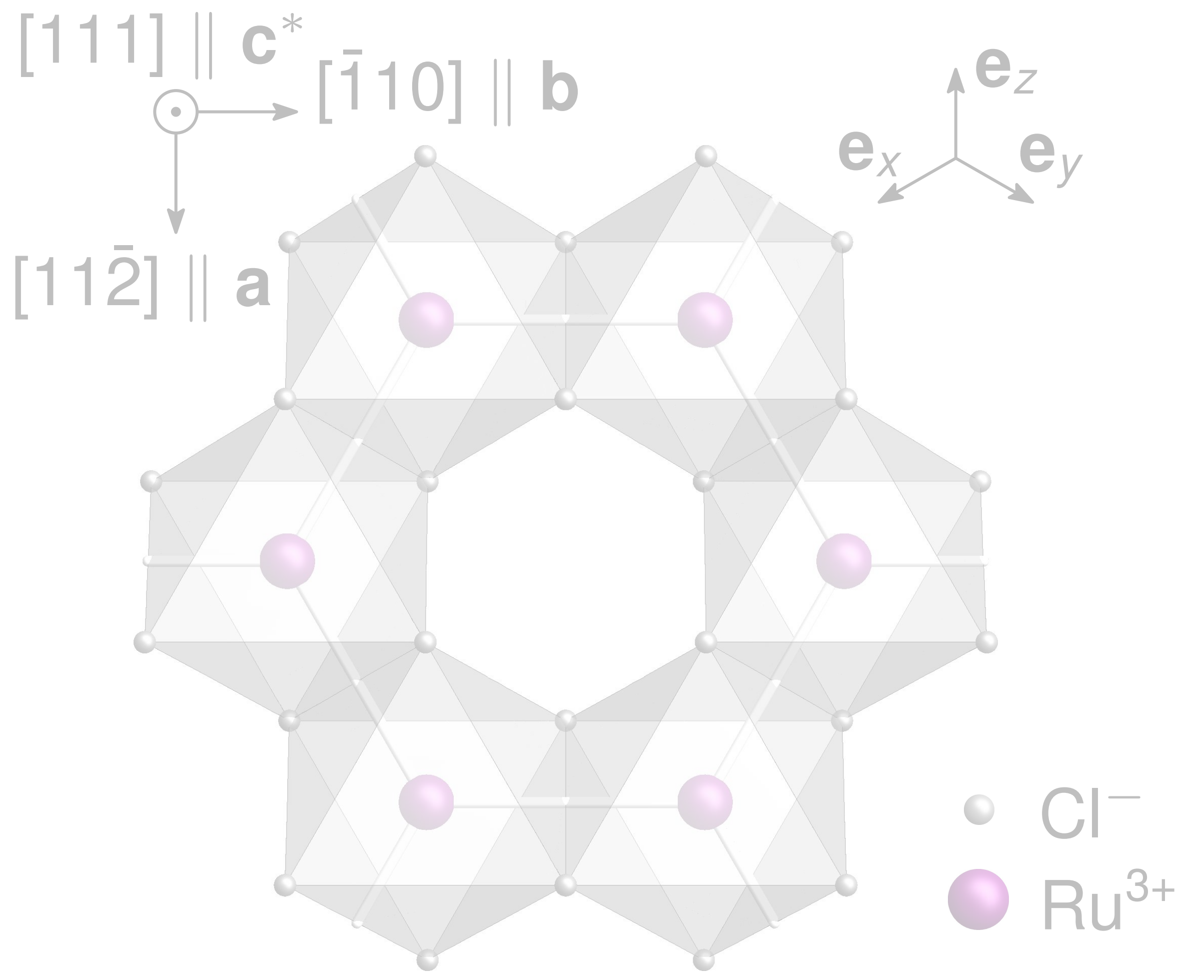


$$J = A \cos\varphi$$

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

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

Kitaev-Heisenberg spin-1/2 model



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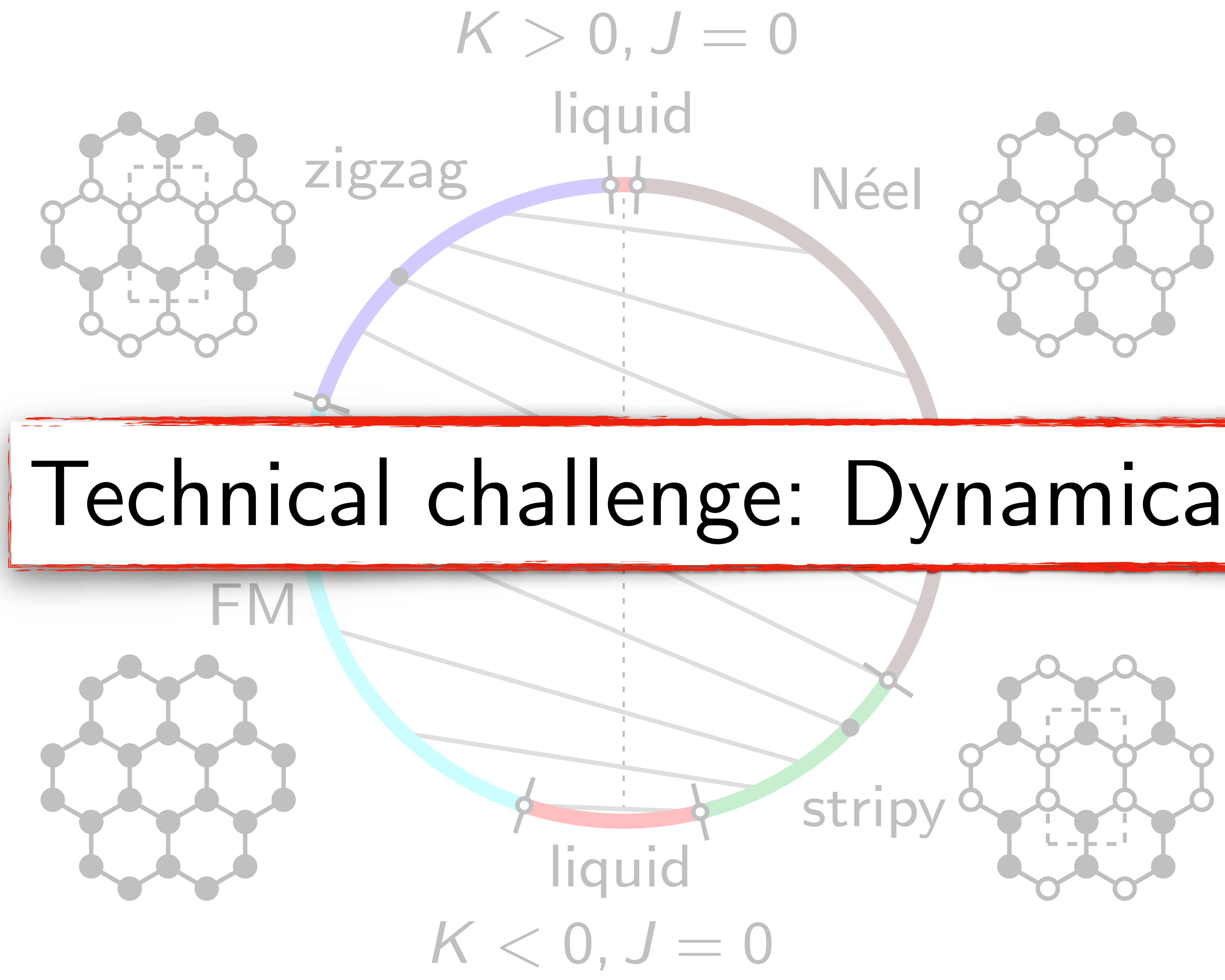


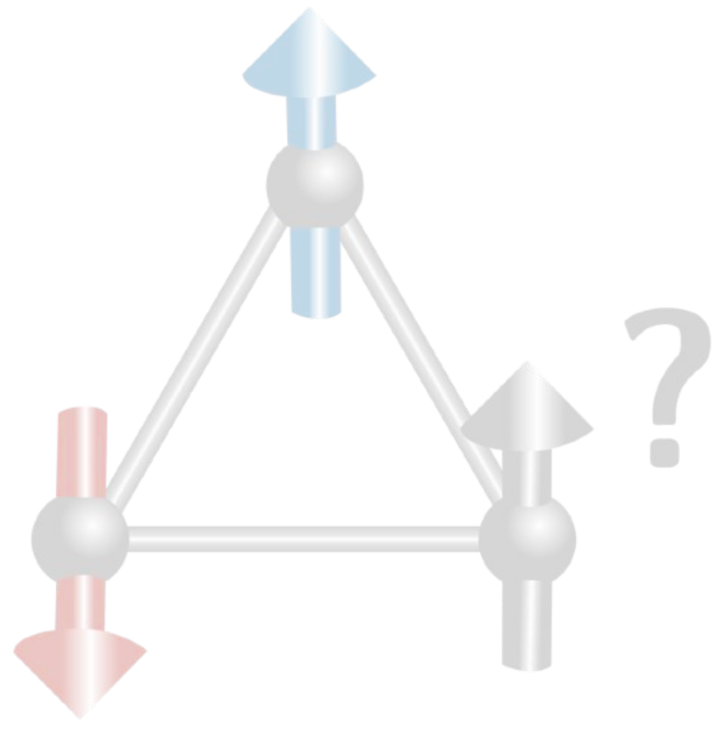
Technical challenge: Dynamical $\mathbb{Z}_2$ gauge field!

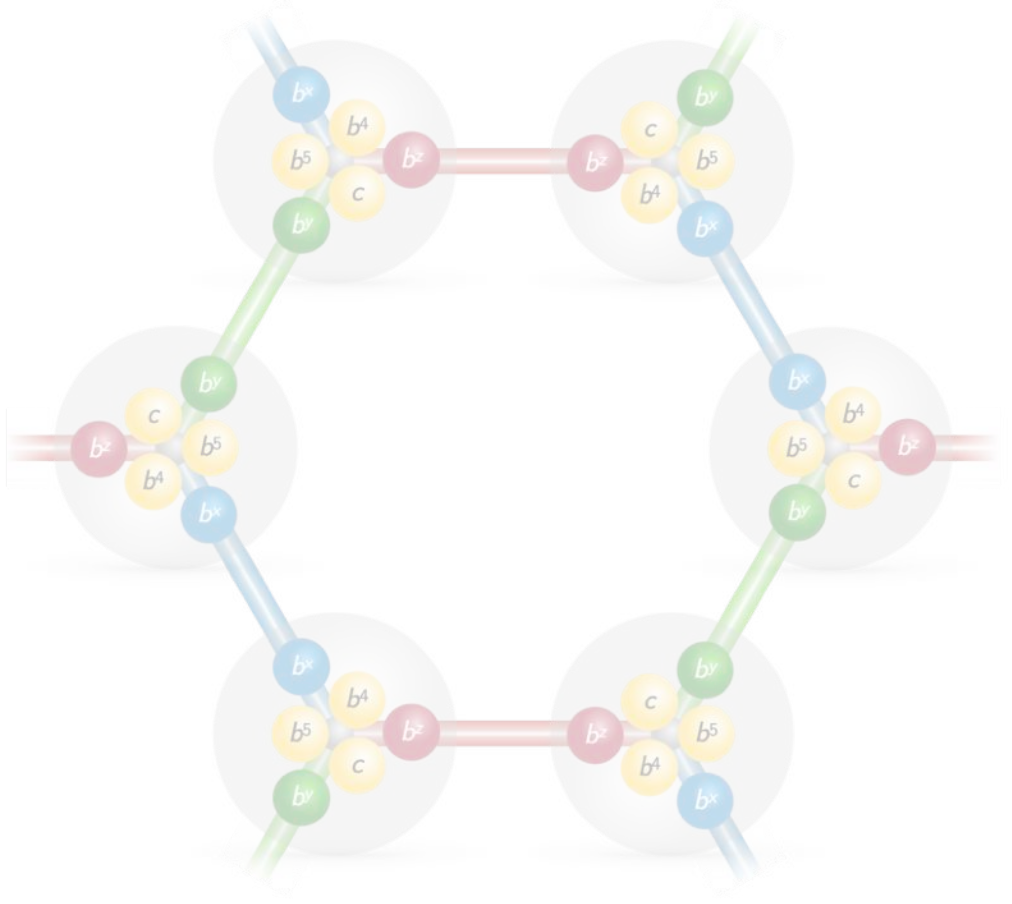
... no sign-problem-free QMC available: [Sato & Assaad, PRB ’21]

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

Outline

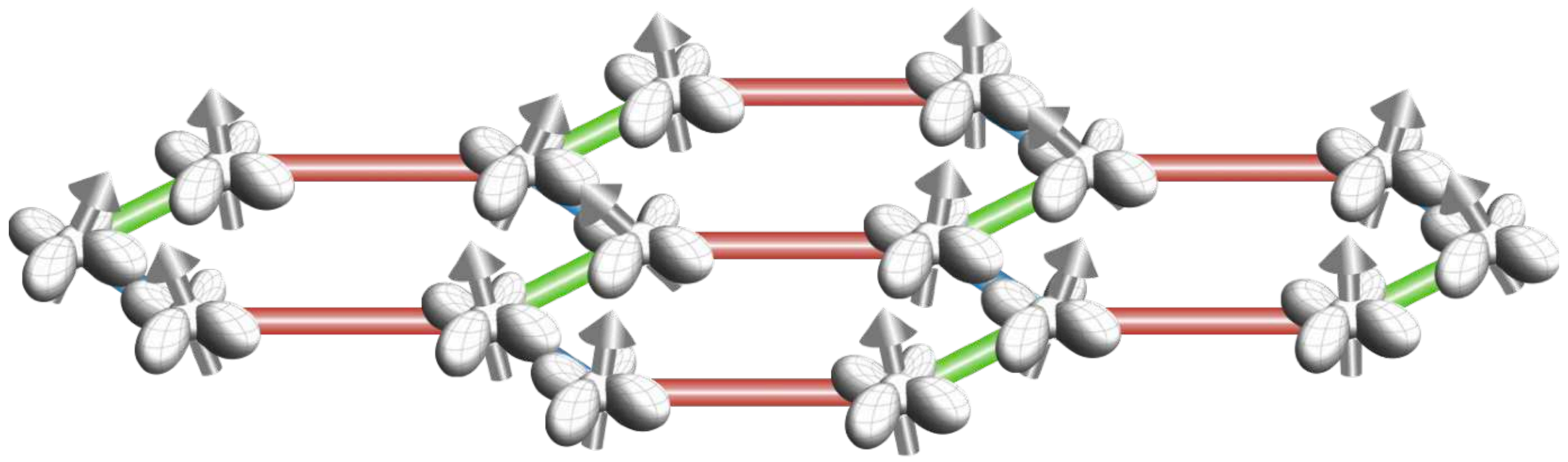
(1) Introduction



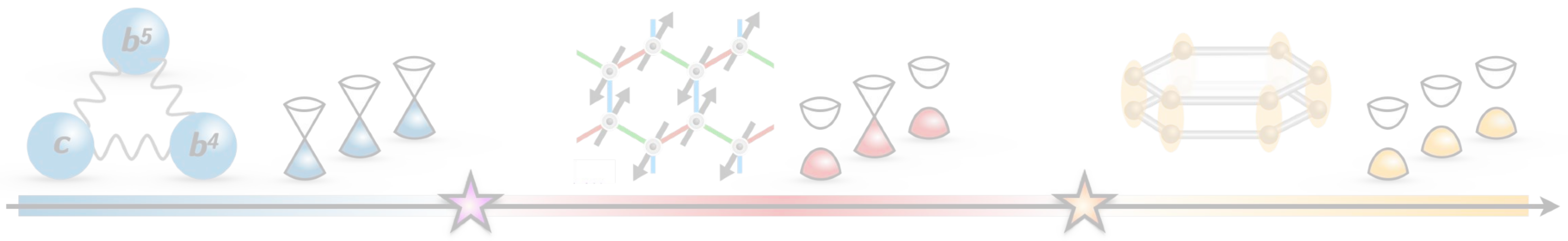


(2) Kitaev spin-1/2 model

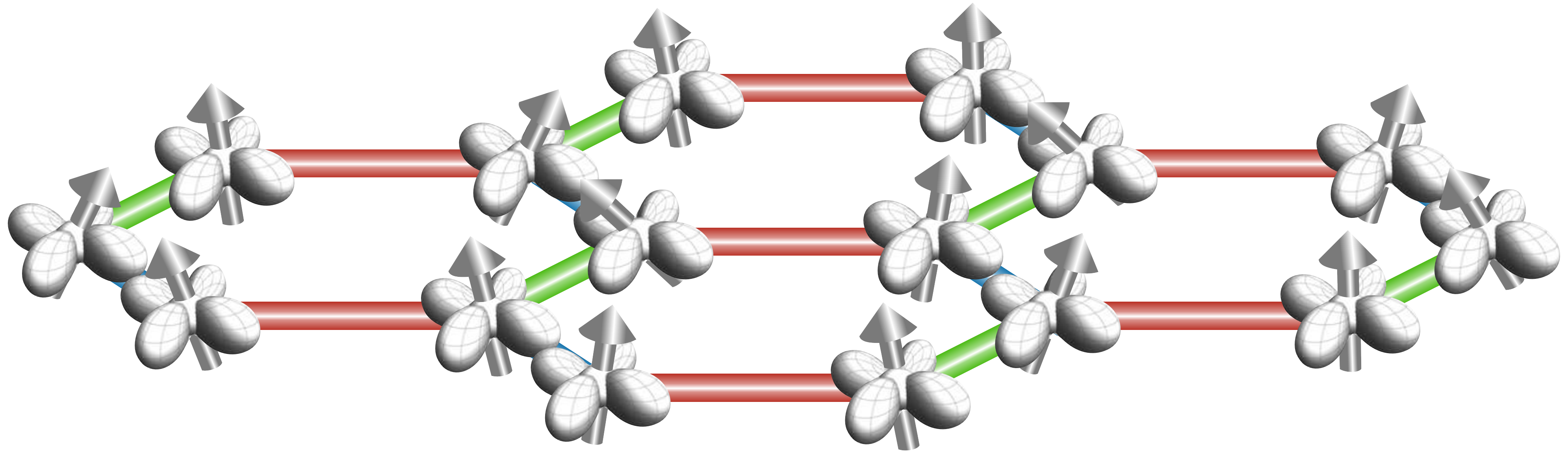
(3) Kitaev-Heisenberg spin-orbital model



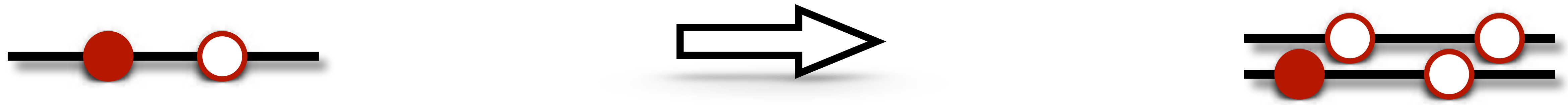
(4) Conclusions



Beyond Kitaev spin-1/2



Spin-orbital generalization:

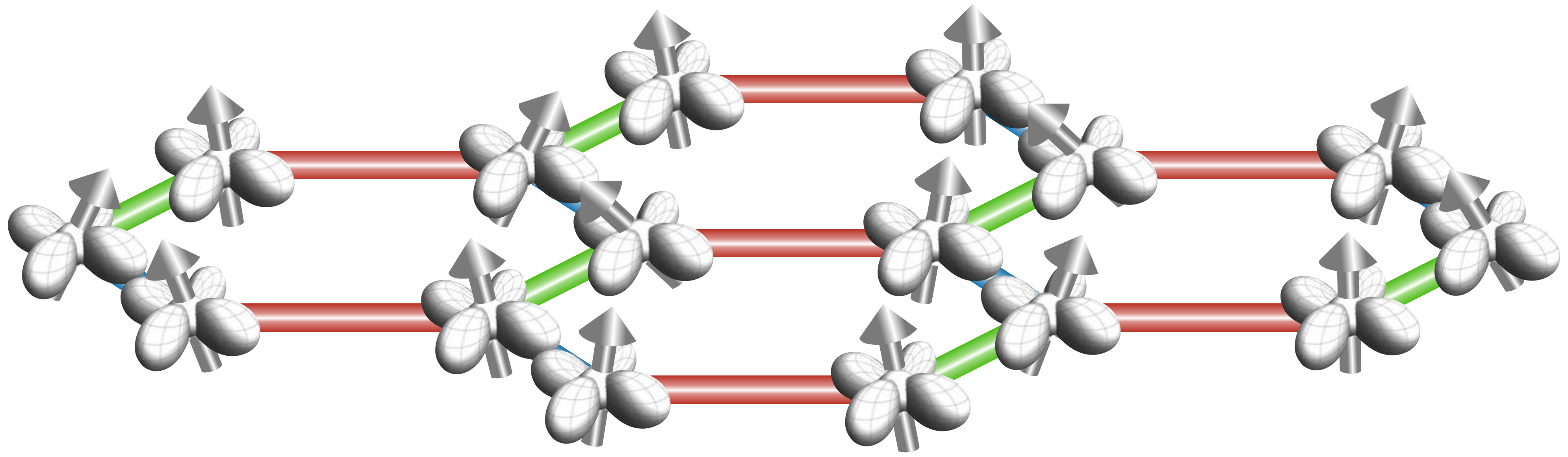


$\sigma^\alpha \quad 2 \times 2$

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

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

Beyond Kitaev spin-1/2



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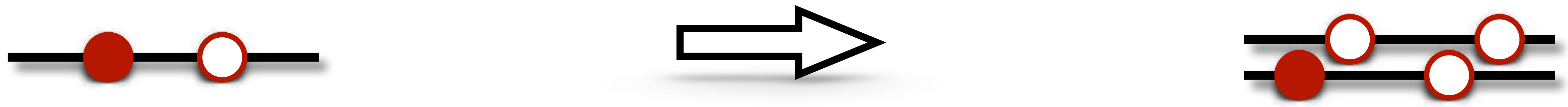

$\sigma^{\alpha} \quad 2 \times 2$

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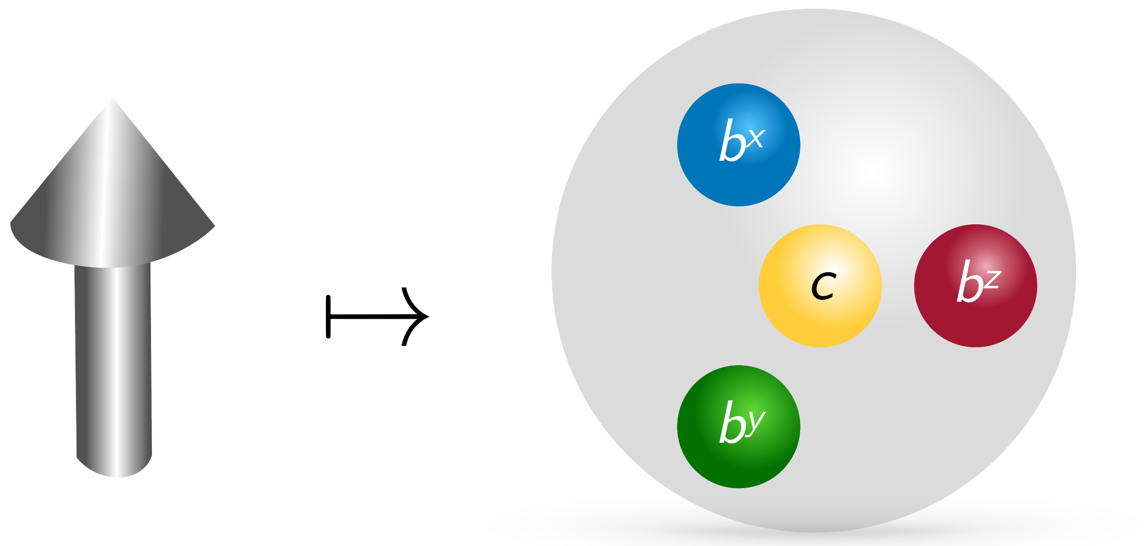
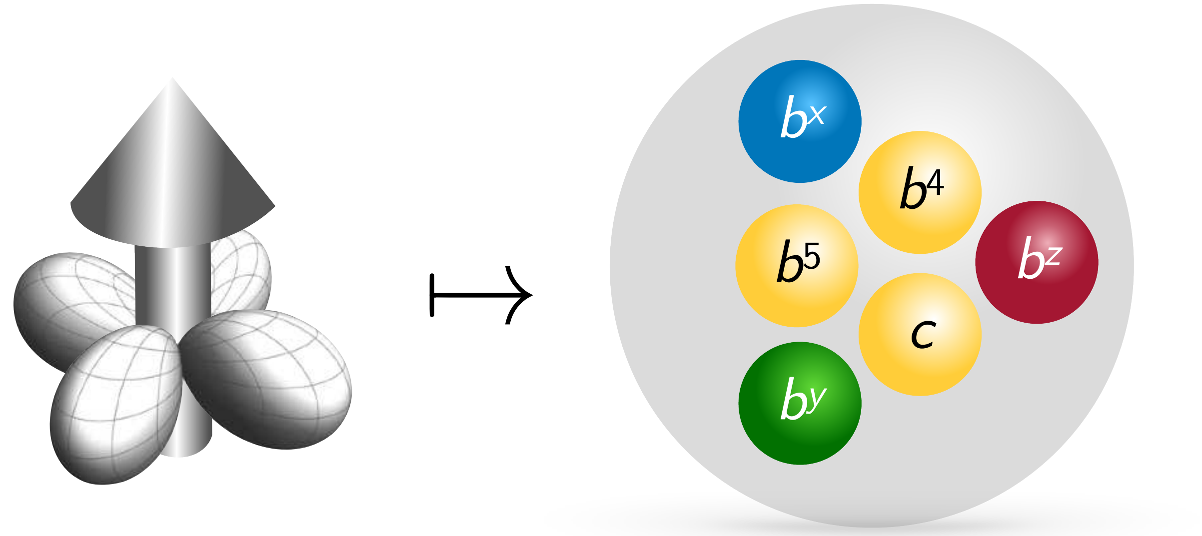


Spin

4 Majoranas
with gauge constraint



Spin + orbital

6 Majoranas
with gauge constraint

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

Kitaev spin-orbital models

Hamiltonian:

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

Heisenberg spin

Kitaev orbital

Kitaev spin-orbital models

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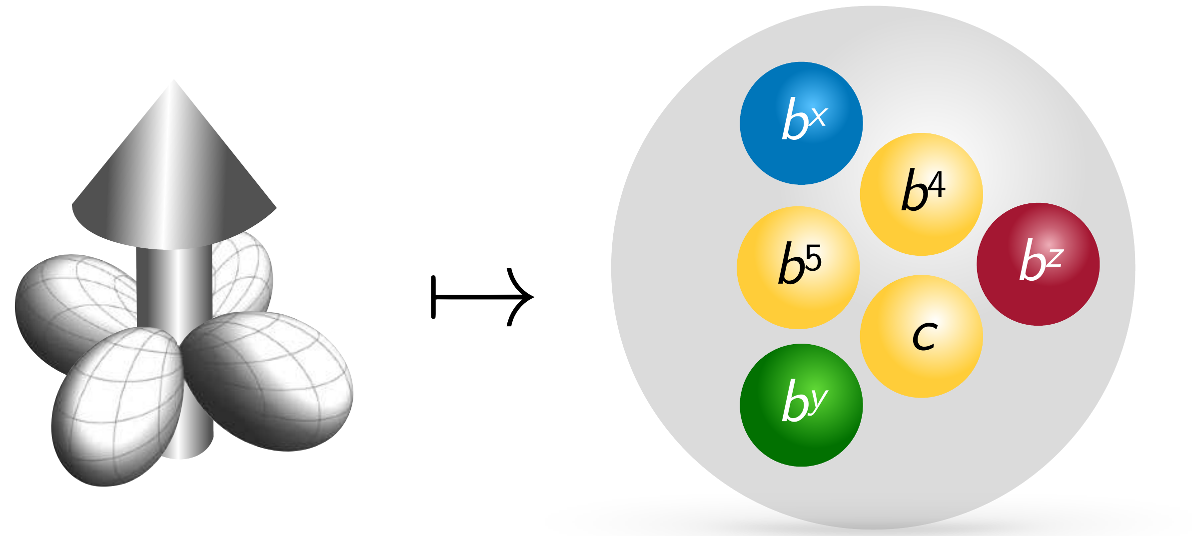
Heisenberg spin

Kitaev orbital

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

Spin-orbital representation:

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



Spin + orbital

6 Majoranas
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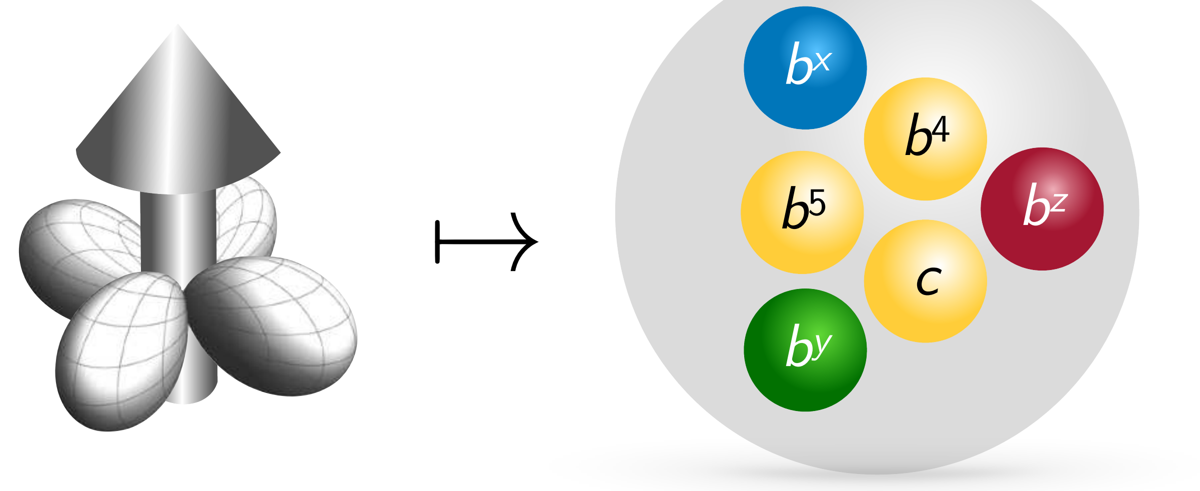
Gauge constraint:

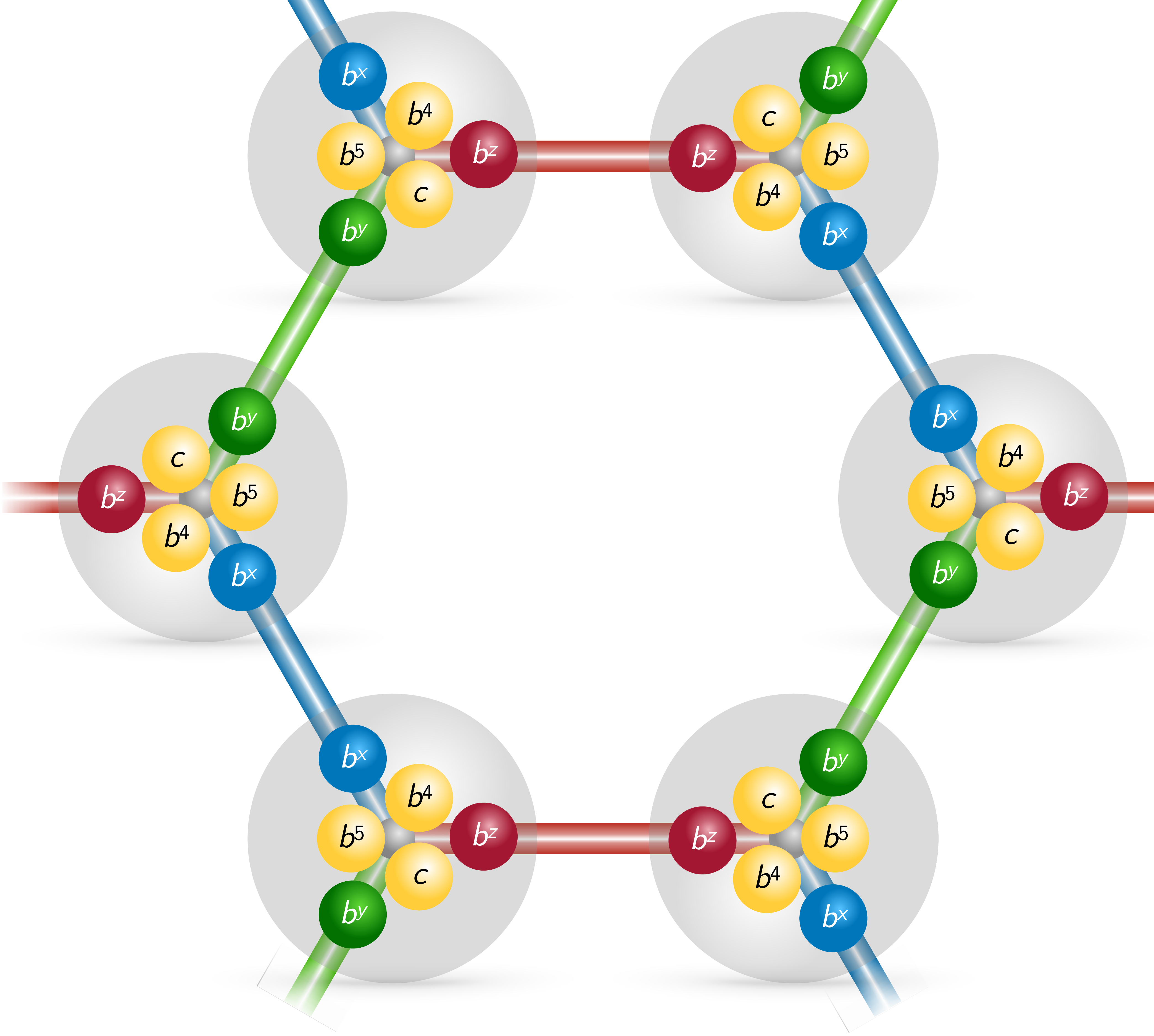
$$|\xi\rangle \in \mathcal{H} \qquad \Leftrightarrow \qquad D|\xi\rangle = |\xi\rangle, \qquad D = \mathrm{i} b^x b^y b^z b^4 b^5 c$$



Spin + orbital

6 Majoranas
with gauge constraint

Gauge-theory representation



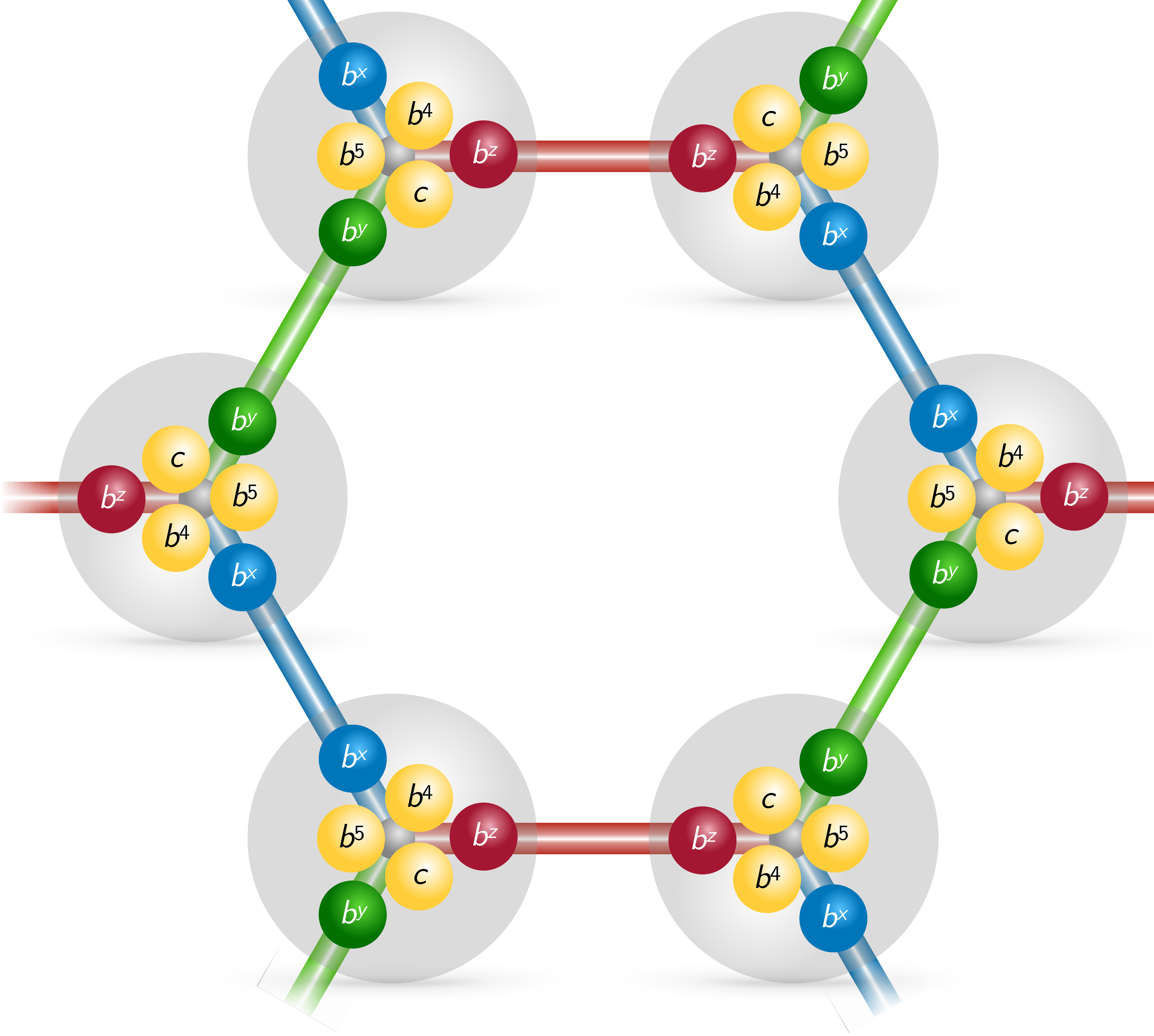
Gauge-theory representation

Ground state:

$$\hat{u}_{ij} \mapsto u_{ij} \equiv 1 \qquad \Longrightarrow \qquad \tilde{H}_u = \mathrm{i}K \sum_{\langle ij \rangle} \boldsymbol{c}_i^\top \boldsymbol{c}_j$$

[Lieb, PRL '94]

$$\text{with } \boldsymbol{c}_j \equiv \begin{pmatrix} c_j \\ b_j^4 \\ b_j^5 \end{pmatrix}$$



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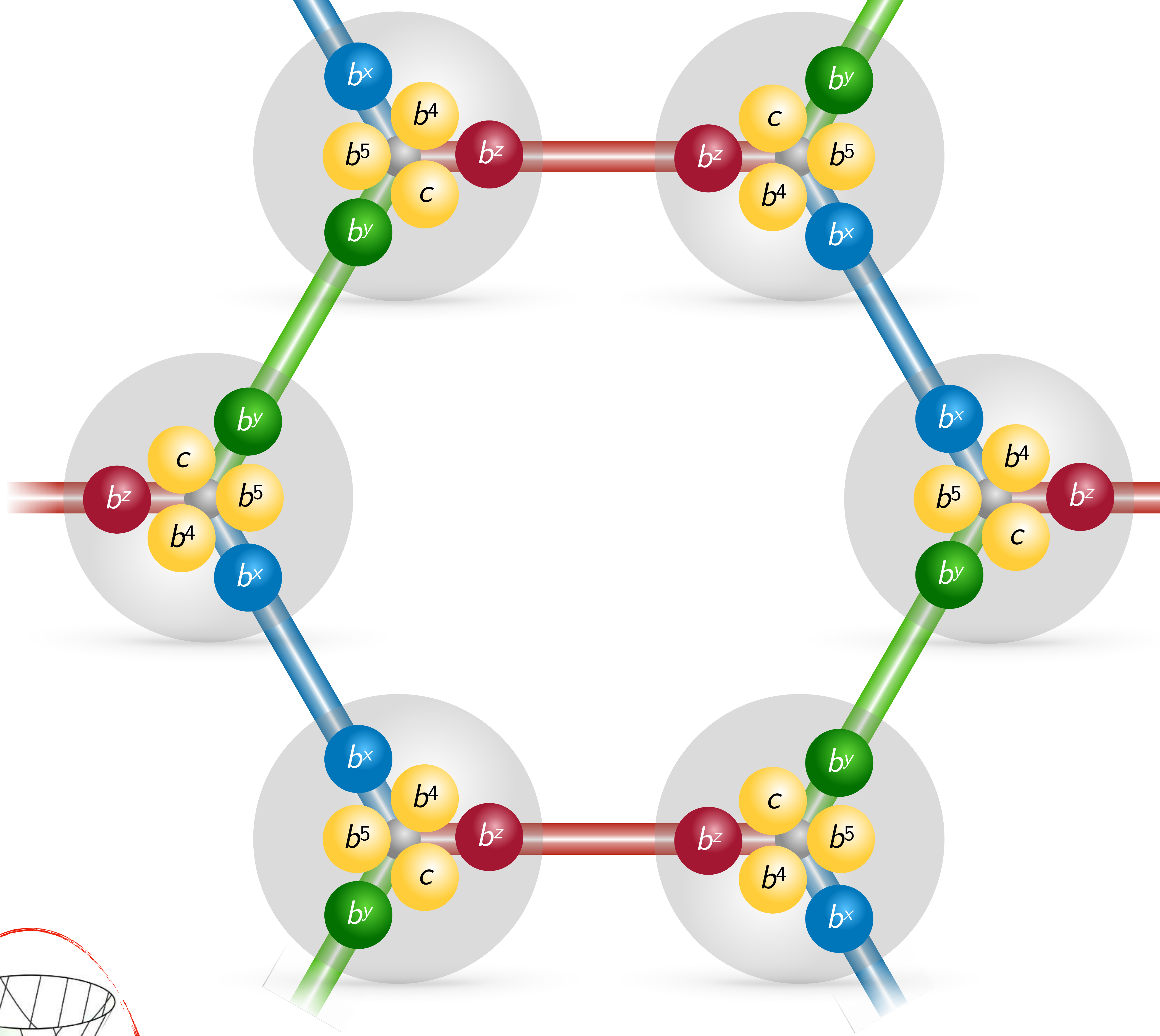

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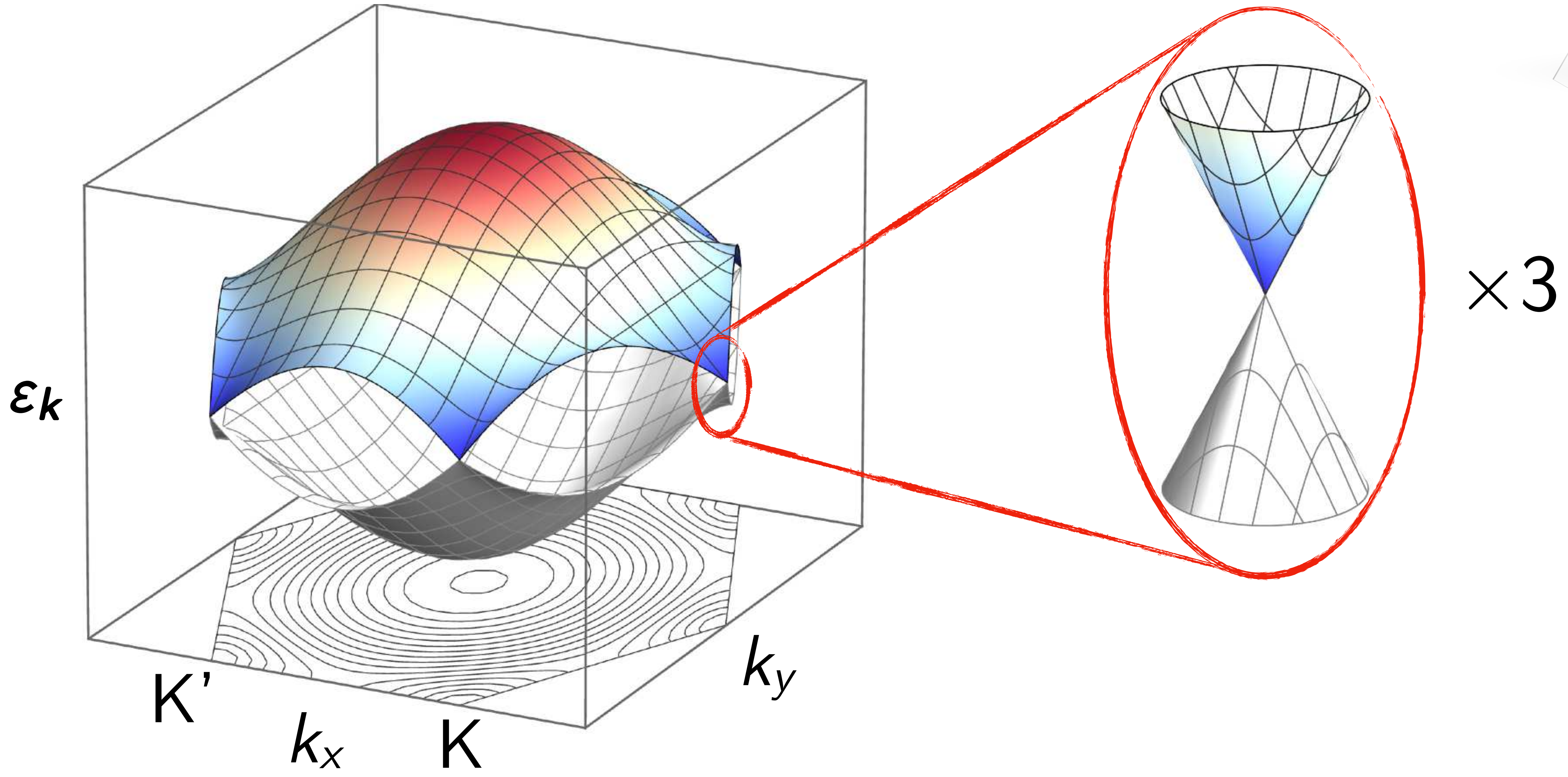
Majorana spectrum:



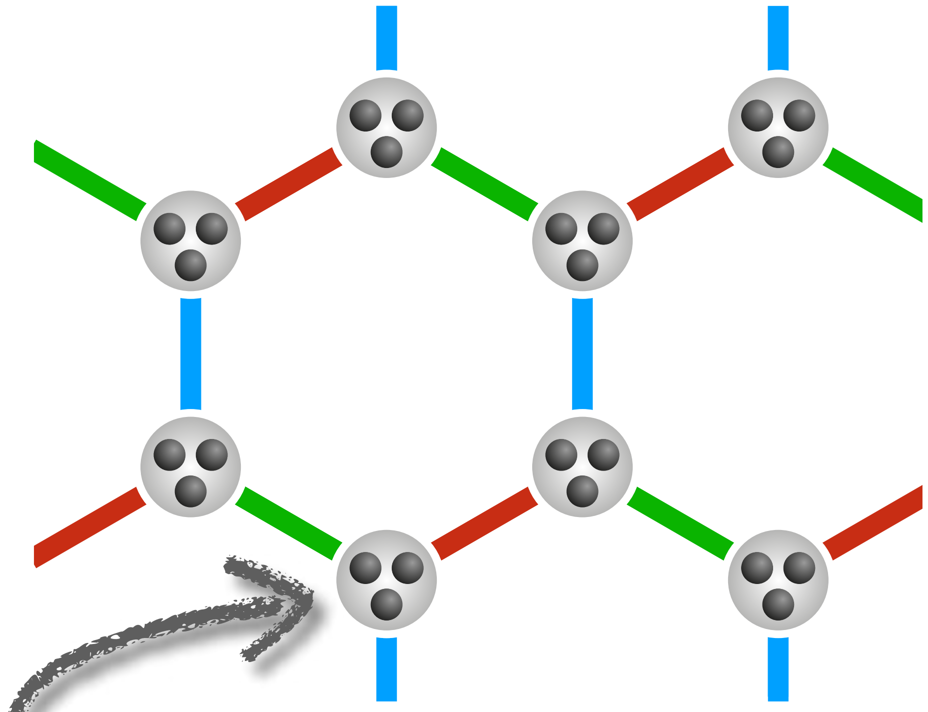
“3/2” of graphene!

Kitaev-Heisenberg spin-orbital model

Hamiltonian:

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

Kitaev-Heisenberg spin-orbital model


3 itinerant fermions

Hamiltonian:

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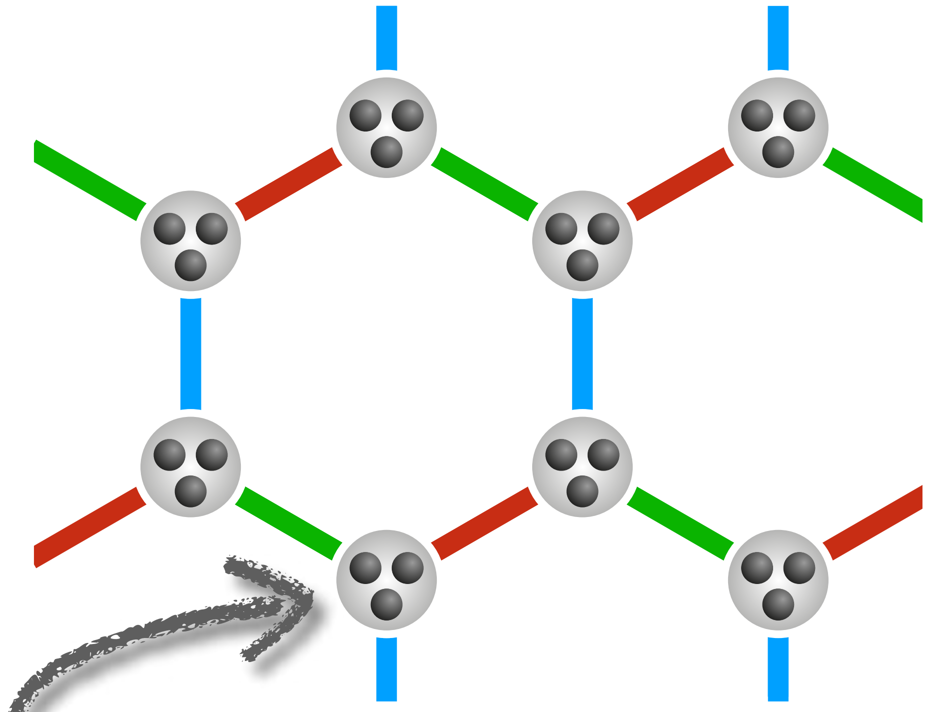
$$\mapsto \quad \hat{u}_{ij} \boldsymbol{c}_i^\top \boldsymbol{c}_j$$

Kitaev-Heisenberg spin-orbital model



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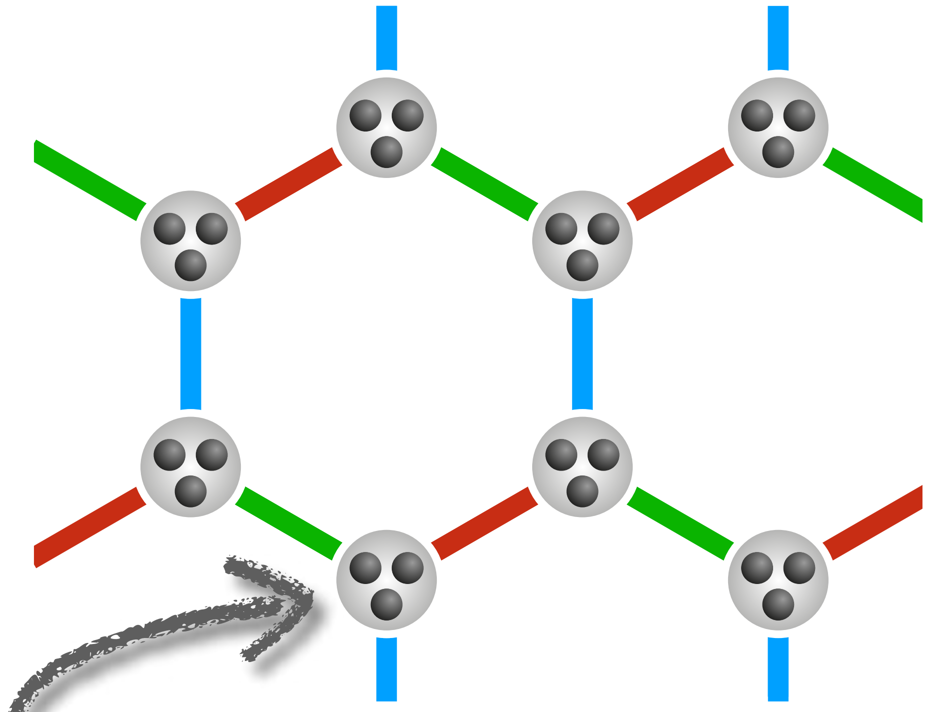
spin-1 matrices

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

Kitaev-Heisenberg spin-orbital model



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spin-1 matrices

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

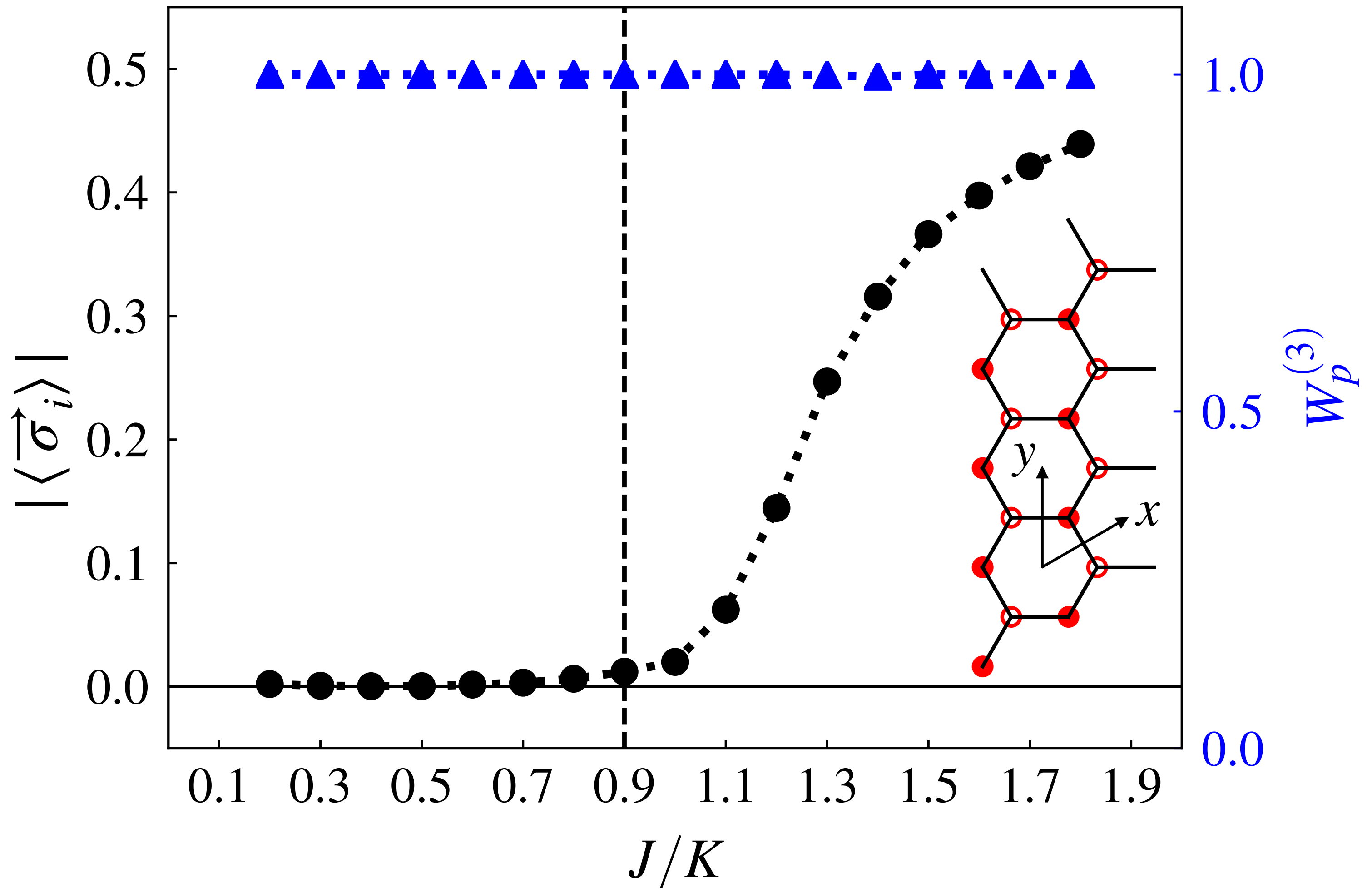
Phase diagram:

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

“spin density wave”

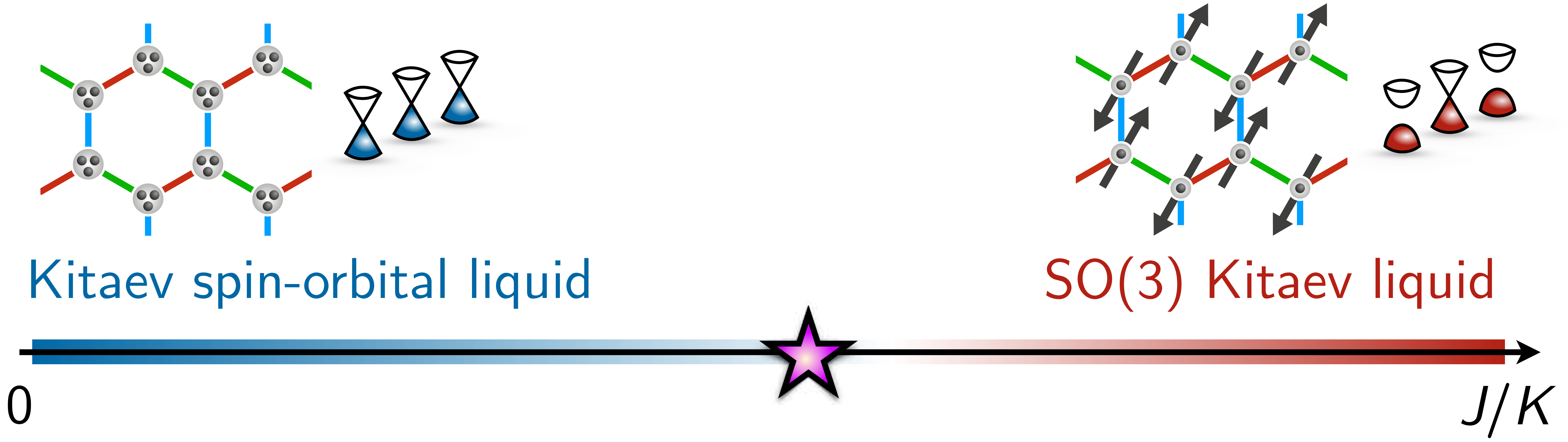
Fractionalized fermionic quantum criticality

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)”

Effective field theory

Gradient expansion:

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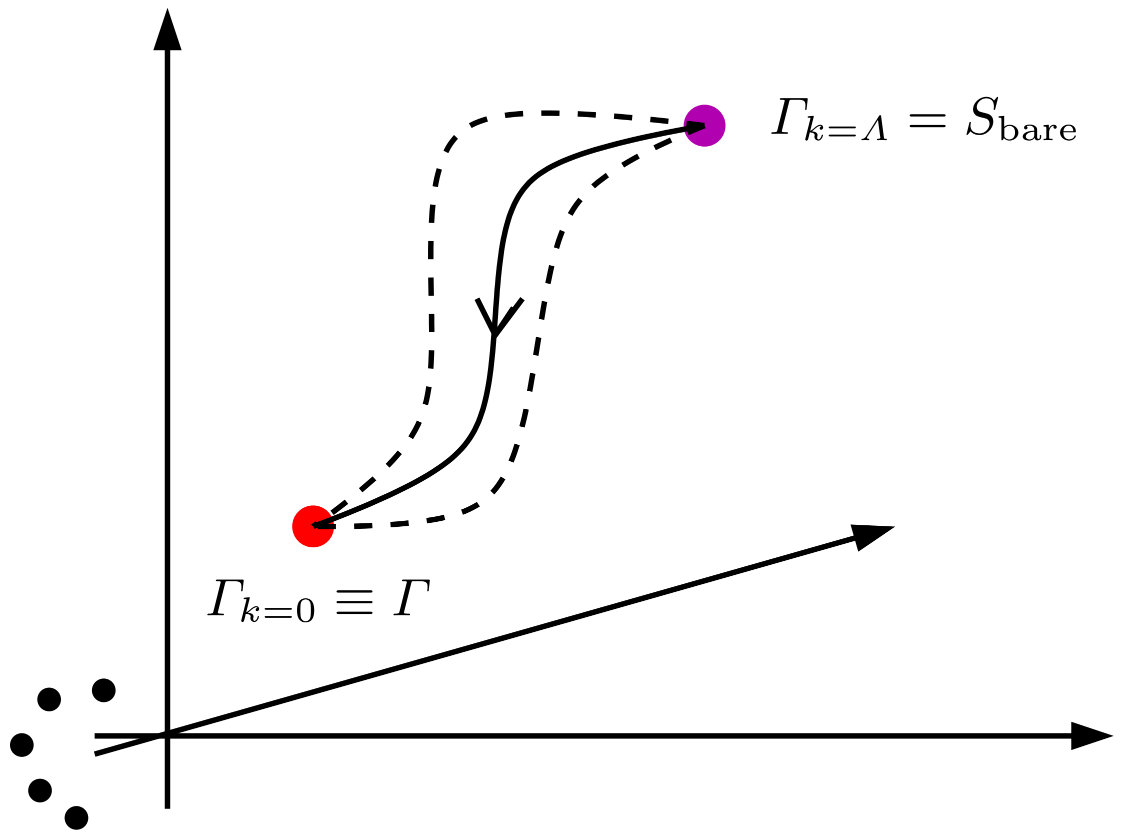
“Gross-Neveu-SO(3)”

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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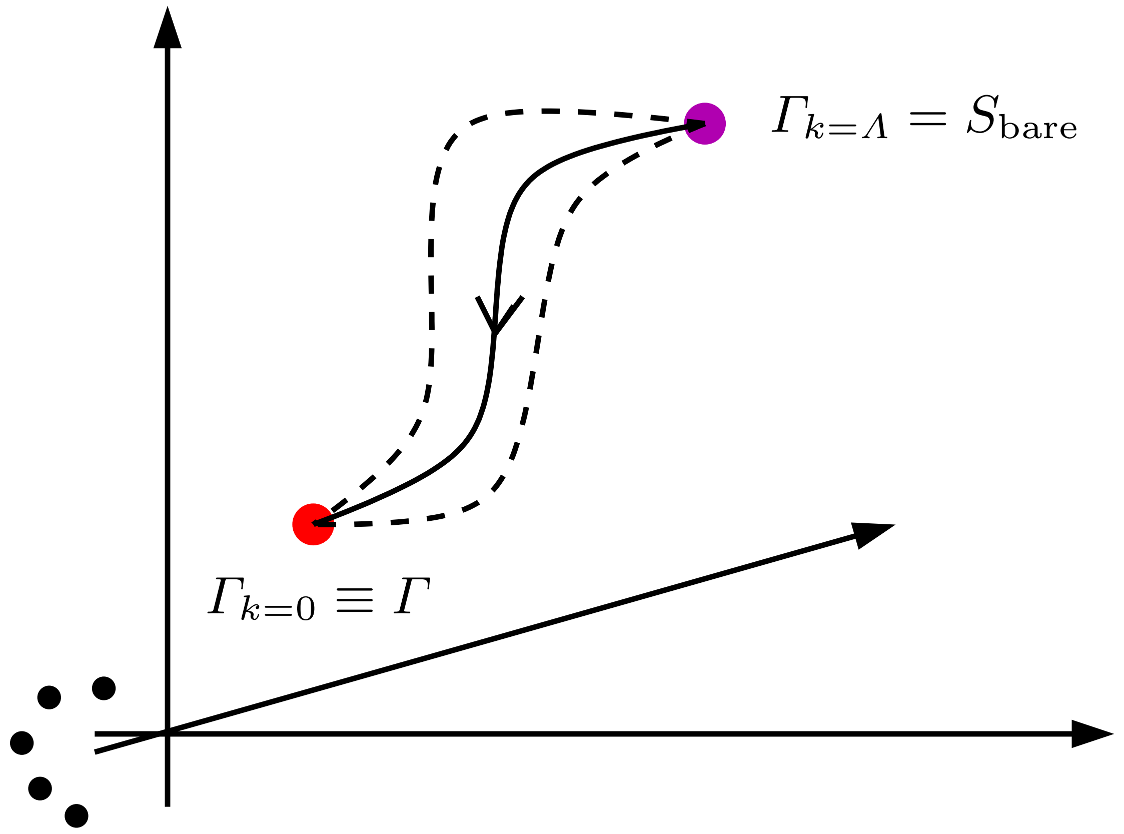


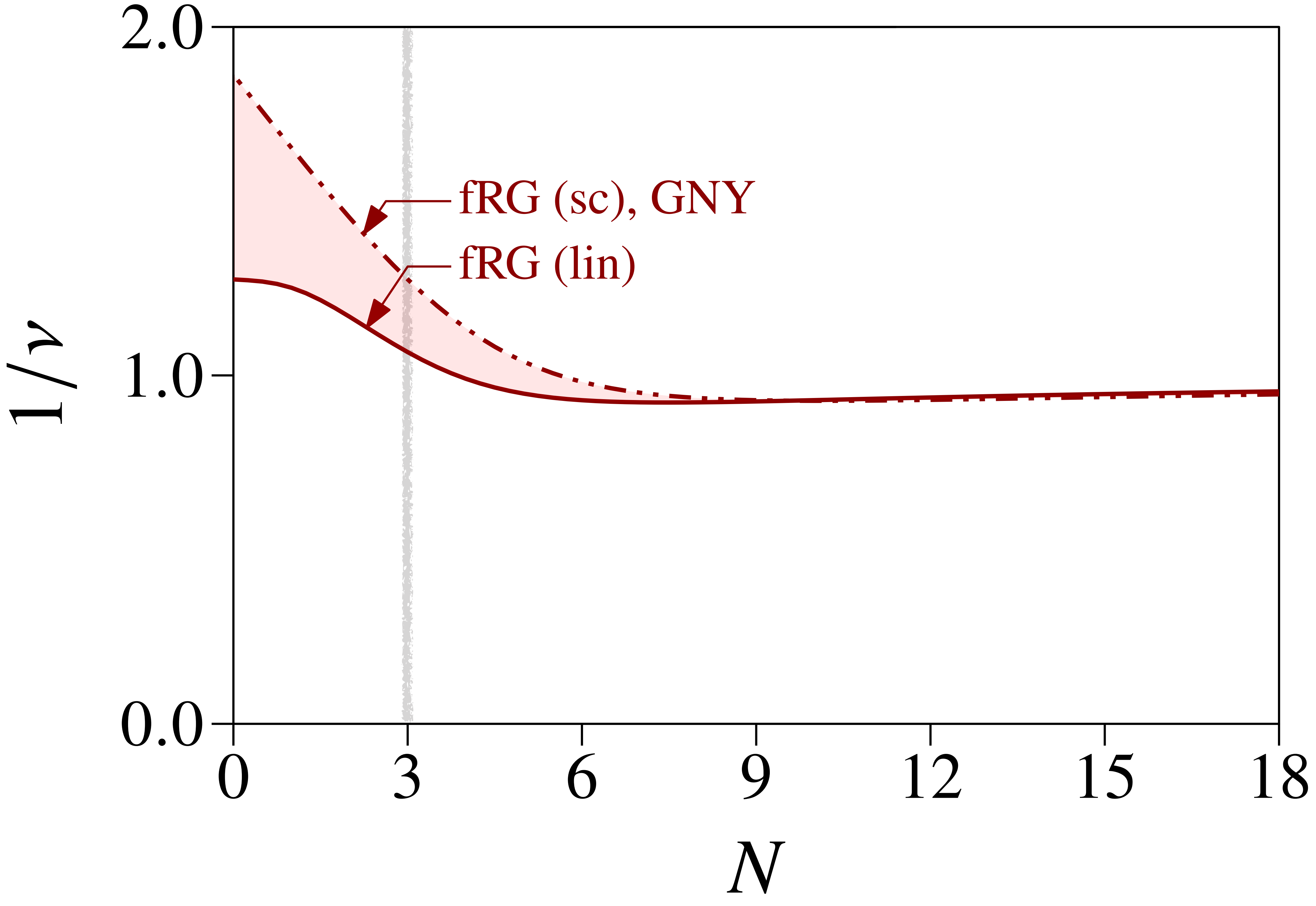
[Gies, Lect. Notes Phys. '12]

Effective action (LPA'):

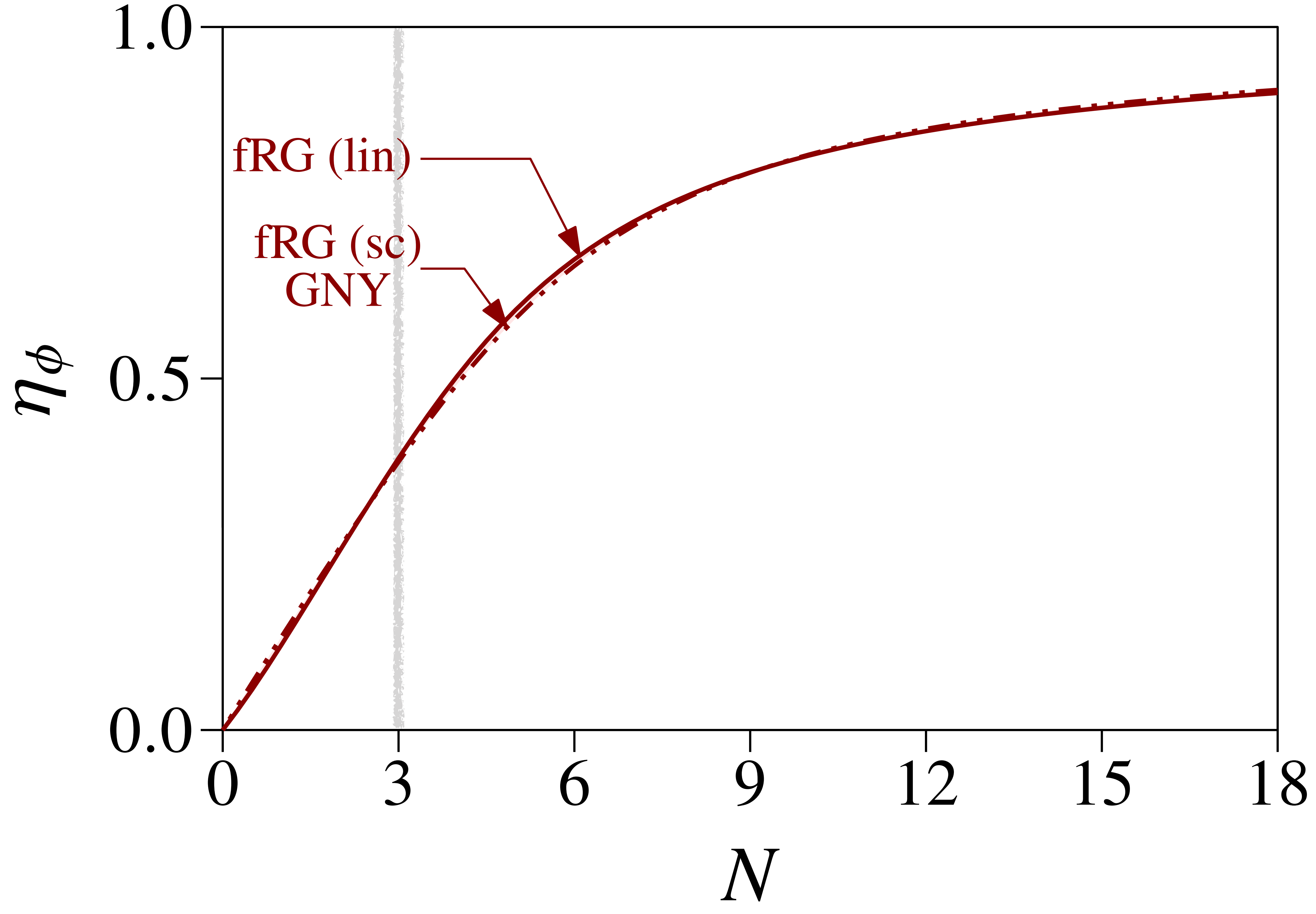
$$\Gamma_k = \int d^{2+1}x\left[Z_{\psi,k}\bar{\psi}\gamma^\mu\partial_\mu\psi + \frac{1}{2}Z_{\varphi,k}(\partial_\mu\vec{\varphi})^2 - g_k\vec{\varphi}\cdot\bar{\psi}\vec{L}\psi + U_k(\varrho)\right]$$

Fractionalized Gross-Neveu-SO(3) criticality

Correlation length exponent:



Anomalous dimension:



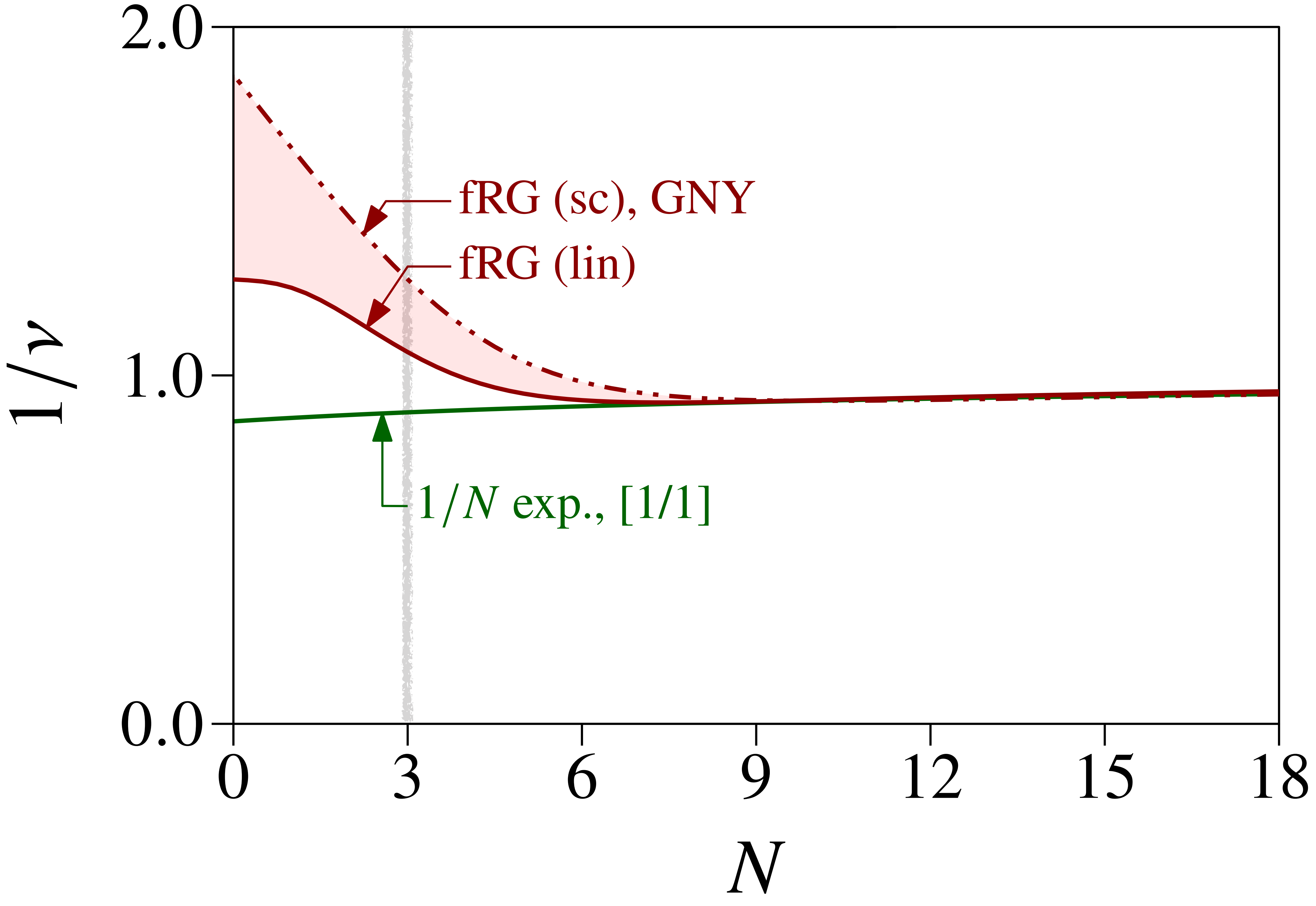
Levels of approximation:

- Functional RG @ LPA’

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

Fractionalized Gross-Neveu-SO(3) criticality

Correlation length exponent:



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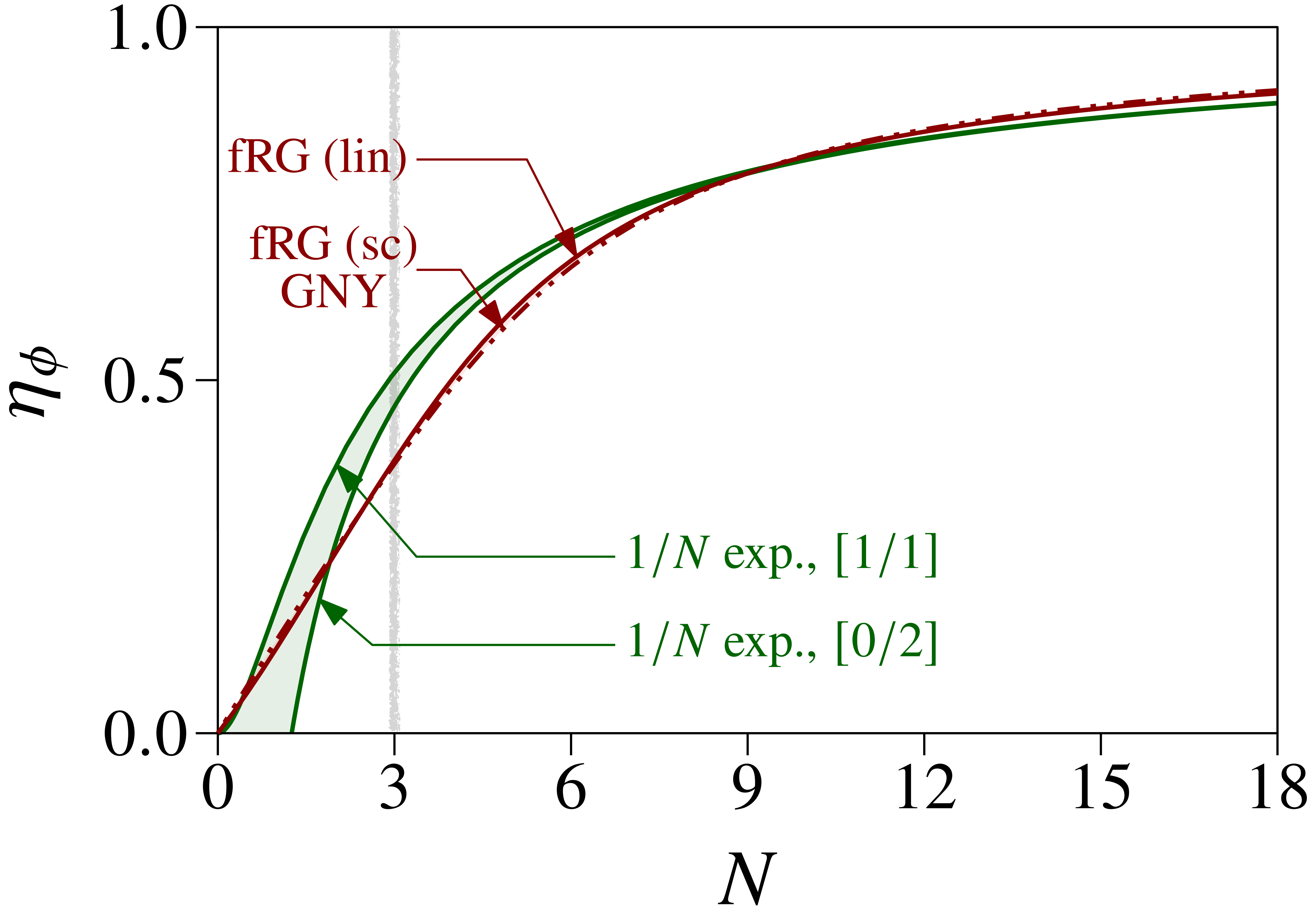

Levels of approximation:

- Functional RG @ LPA'
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Fractionalized Gross-Neveu-SO(3) criticality

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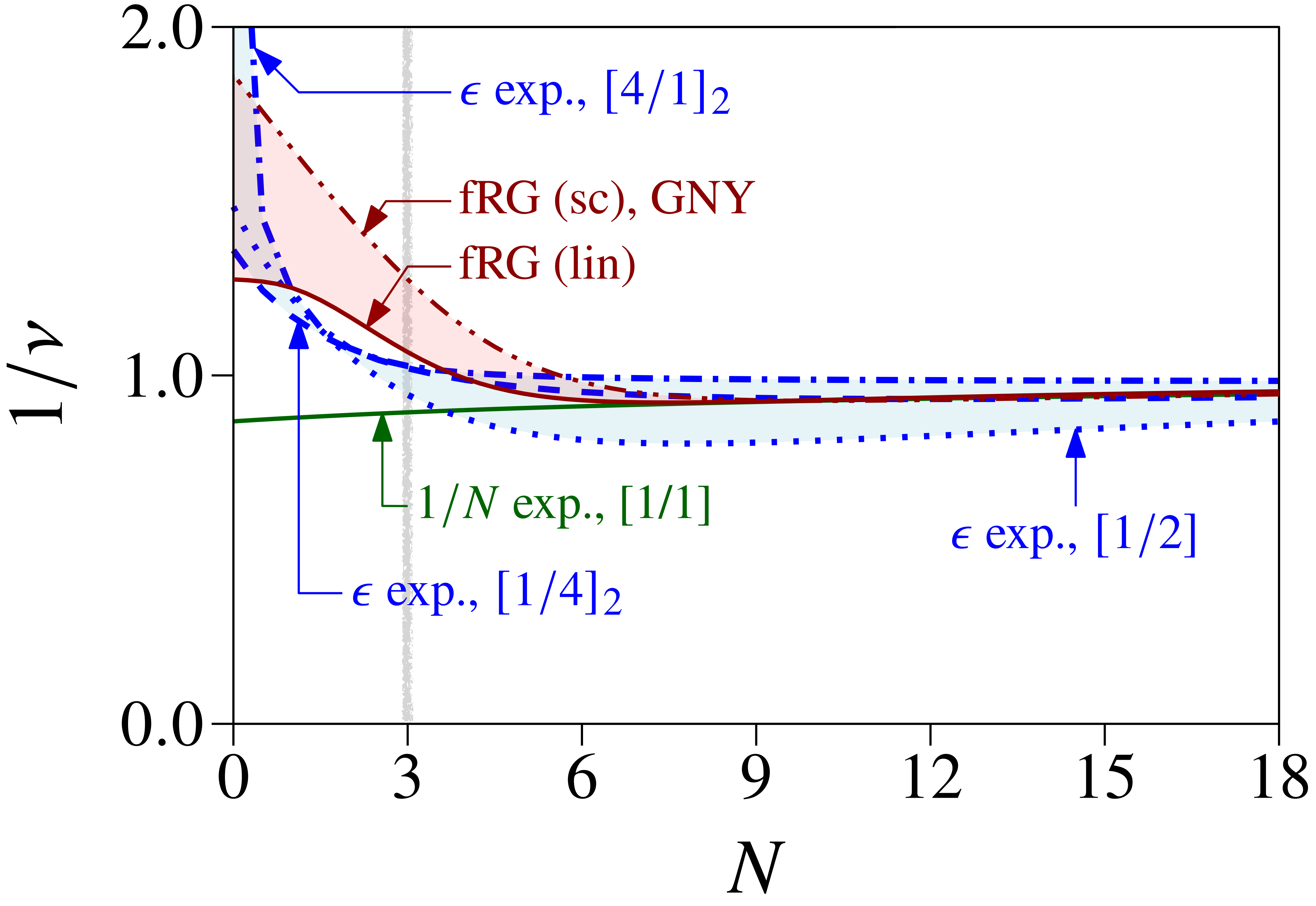

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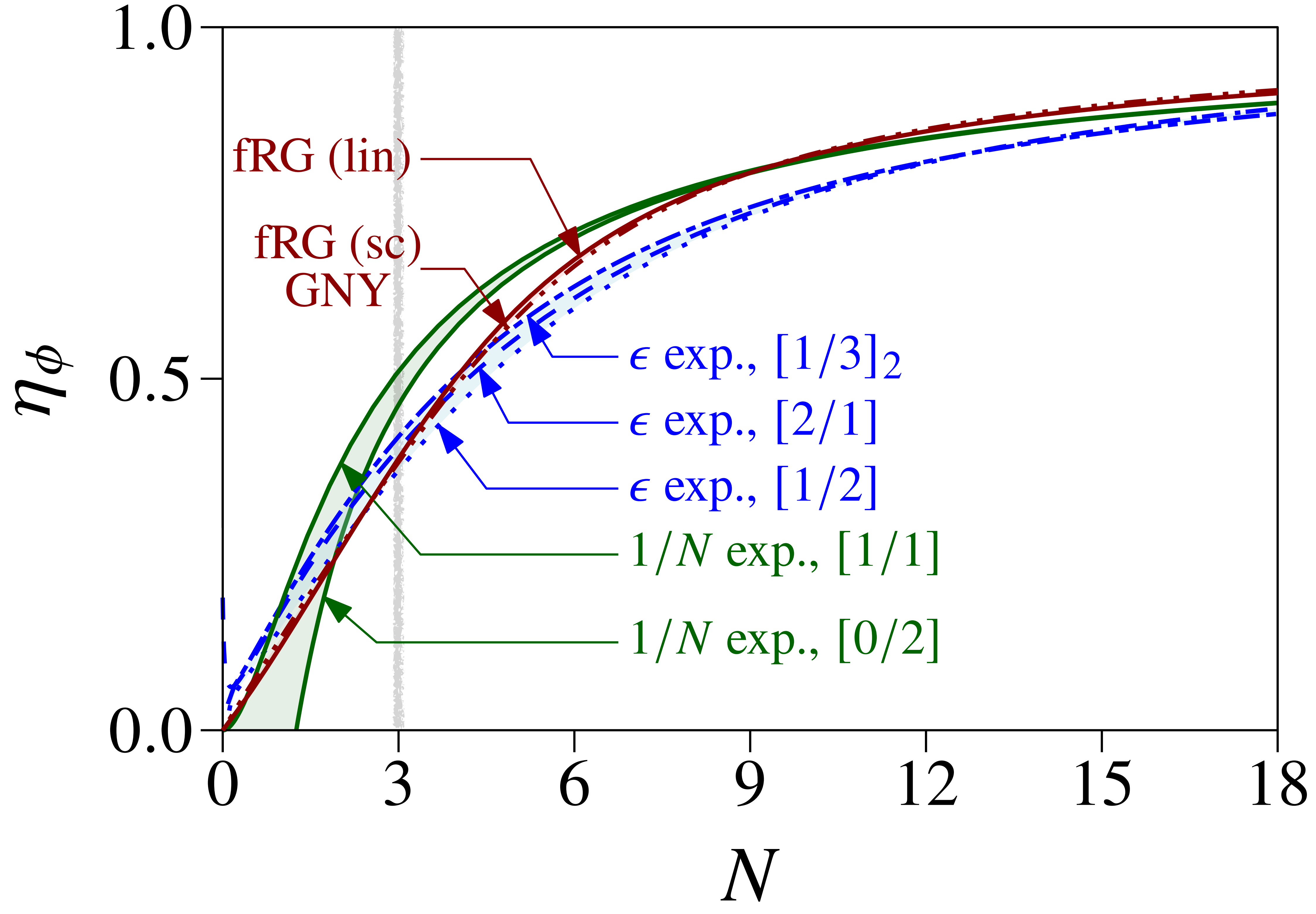

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- Functional RG @ LPA’
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- 4 - ε expansion @ 3 loop

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

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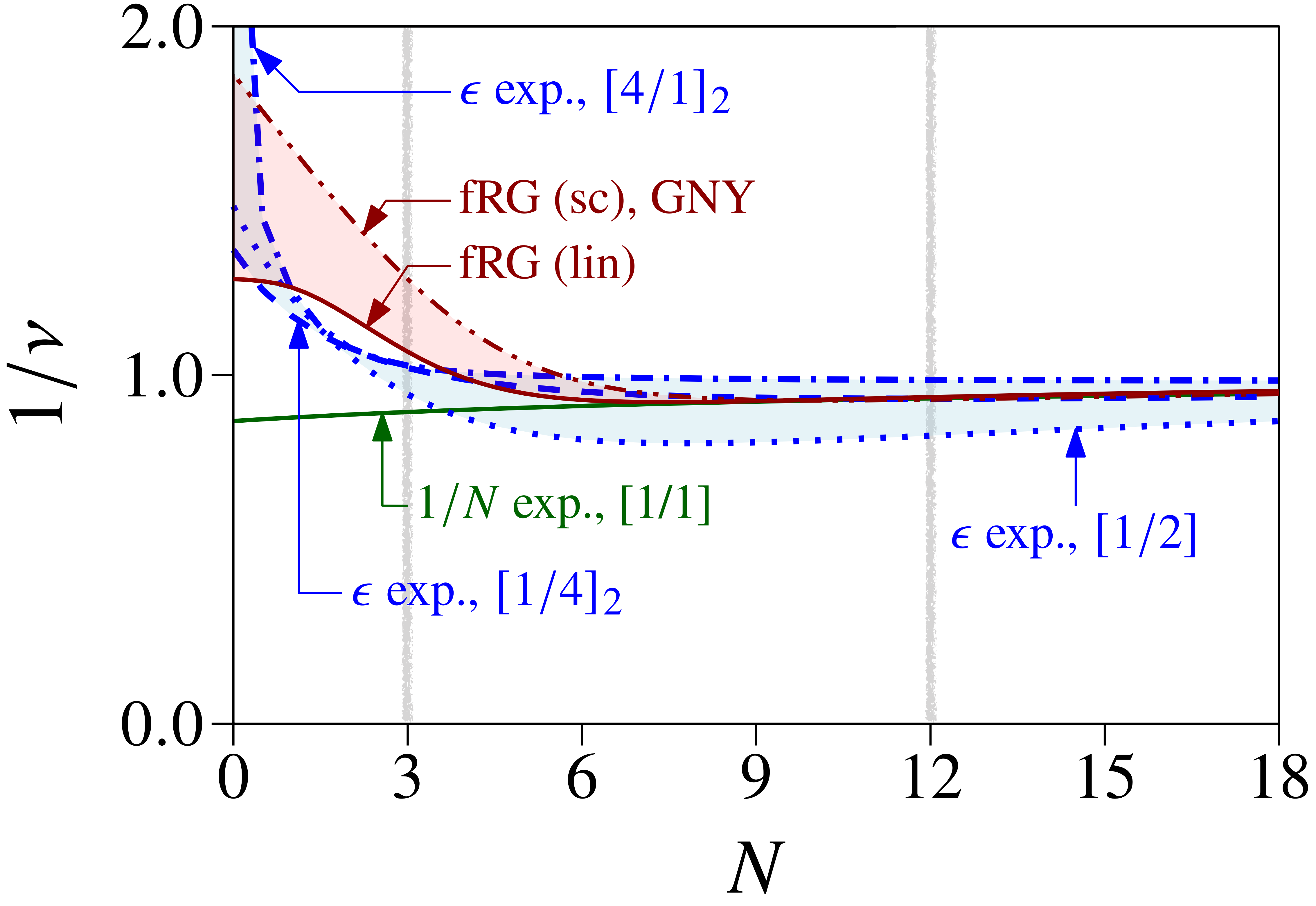

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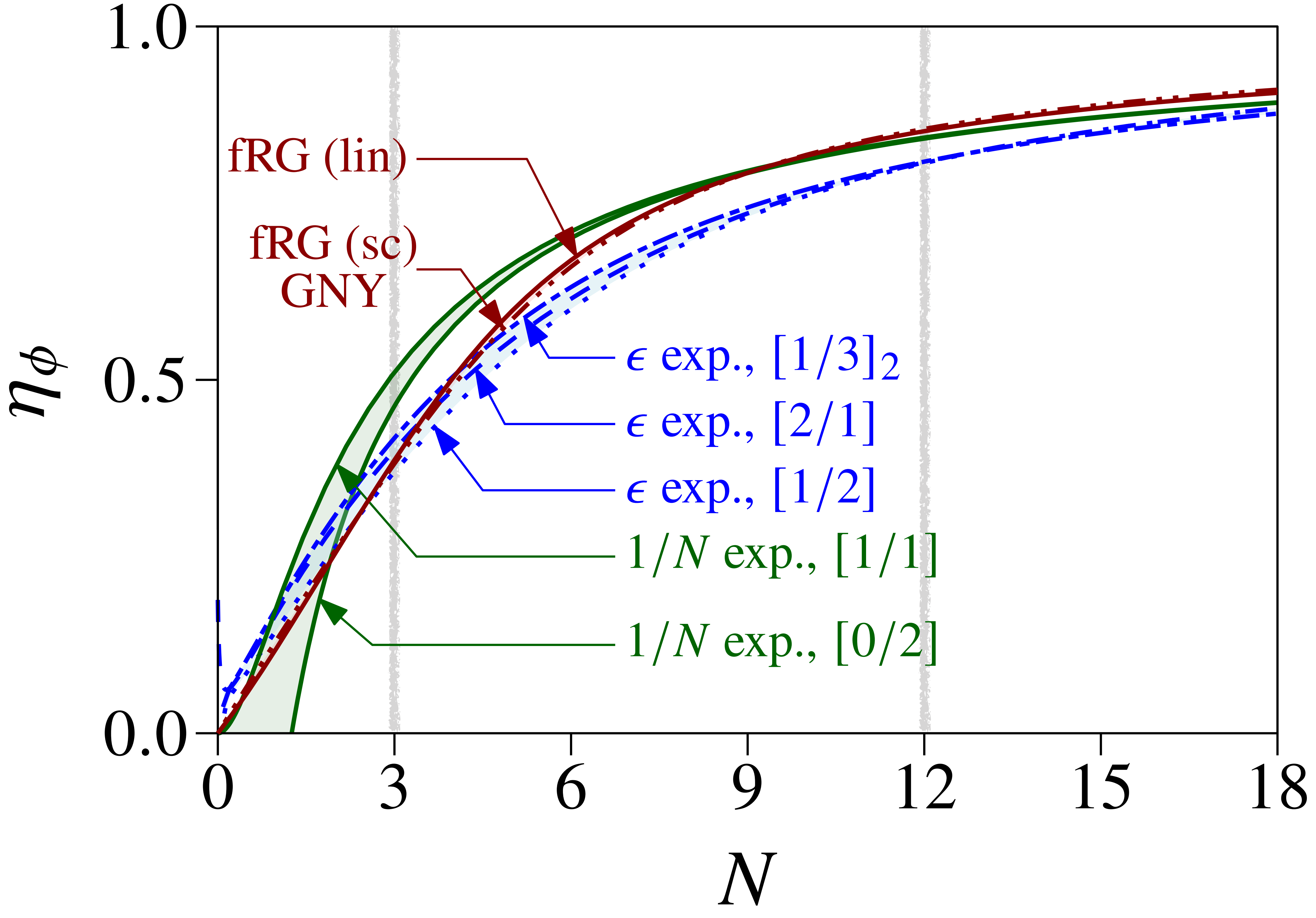

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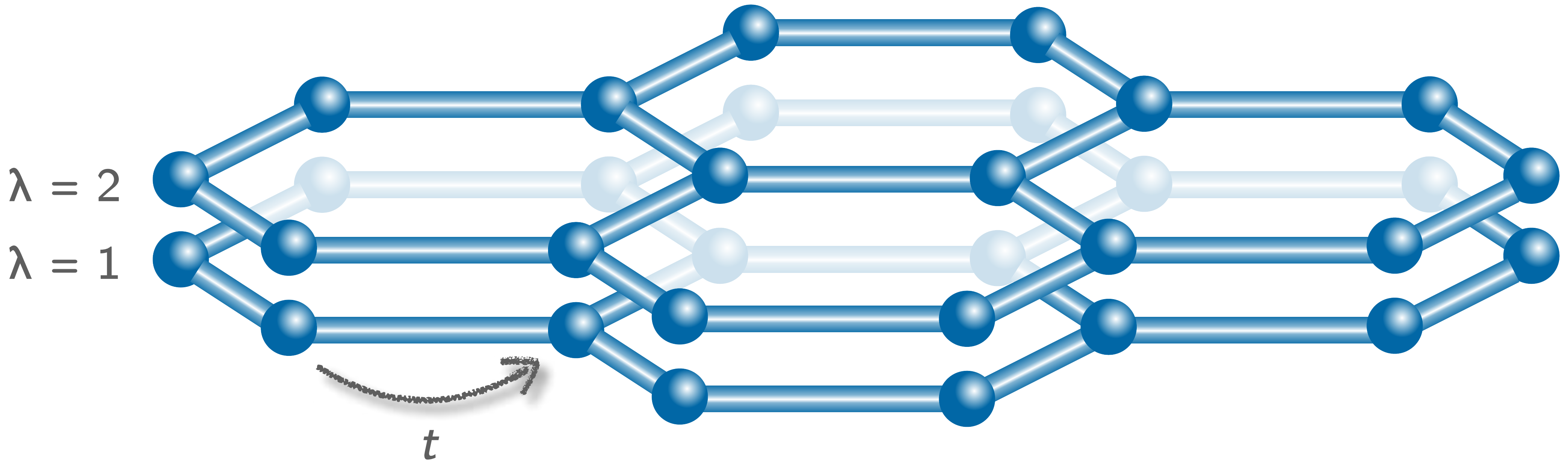
[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB ’21]

Sign-problem-free bilayer model

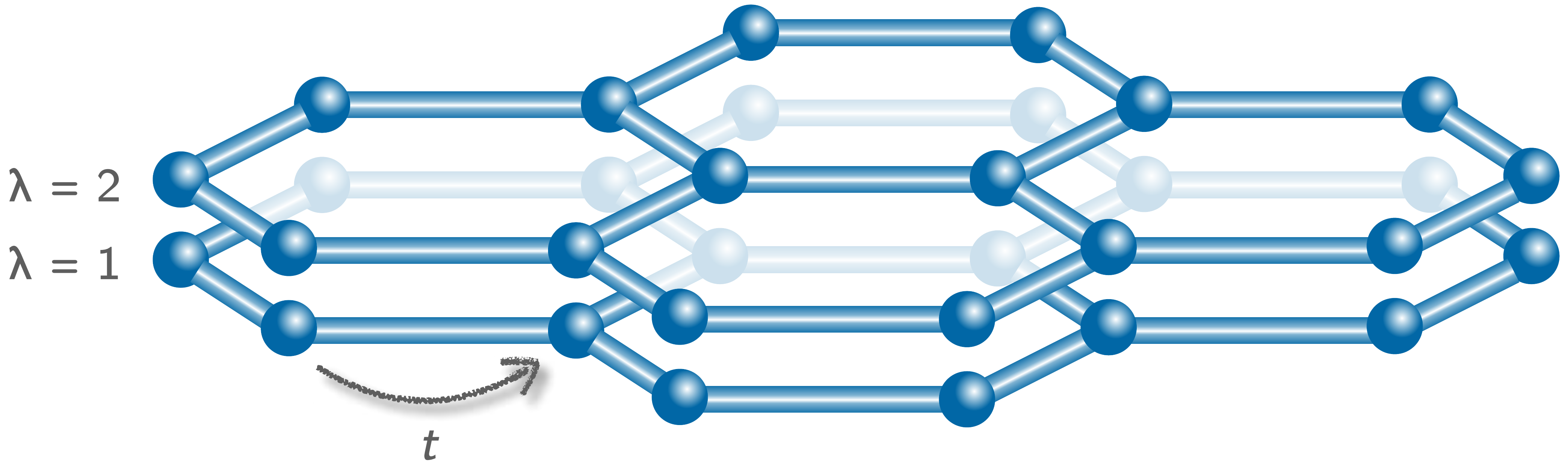
Hamiltonian:

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



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

Sign-problem-free bilayer model



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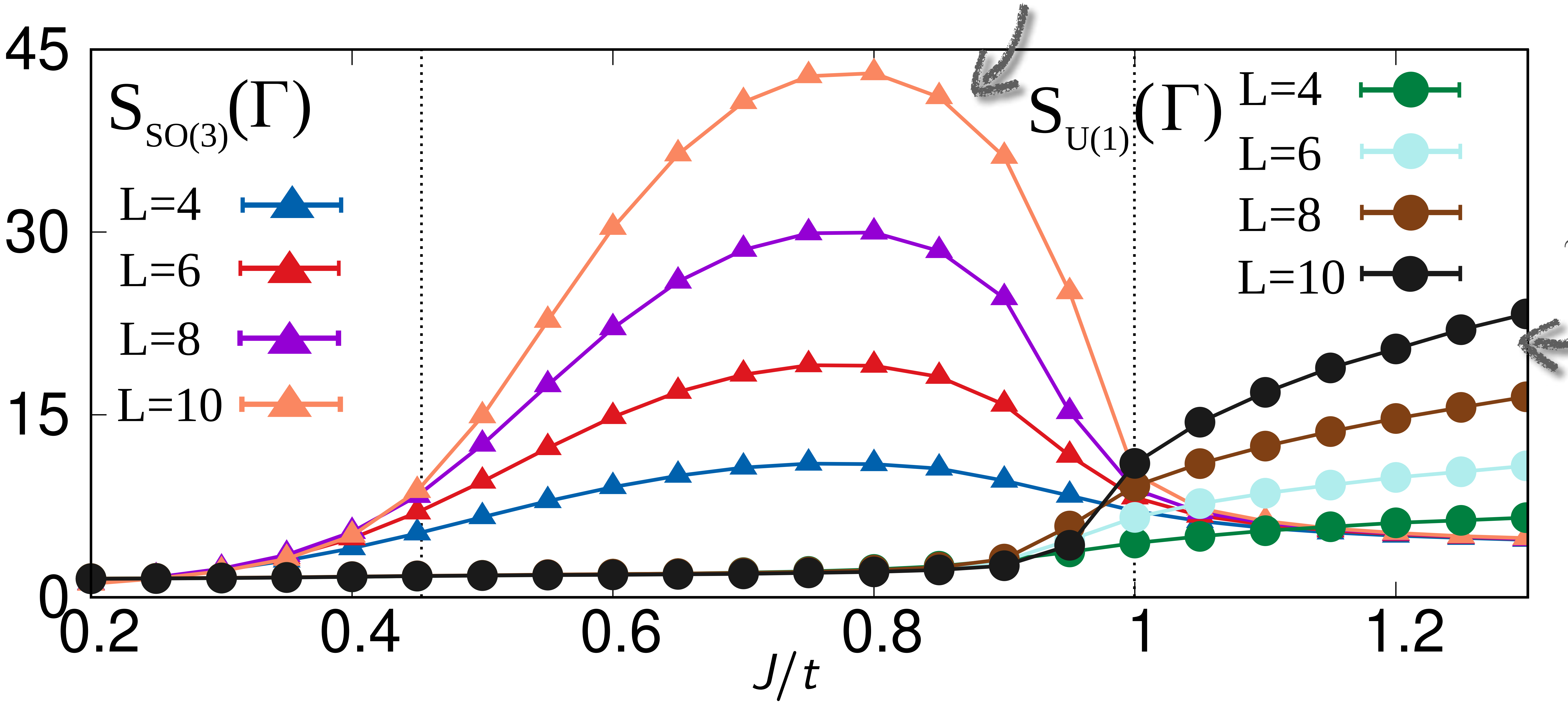
QMC structure factors:

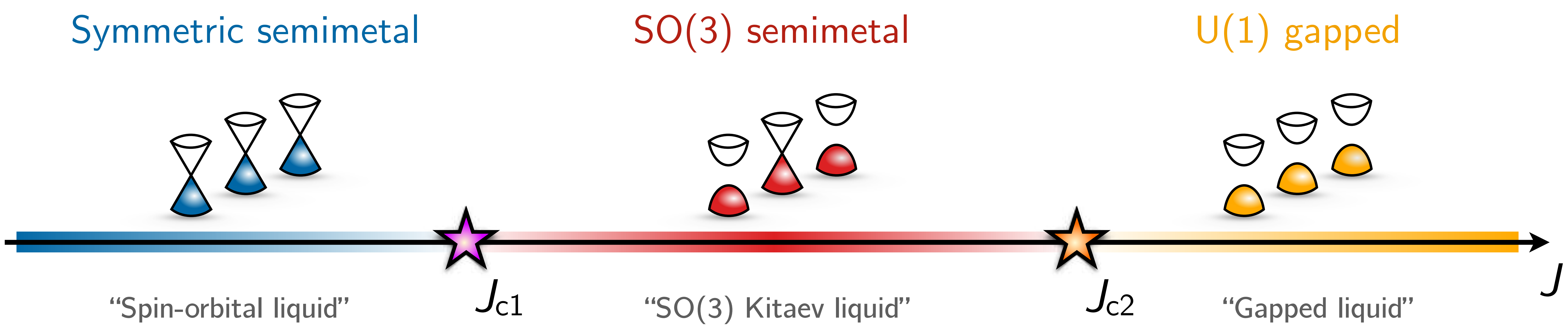
$\sim \langle c^\dagger \vec{L} c \rangle$ "SO(3) semimetal"

$\sim \langle c_1^\dagger c_2 \rangle$ "interlayer coherence"



Sign-problem-free bilayer model

Phase diagram:



Symmetric semimetal

SO(3) semimetal

U(1) gapped

“Spin-orbital liquid”

J_{c1}

“SO(3) Kitaev liquid”

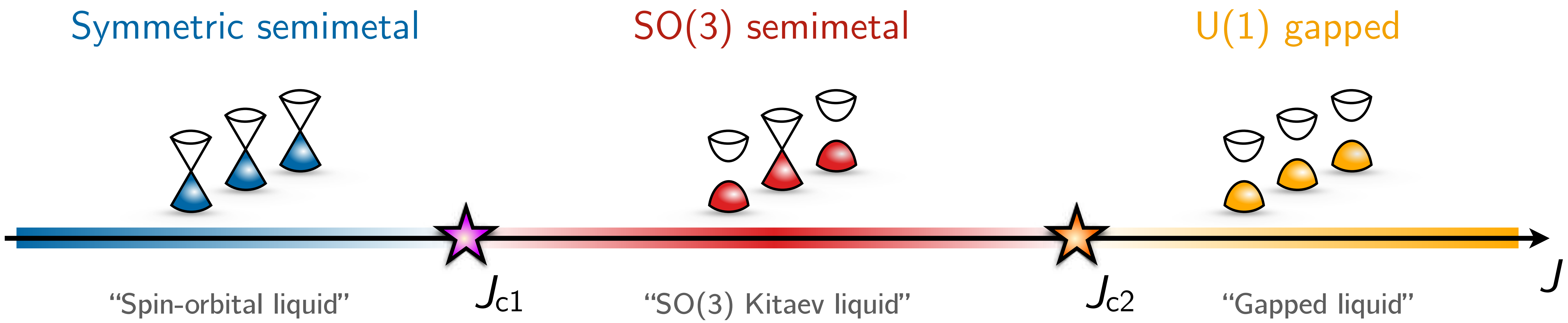
J_{c2}

“Gapped liquid”

J

Sign-problem-free bilayer model

Phase diagram:



Symmetric semimetal

SO(3) semimetal

U(1) gapped

“Spin-orbital liquid”

J_{c1}

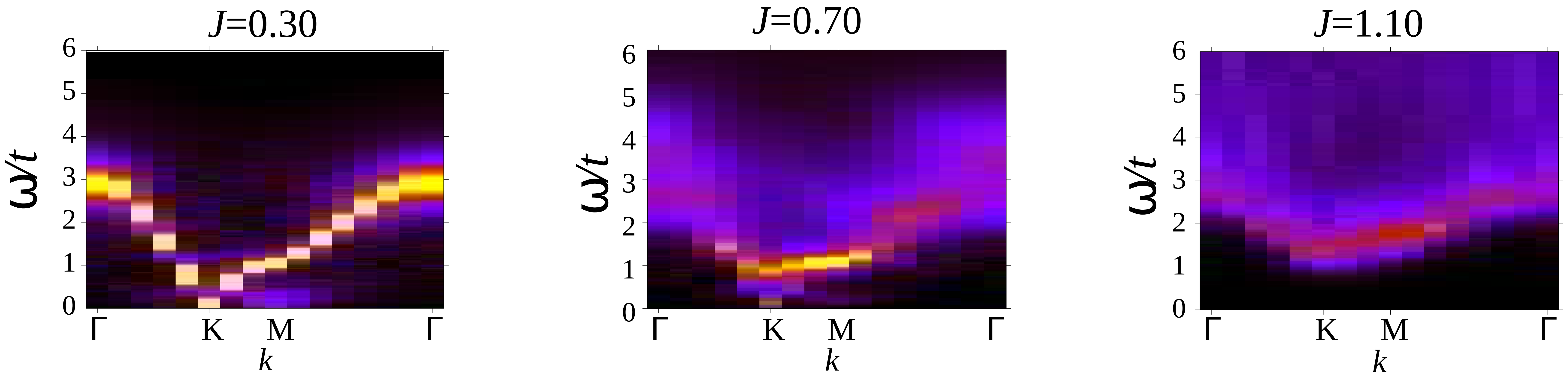
“SO(3) Kitaev liquid”

J_{c2}

“Gapped liquid”

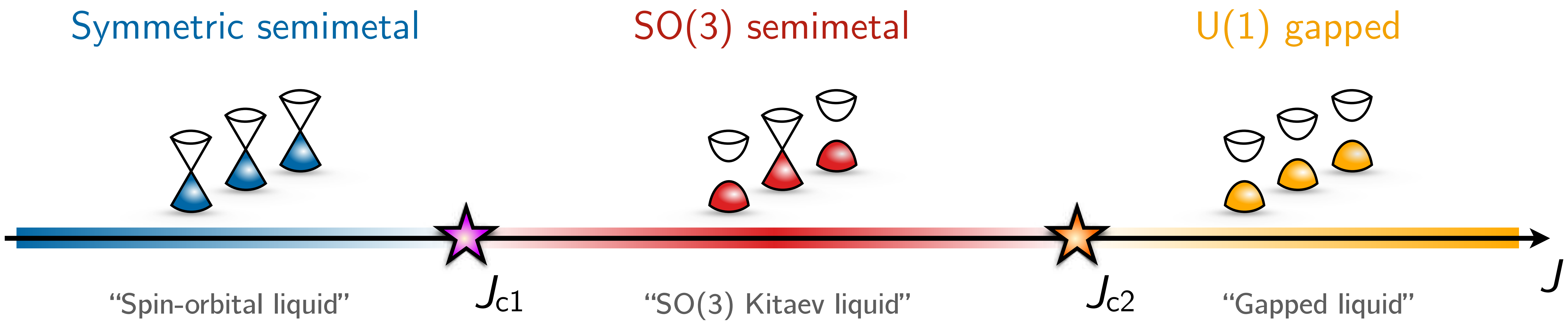
J

Fermion spectral function:



Sign-problem-free bilayer model

Phase diagram:



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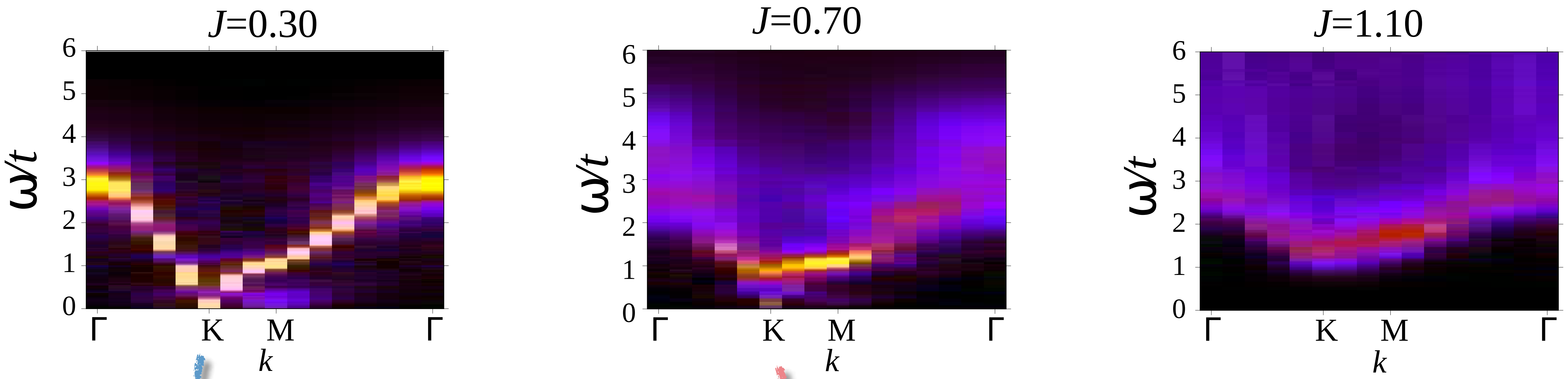
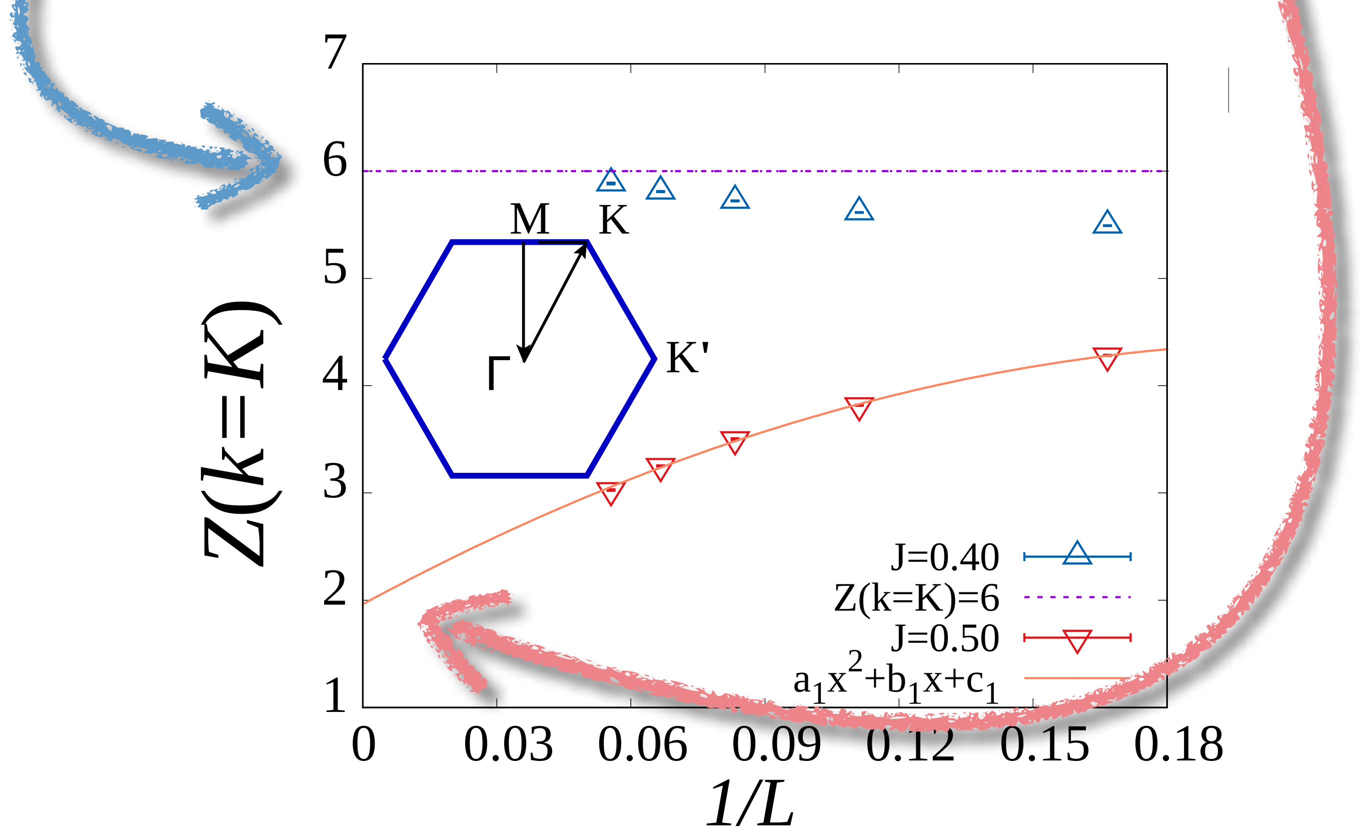
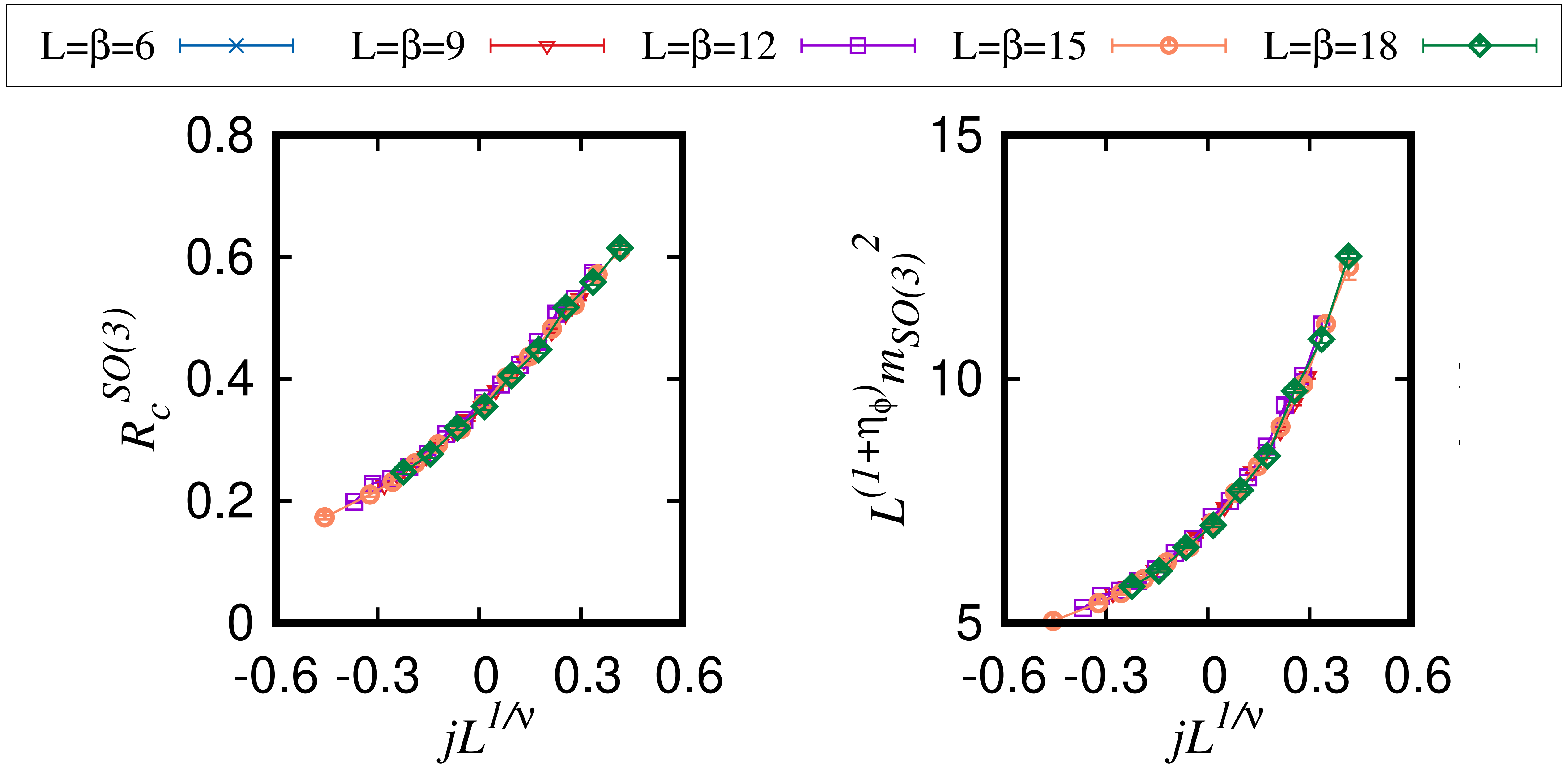


Quasiparticle weight:



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

Scaling collapse:



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

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

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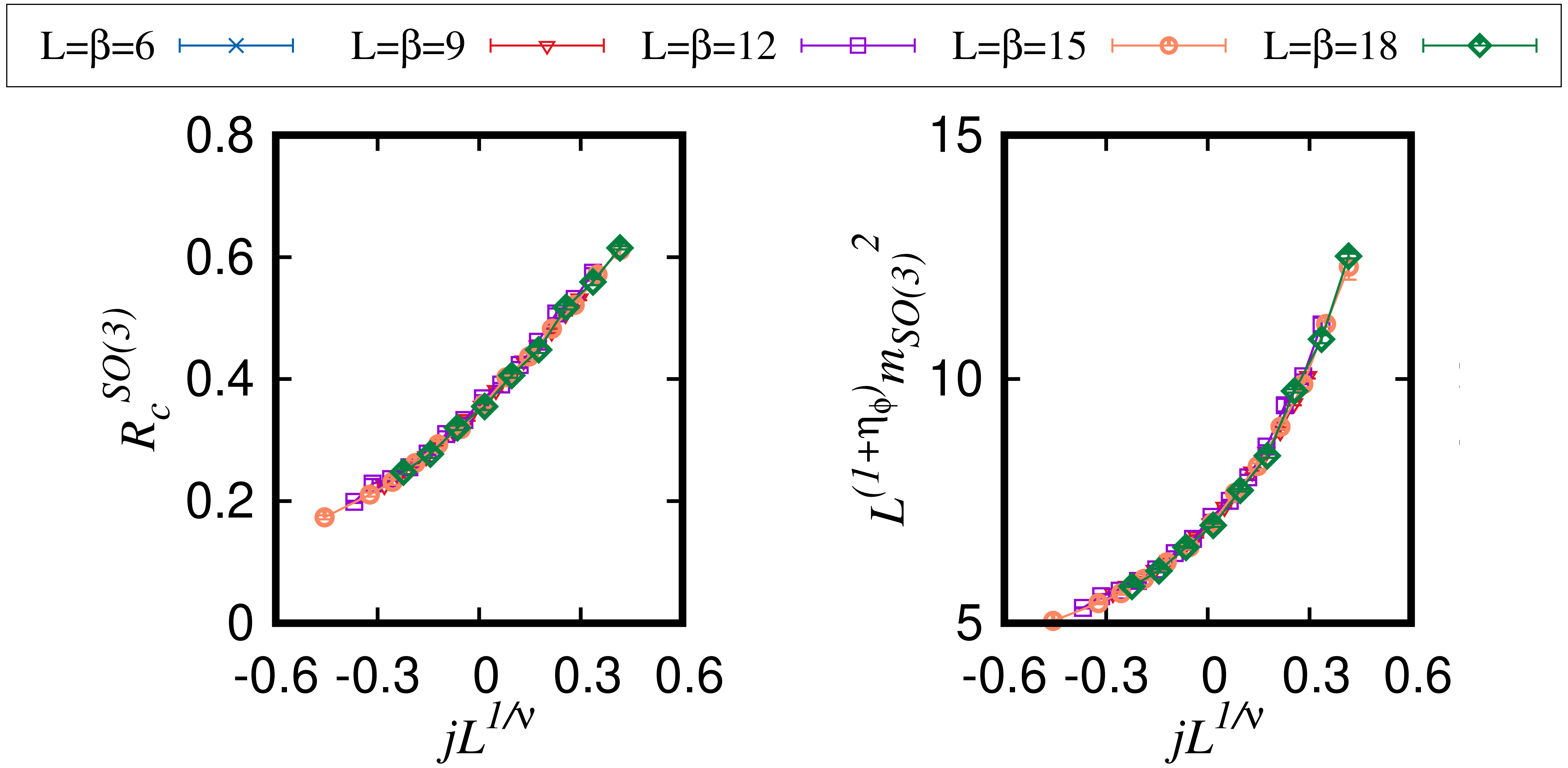
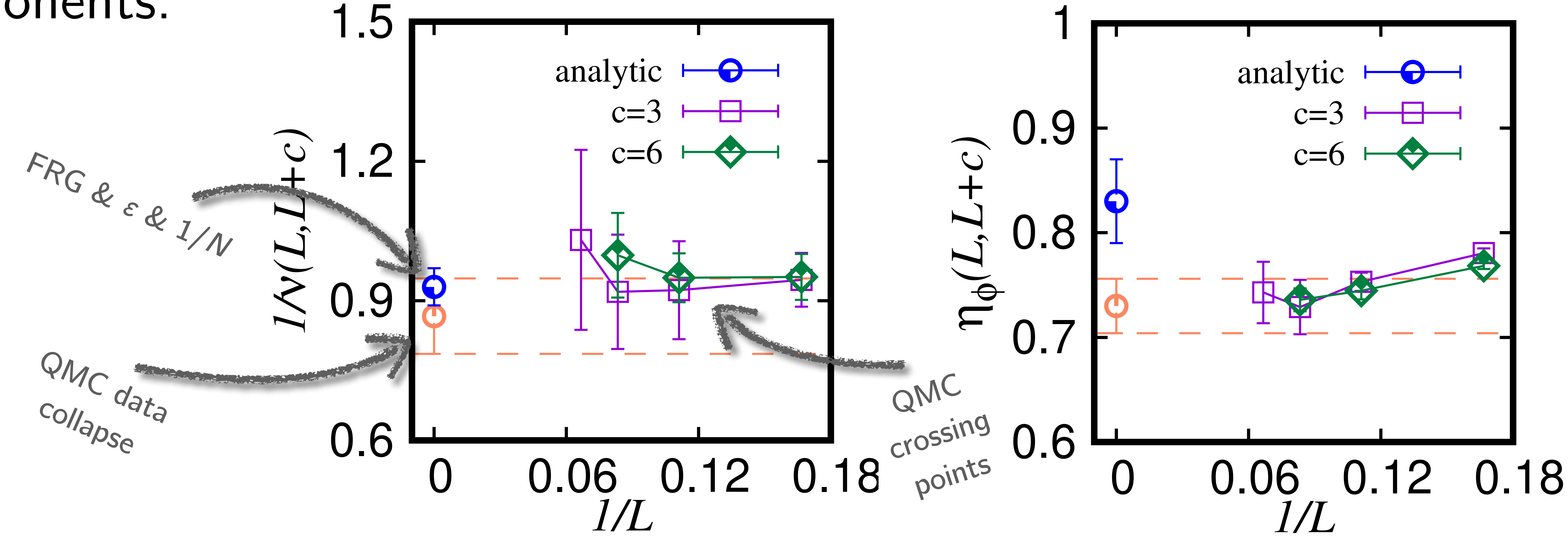


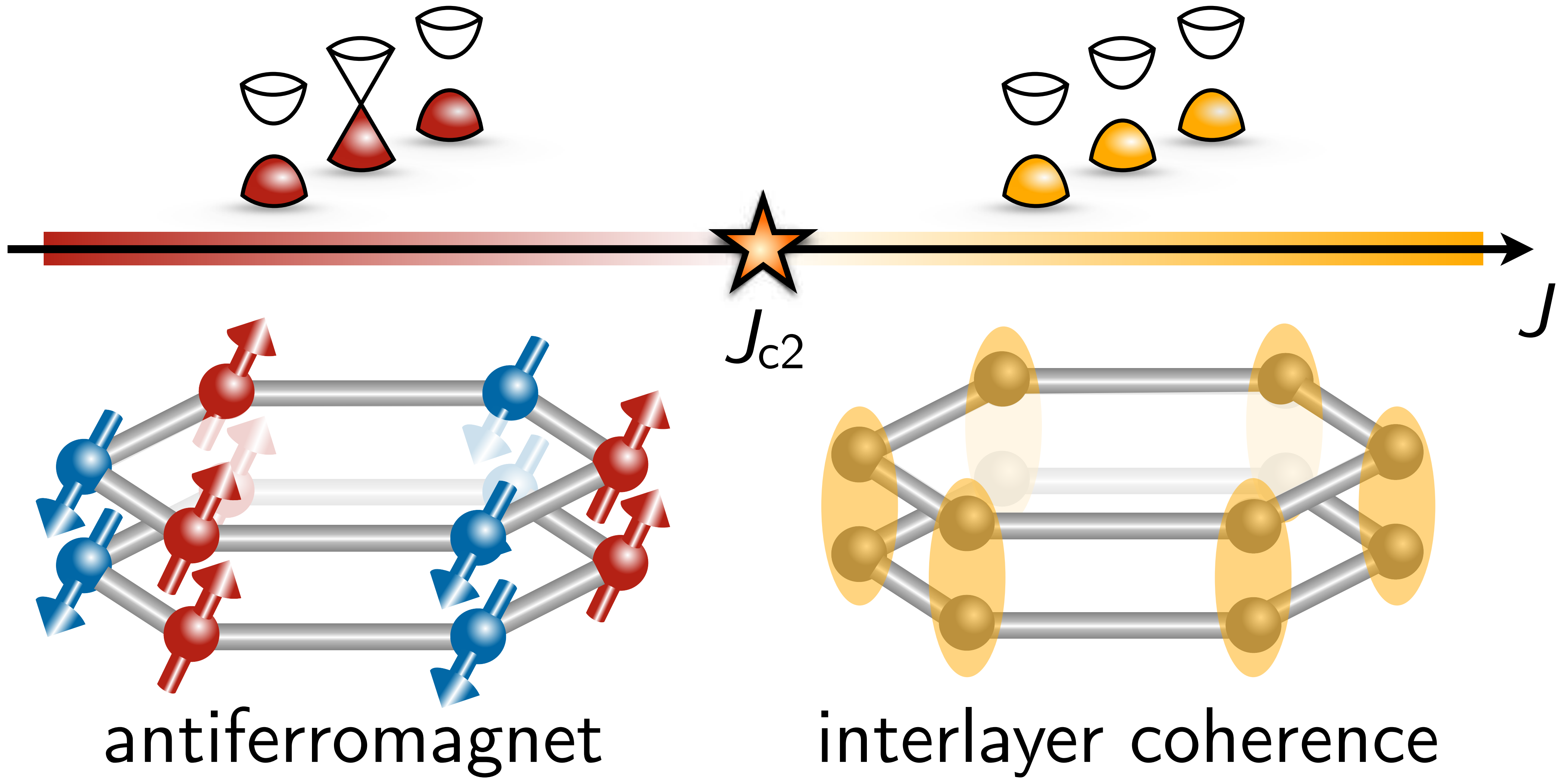
Critical exponents:



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

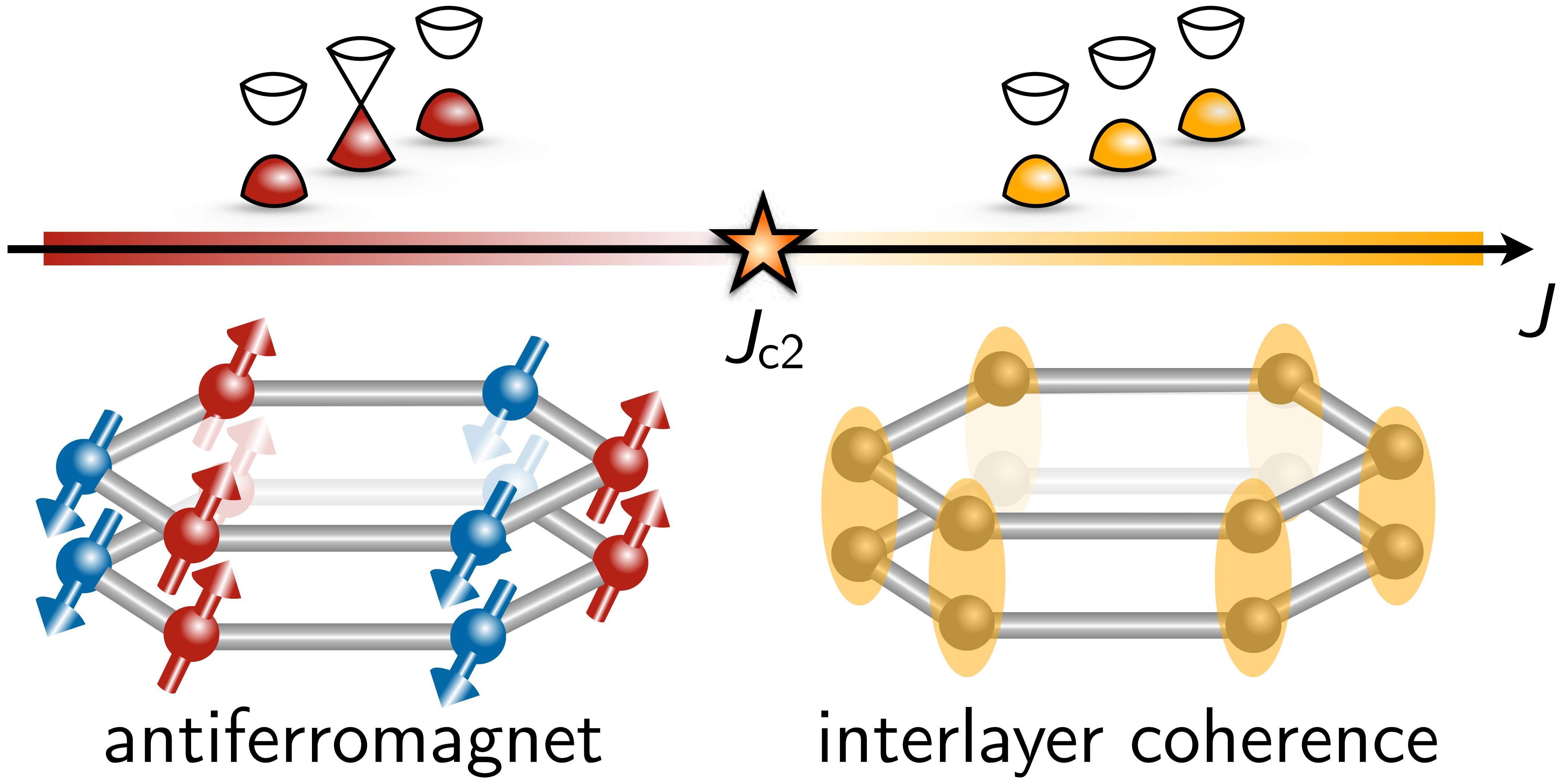
SO(3)-U(1) transition at J_{c2}

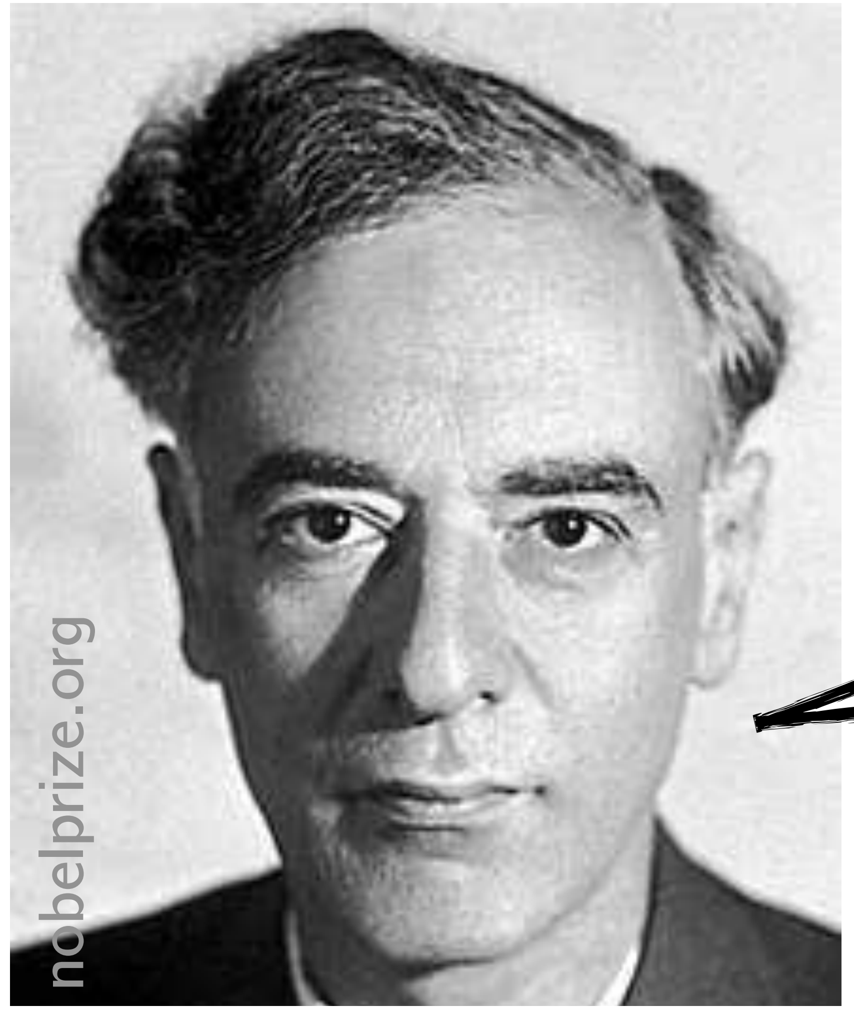
Competing orders:



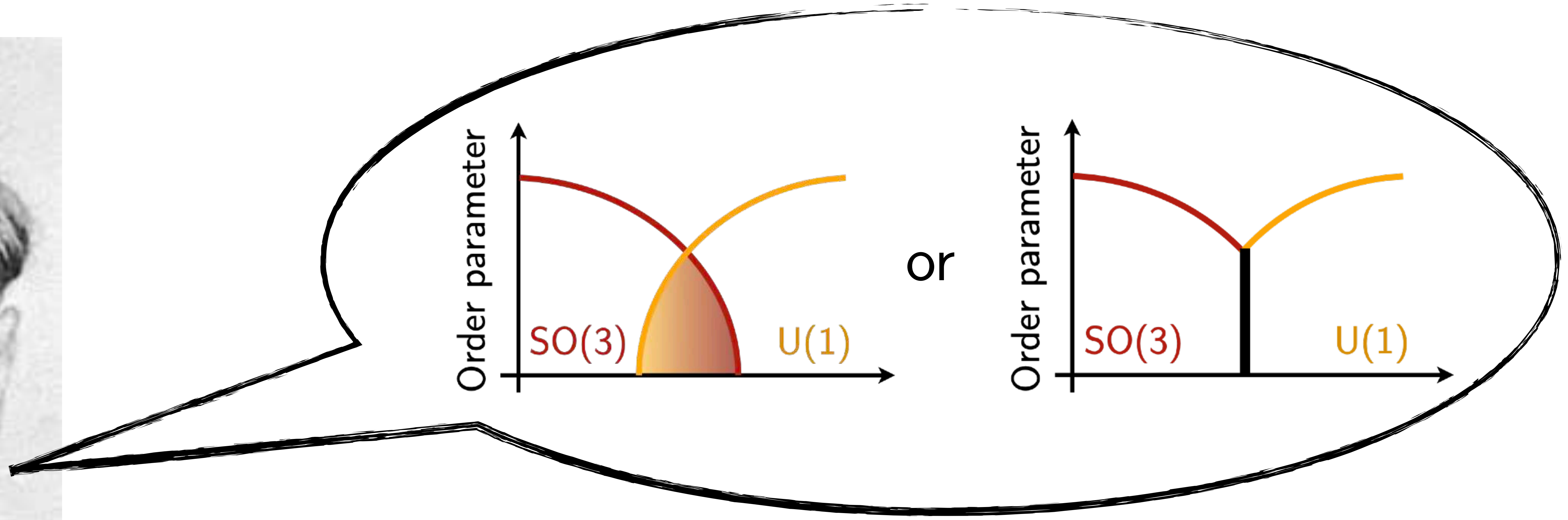
SO(3)-U(1) transition at J_{c2}

Competing orders:



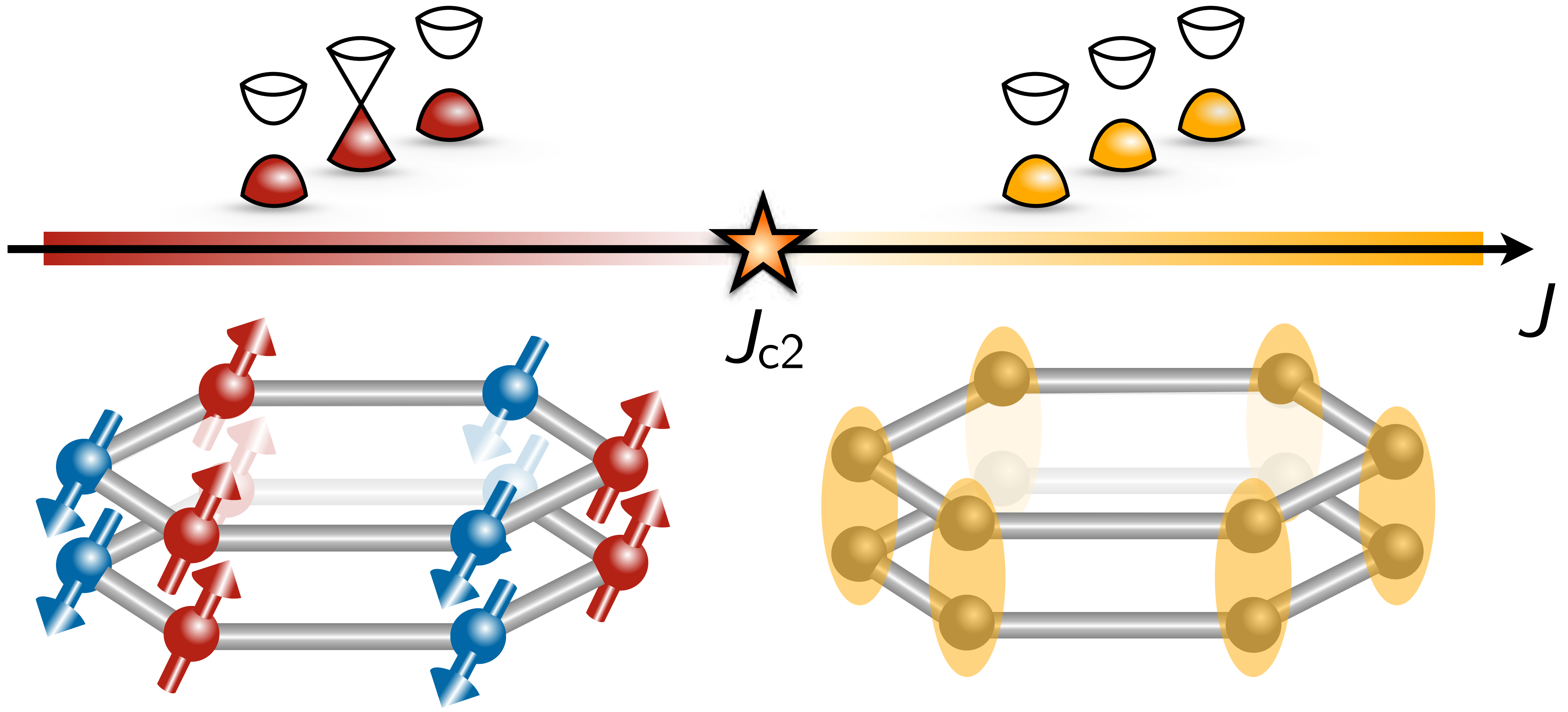


Landau

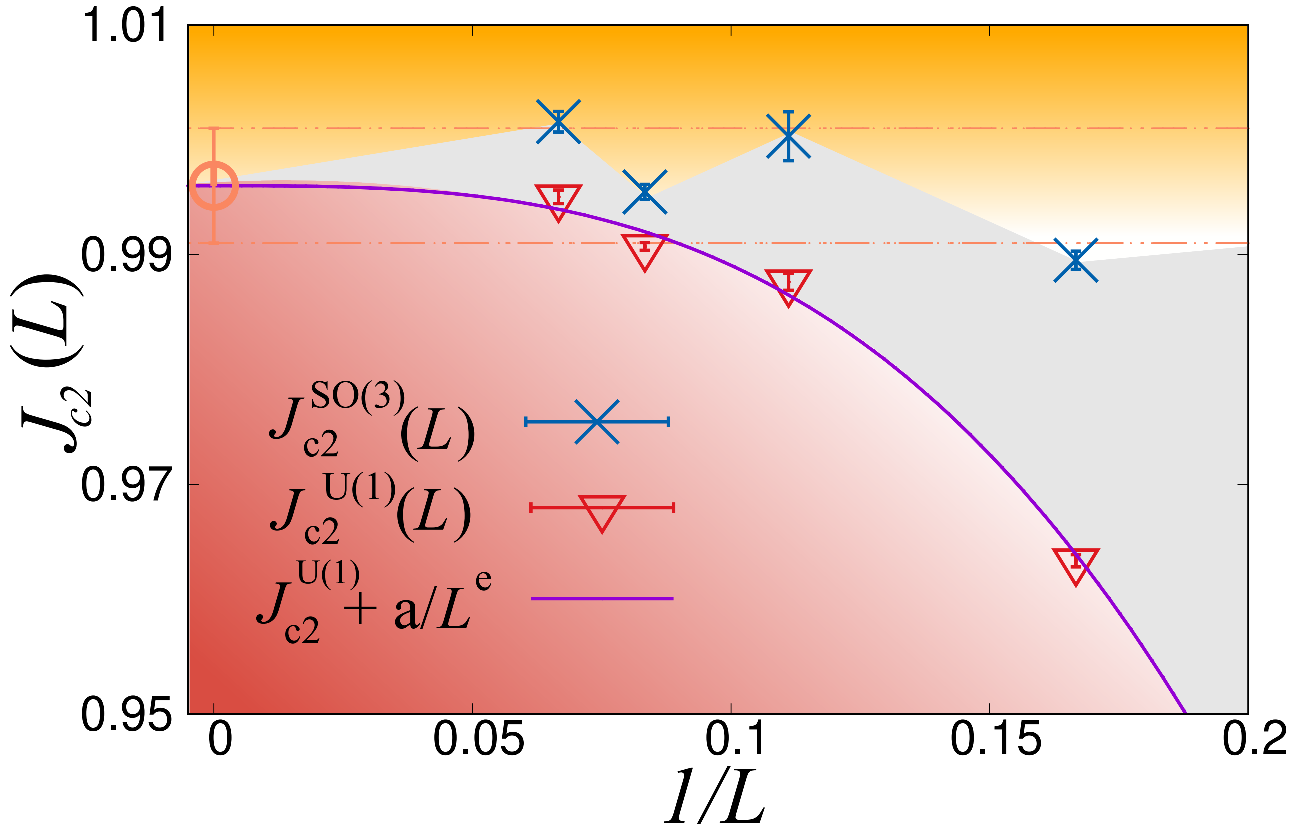


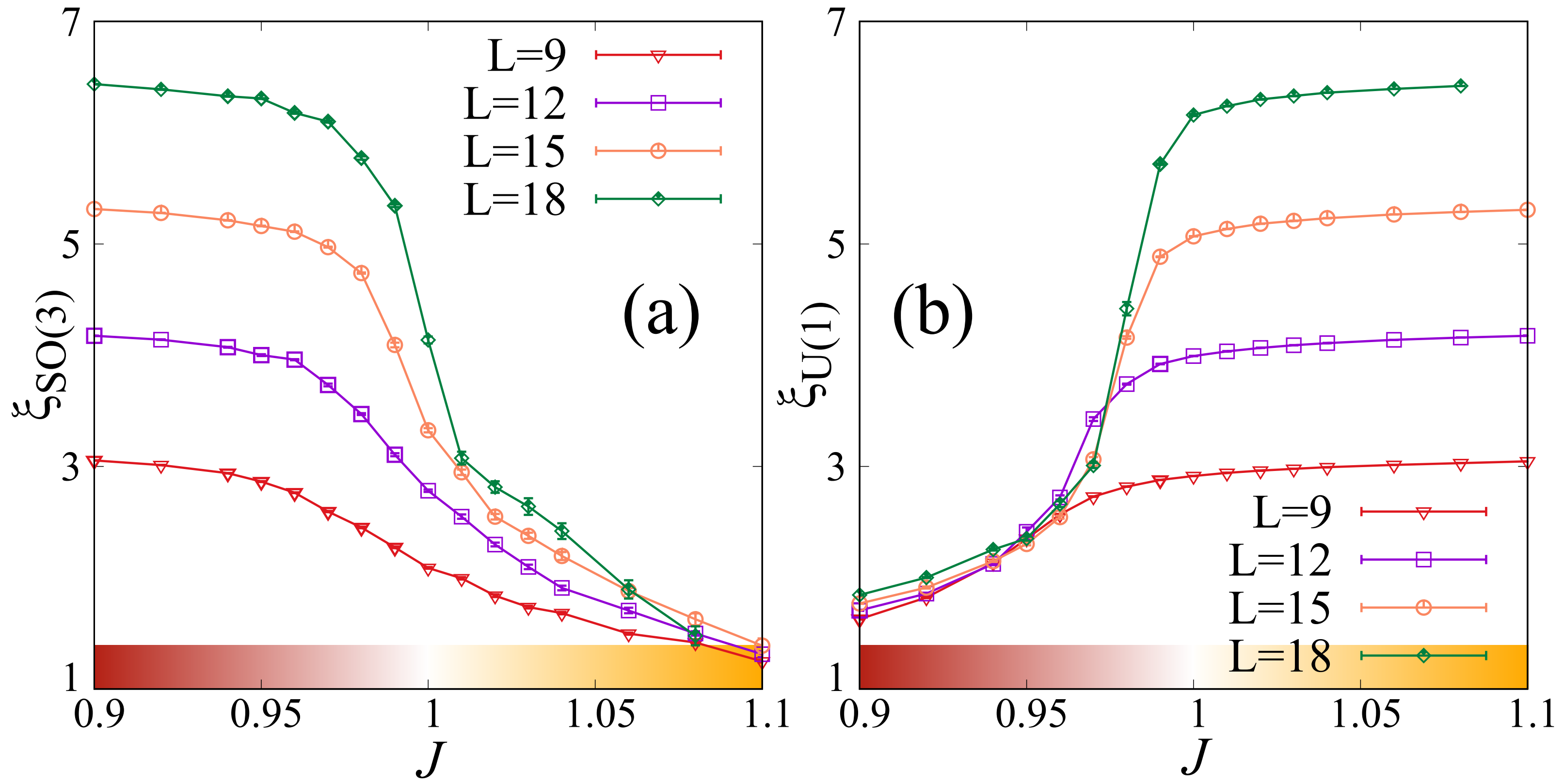
SO(3)-U(1) transition at J_{c2}

Competing orders:



Quantum Monte Carlo:



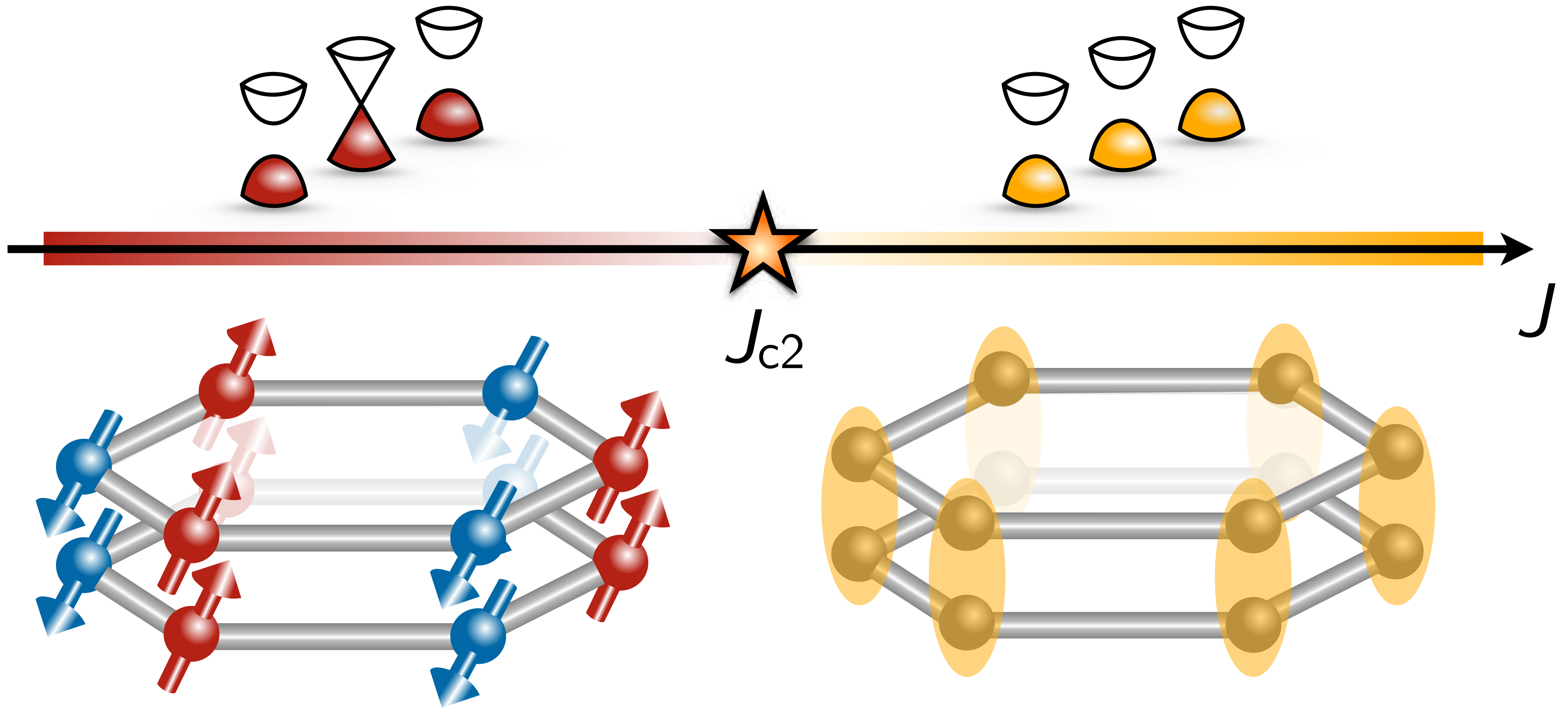


direct … & … continuous

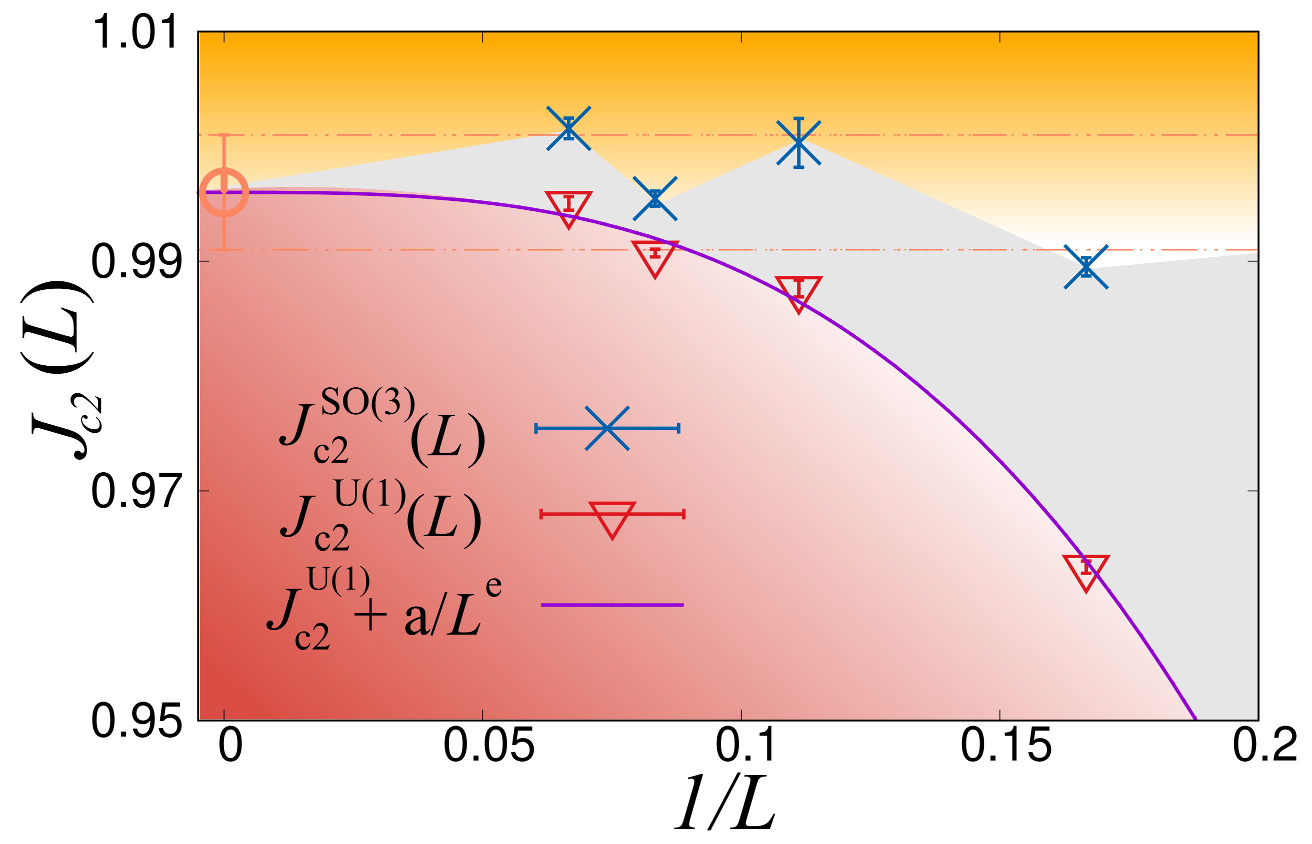
[Liu, Vojta, Assaad, LJ, PRL '22]

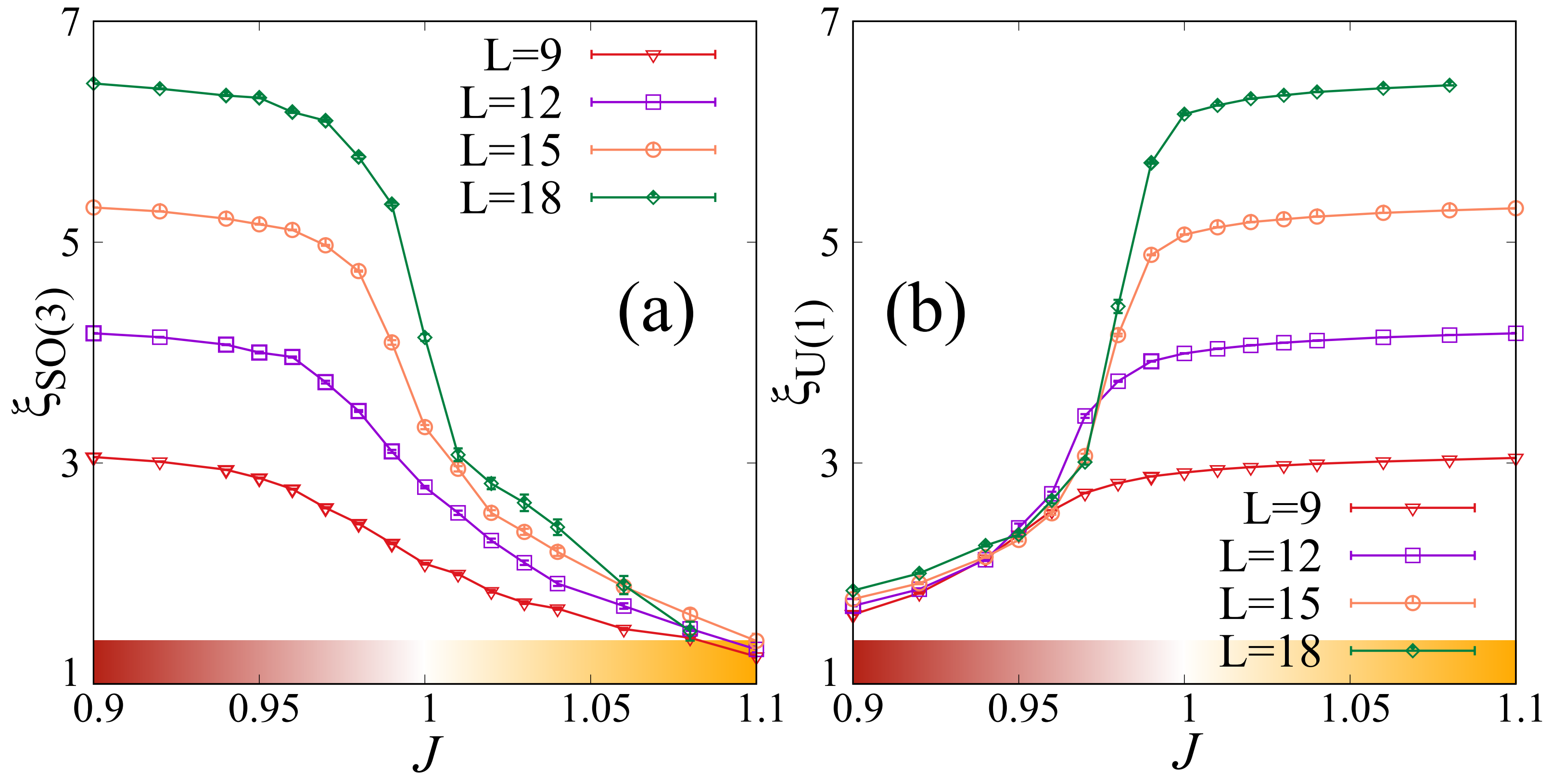
SO(3)-U(1) transition at J_{c2}

Competing orders:



Quantum Monte Carlo:





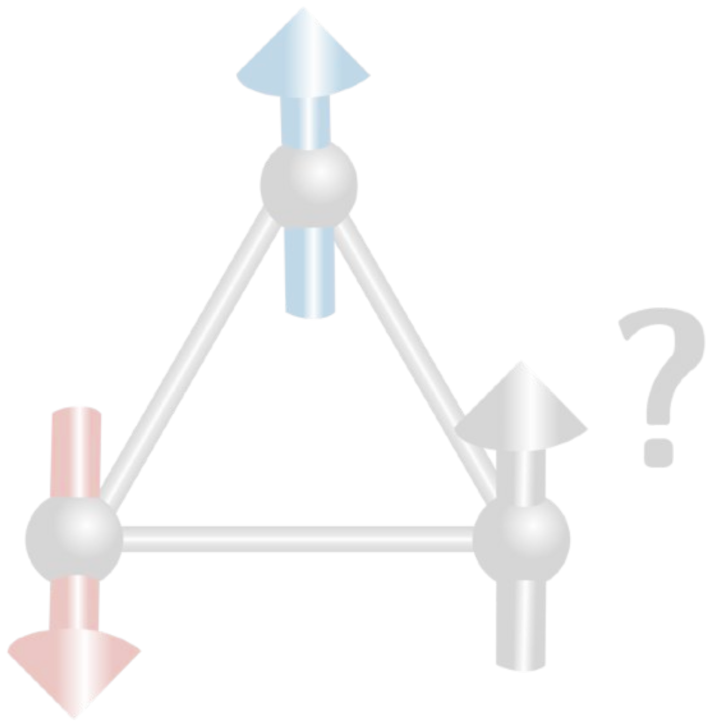
direct … & … continuous

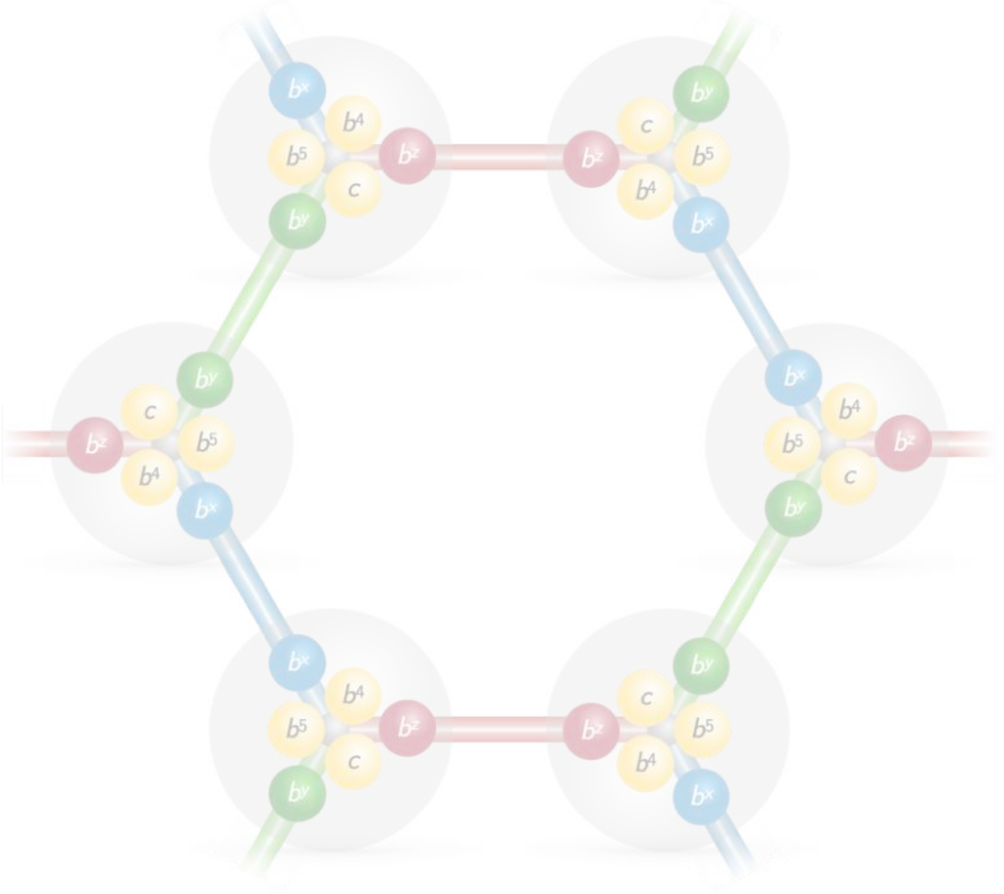
⇨ Metallic deconfined quantum critical point!

[Liu, Vojta, Assaad, LJ, PRL '22]

Outline

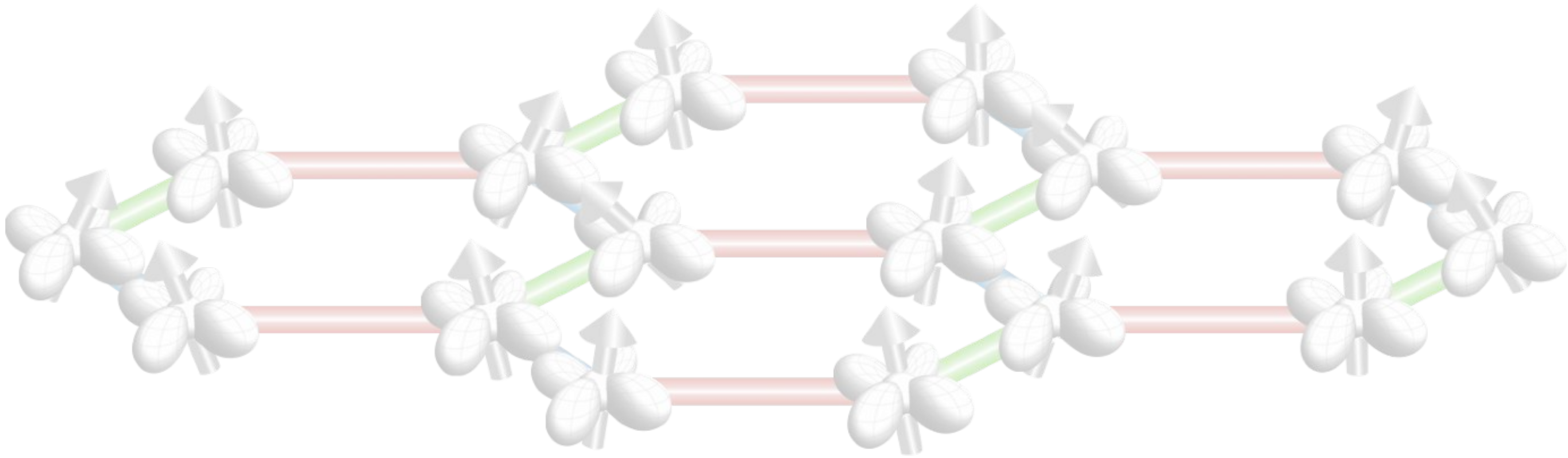
(1) Introduction



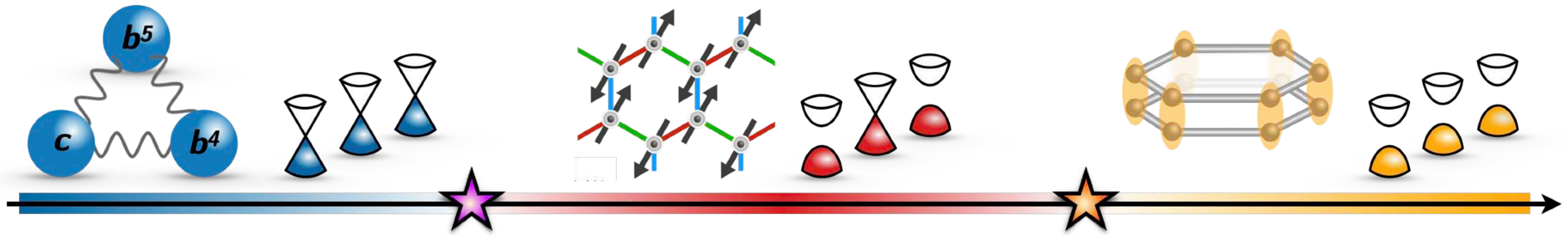


(2) Kitaev spin-1/2 model

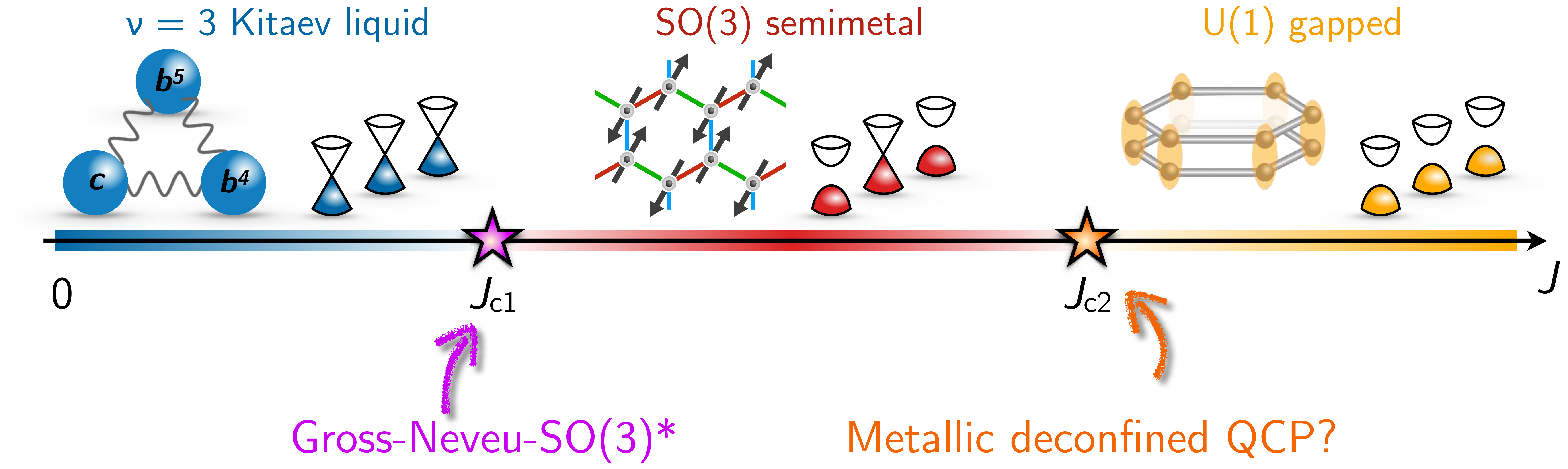
(3) Kitaev-Heisenberg spin-orbital model



(4) Conclusions



Conclusions



$\nu = 3$ Kitaev liquid

SO(3) semimetal

U(1) gapped

Gross-Neveu-SO(3)*

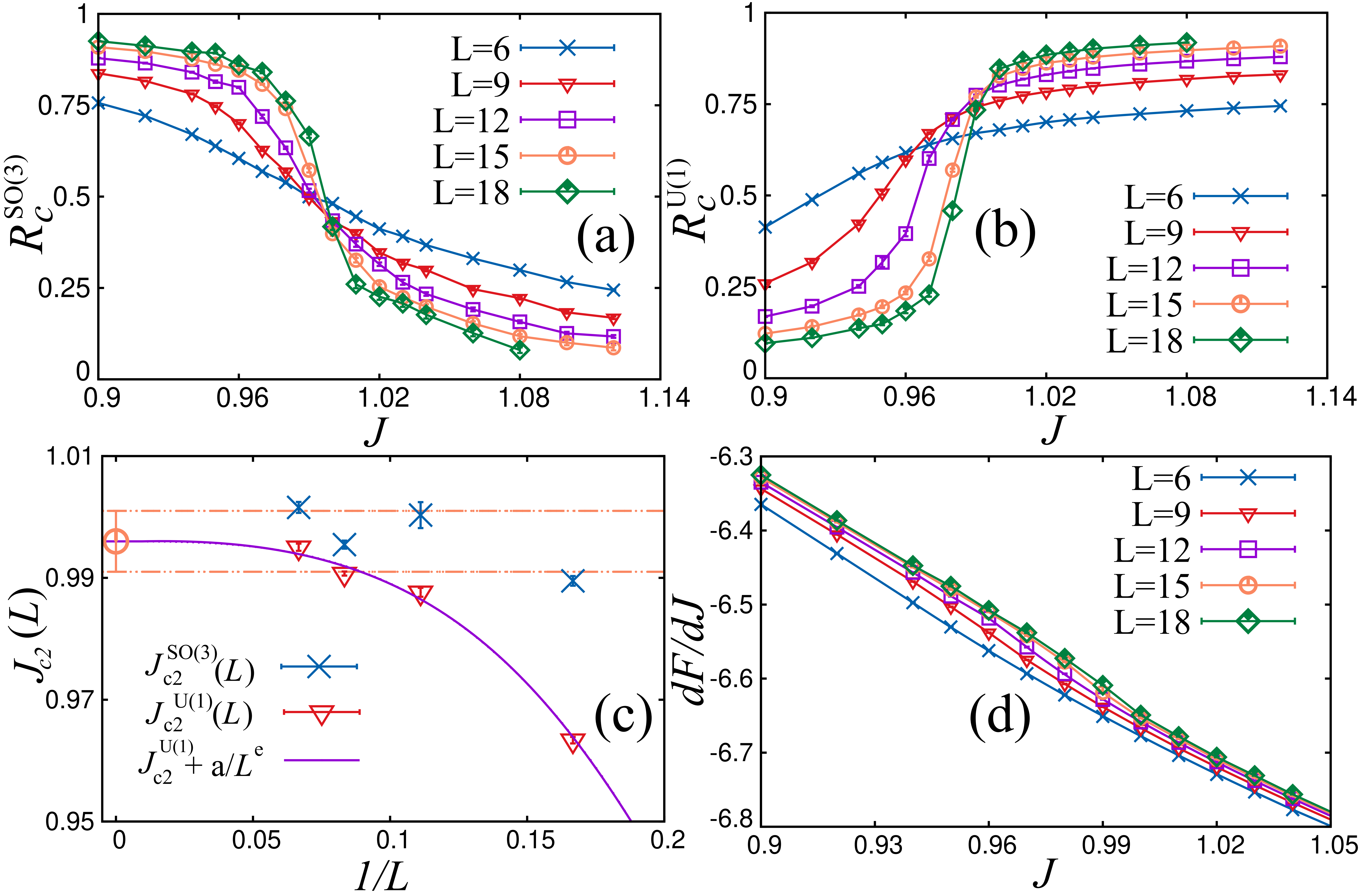
Metallic deconfined QCP?

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

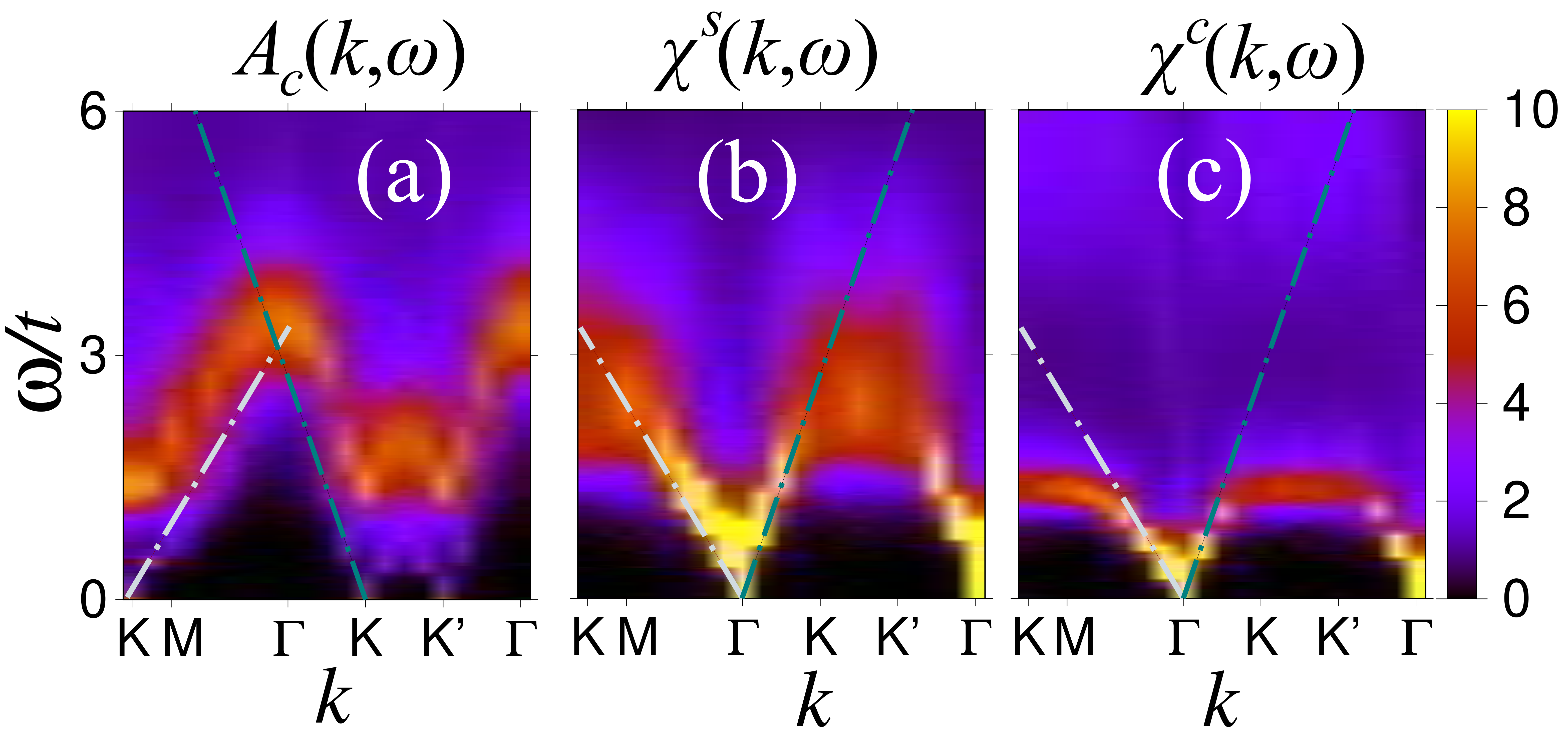
[Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB ’21]

[Liu, Vojta, Assaad, LJ, PRL ’22]

SO(3)-U(1) transition at J_{c2}: Correlation ratios



SO(3)-U(1) transition at J_{c2}: Spectral functions



⇒ Single "velocity of light"

⇒ Emergent Lorentz symmetry

Finite-temperature phase diagram