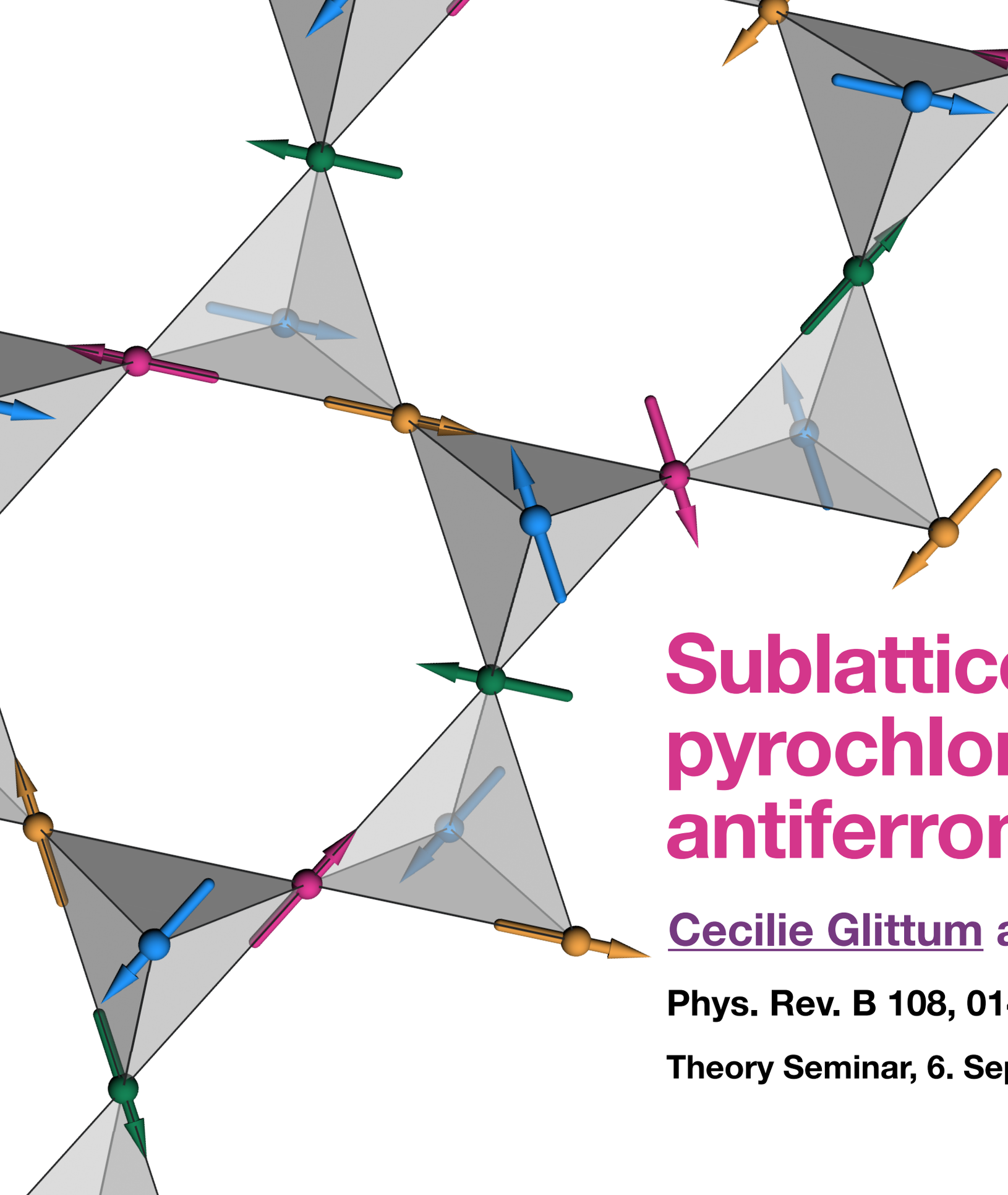


Sublattice pairing in pyrochlore Heisenberg antiferromagnets

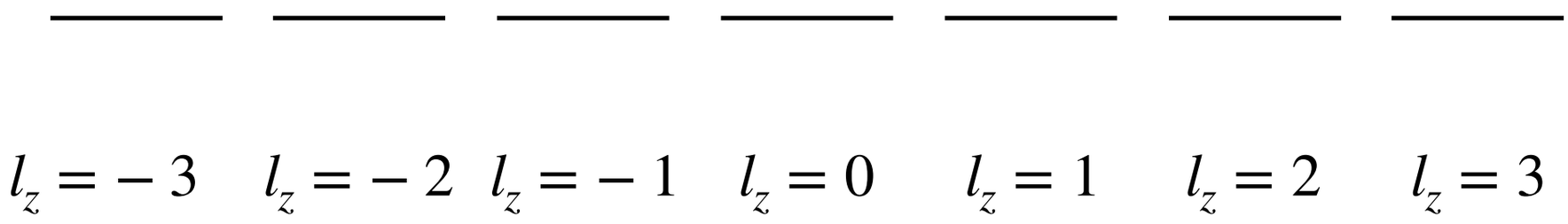
Cecilie Glittum and Olav F. Syljuåsen

Phys. Rev. B 108, 014413 (2023)

Theory Seminar, 6. September 2023

Magnetism in materials originates from partially filled electron shells.

$$\mathrm{Gd}^{3+}: \quad [\mathrm{Xe}]4f^7$$



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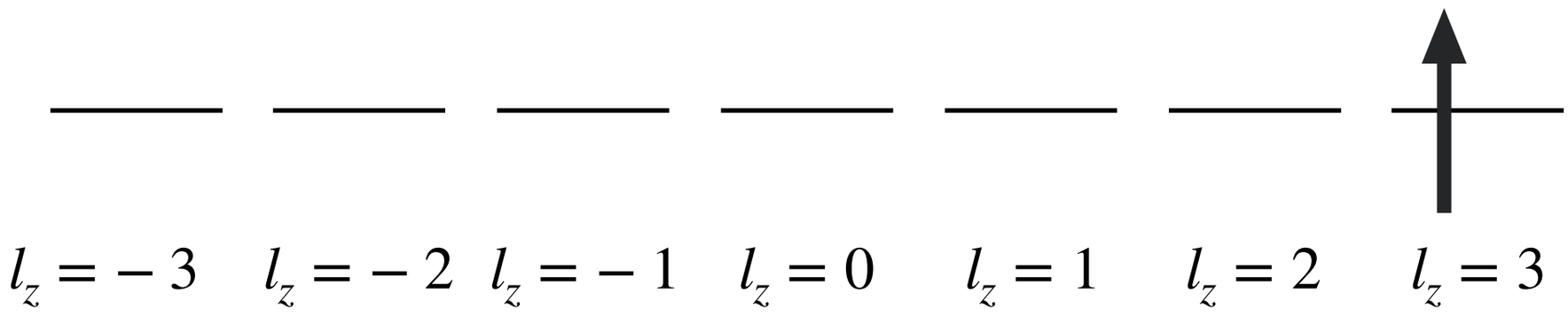

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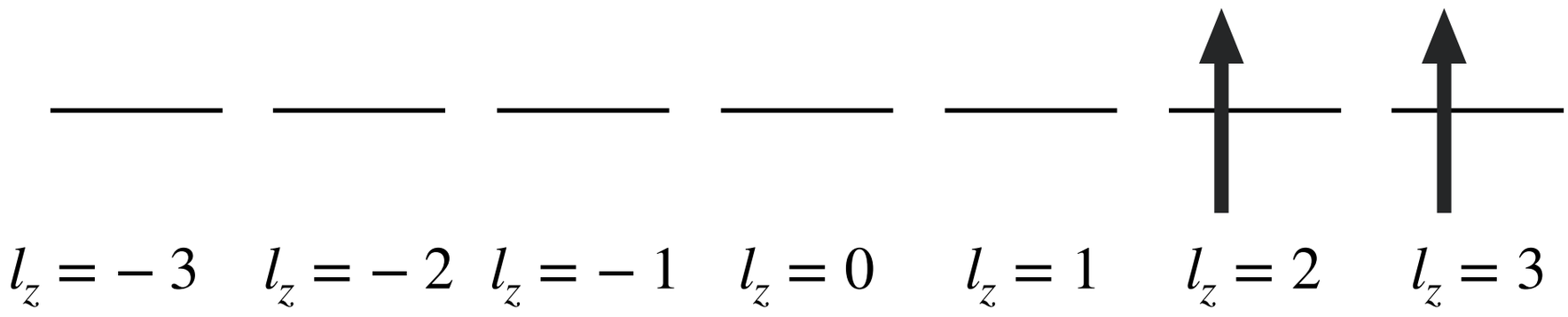

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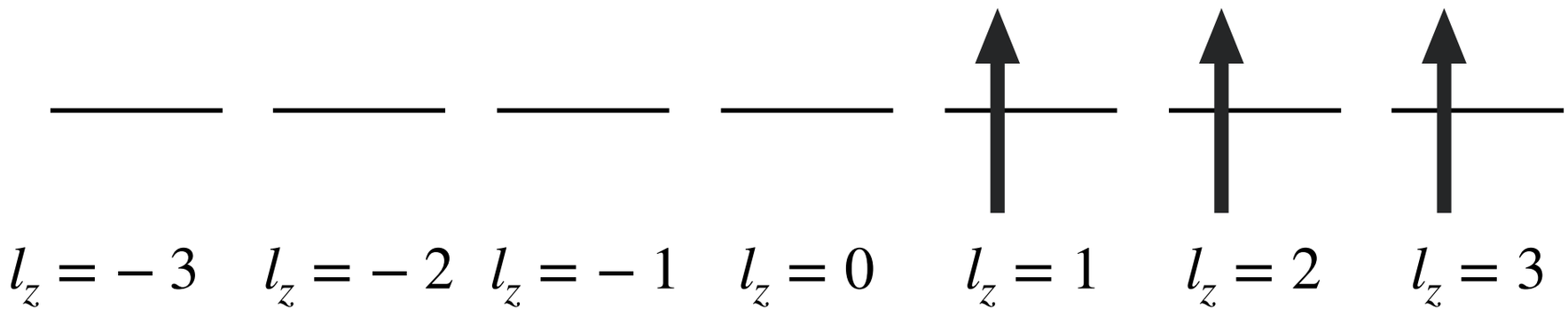

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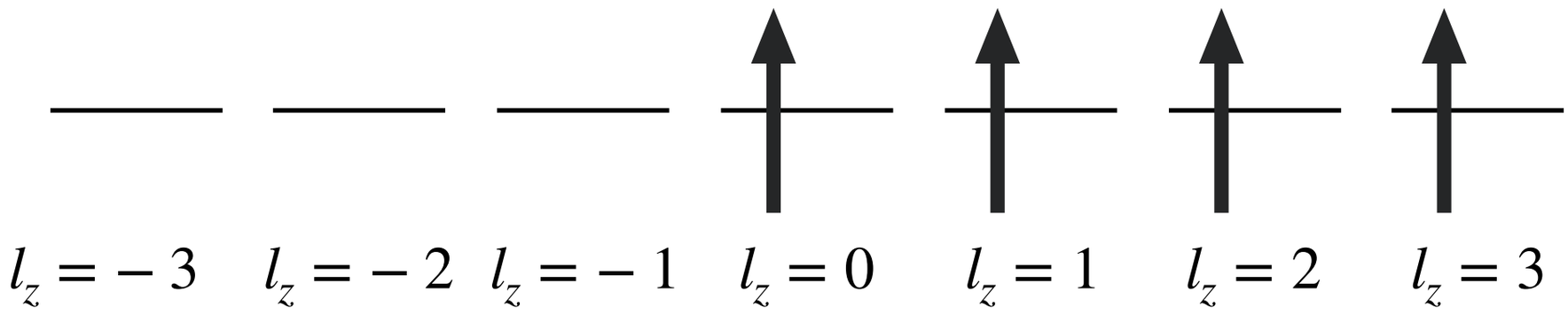

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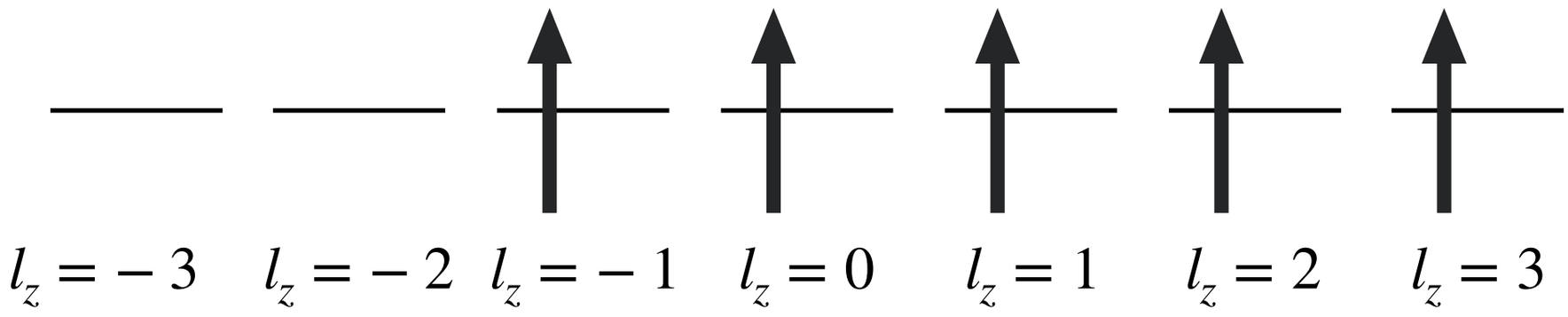

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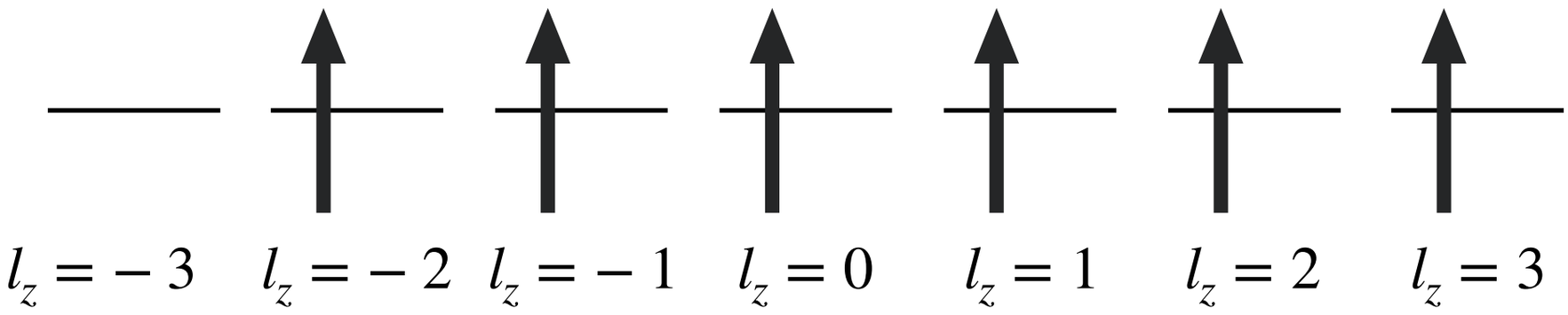

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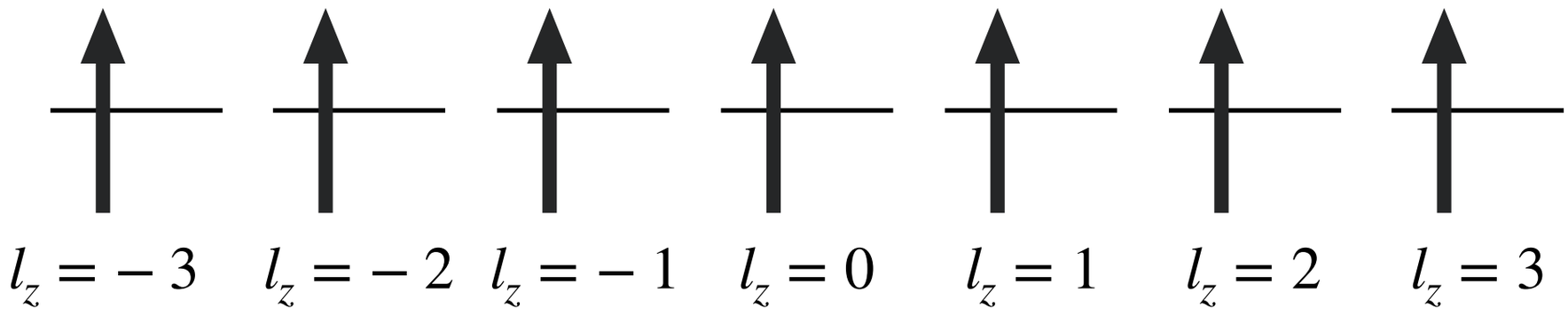

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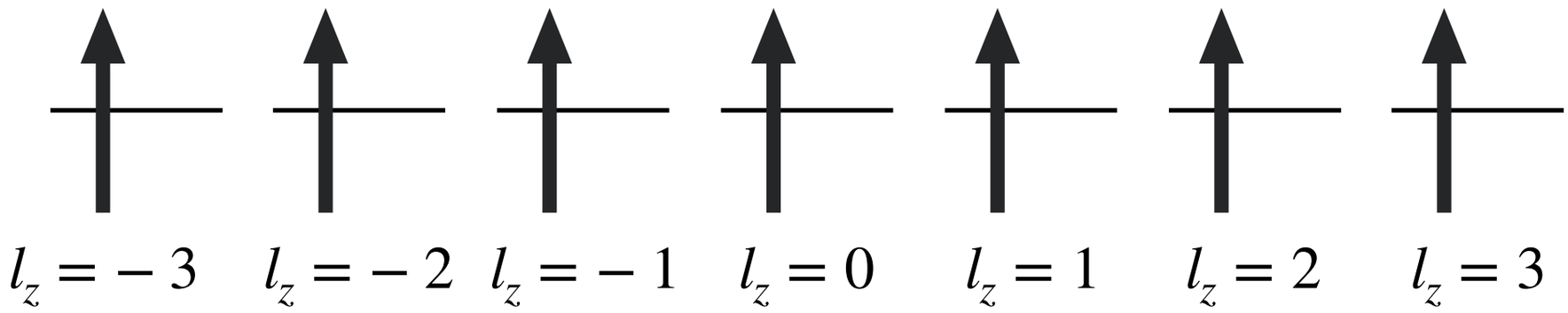

$S = 7/2$

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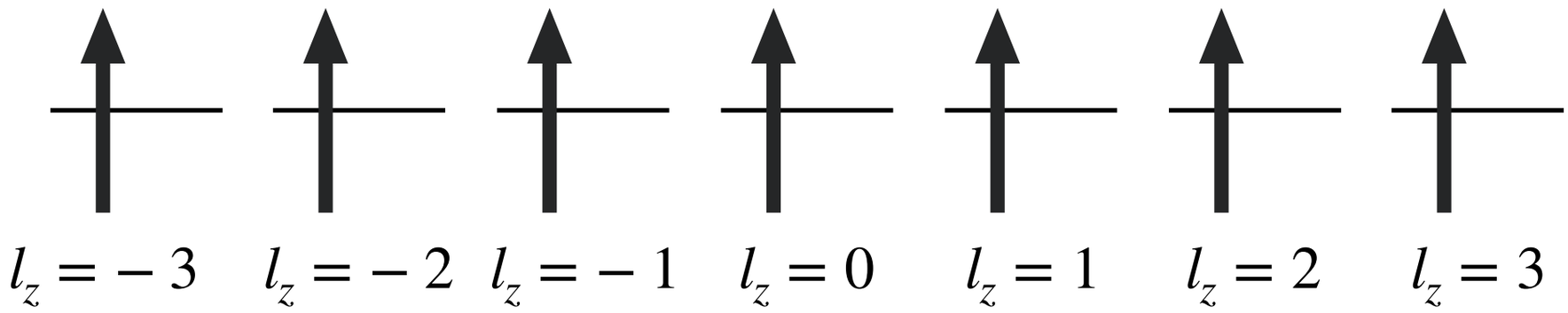

$$S = 7/2 \qquad L = 0$$

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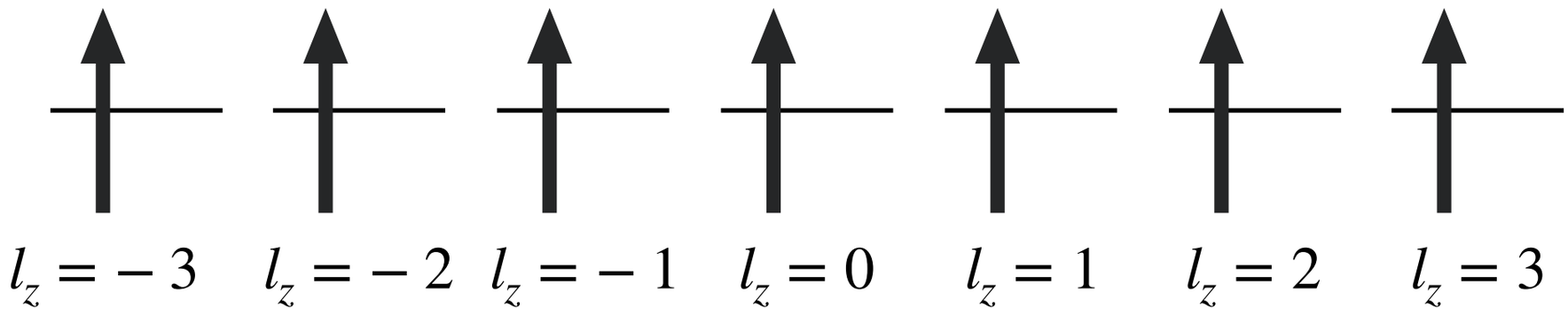

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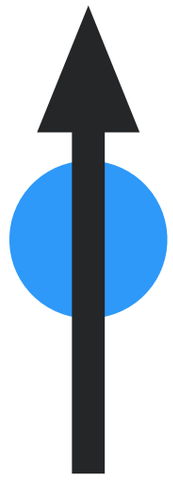

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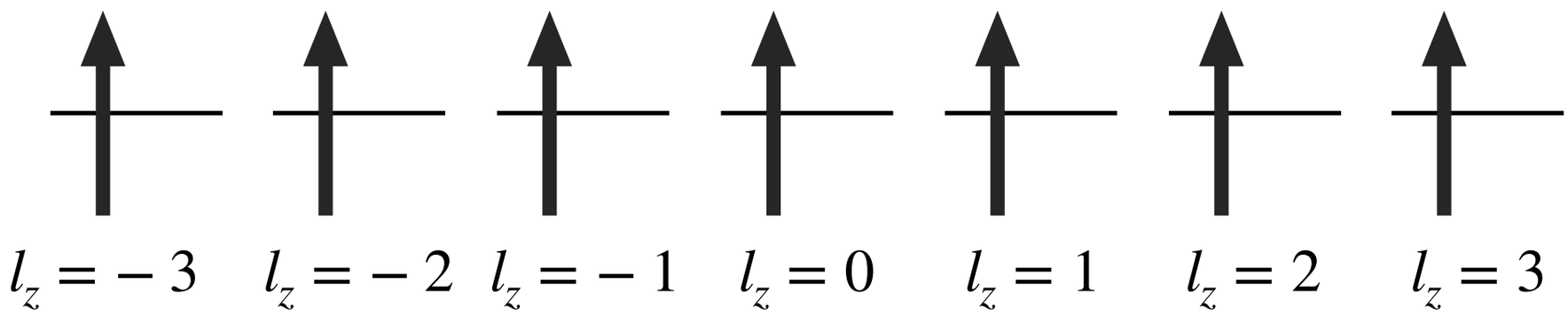

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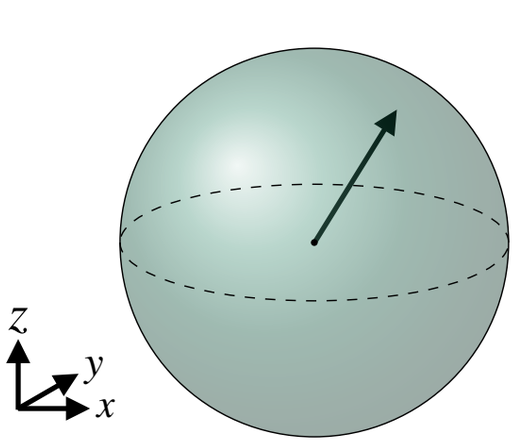

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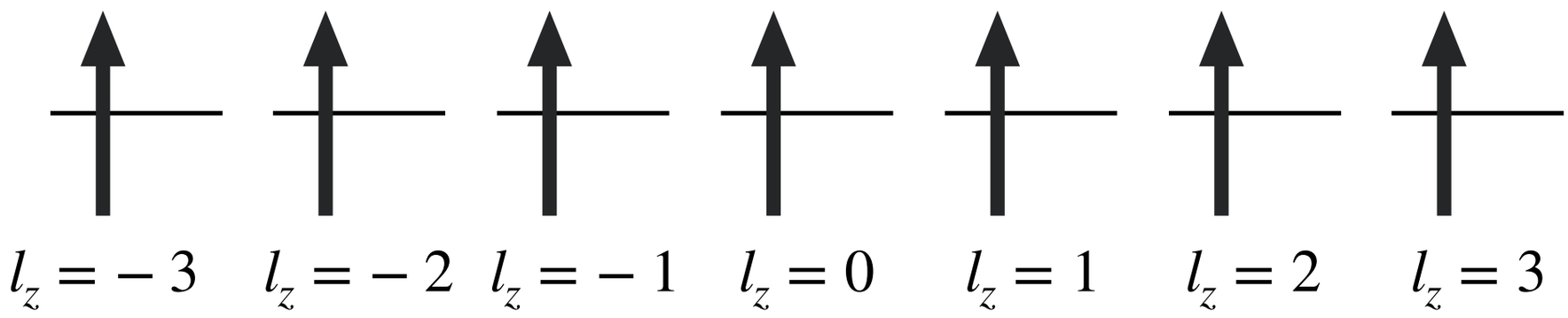

$$S = 7/2 \qquad L = 0 \qquad J = 7/2$$

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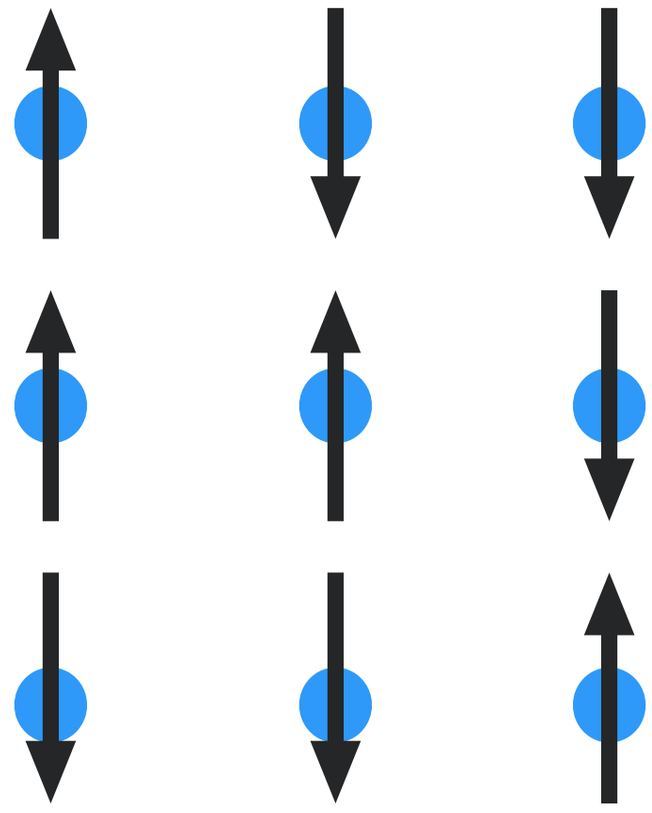

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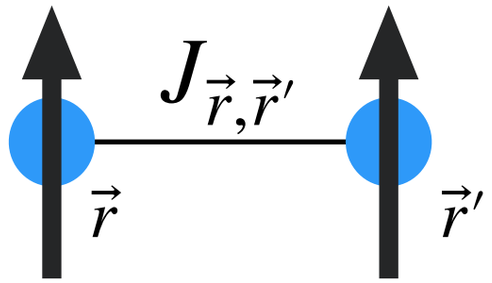
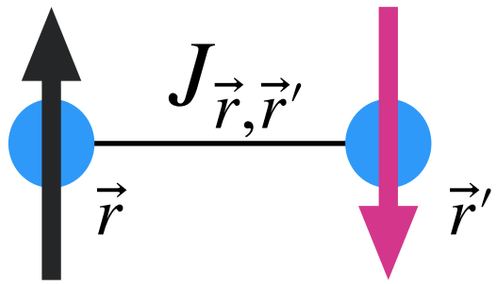
$J_{\vec{r},\vec{r}'} < 0$: Ferromagnetic

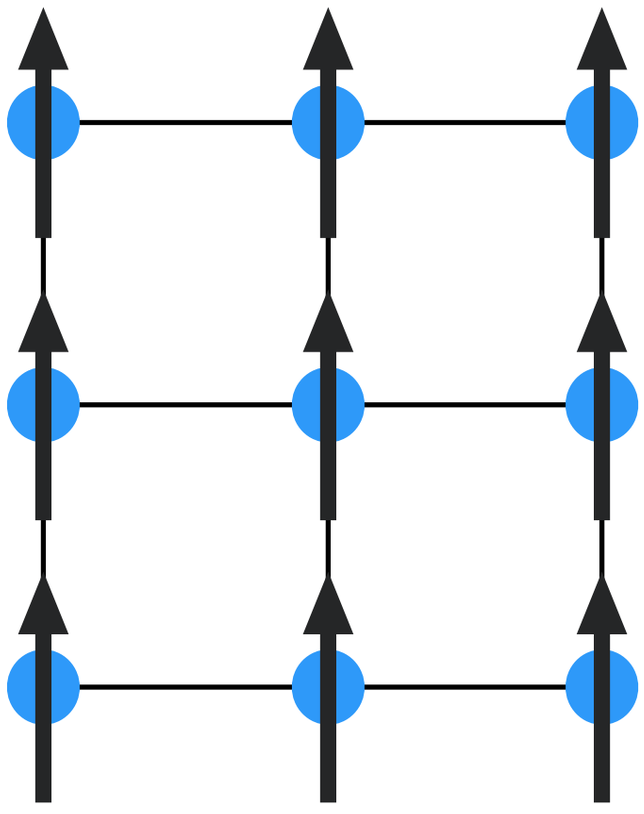


$J_{\vec{r},\vec{r}'} > 0$: Antiferromagnetic



Square lattice with nearest neighbour interactions.

Ferromagnetic



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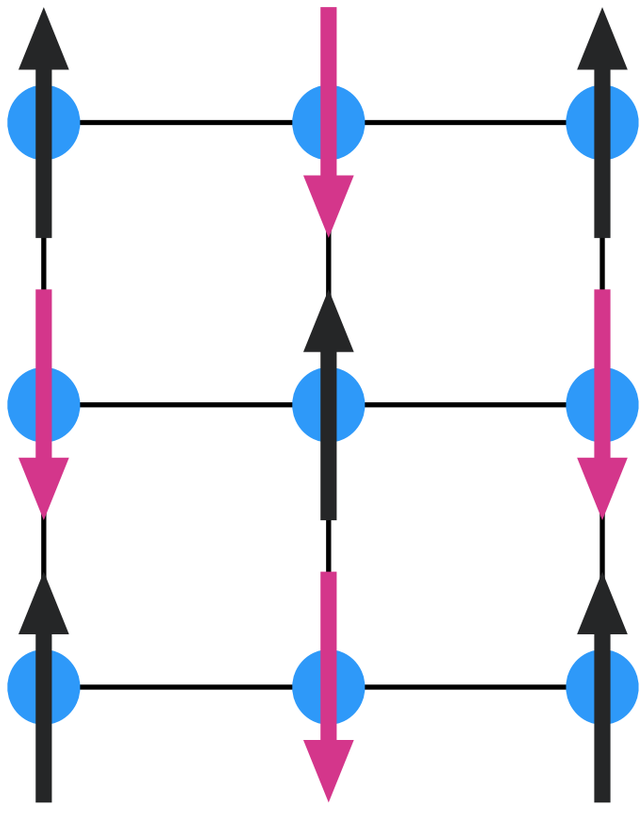
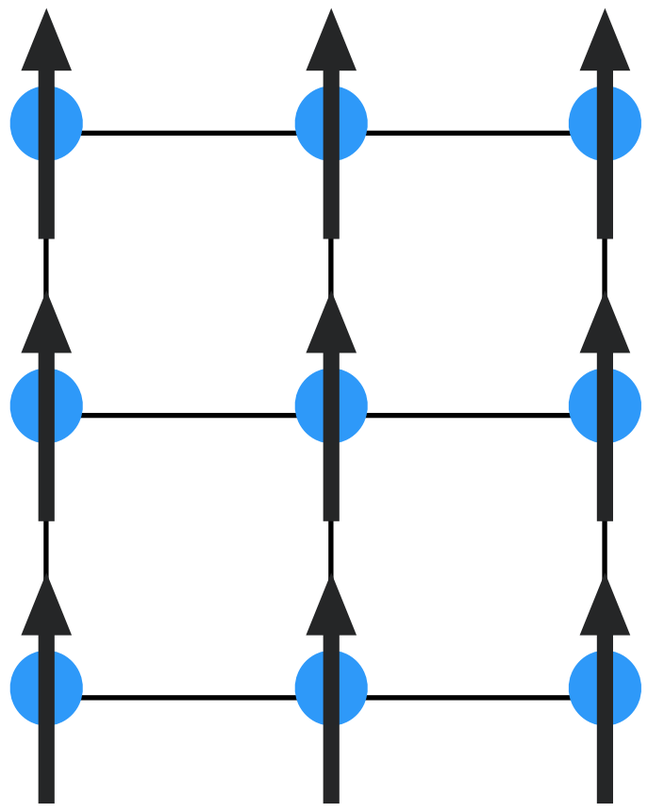
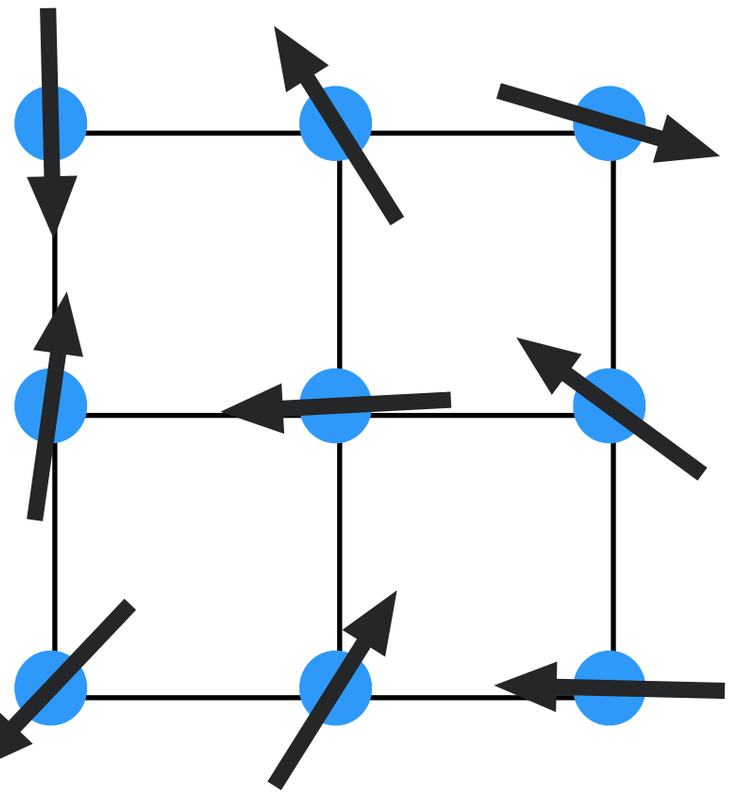


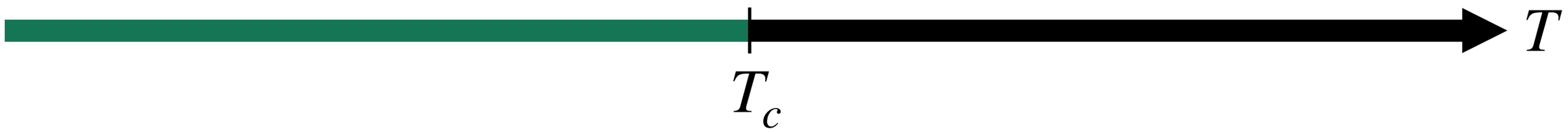
Conventional magnets usually order below a critical temperature.

Ferromagnet



Paramagnet





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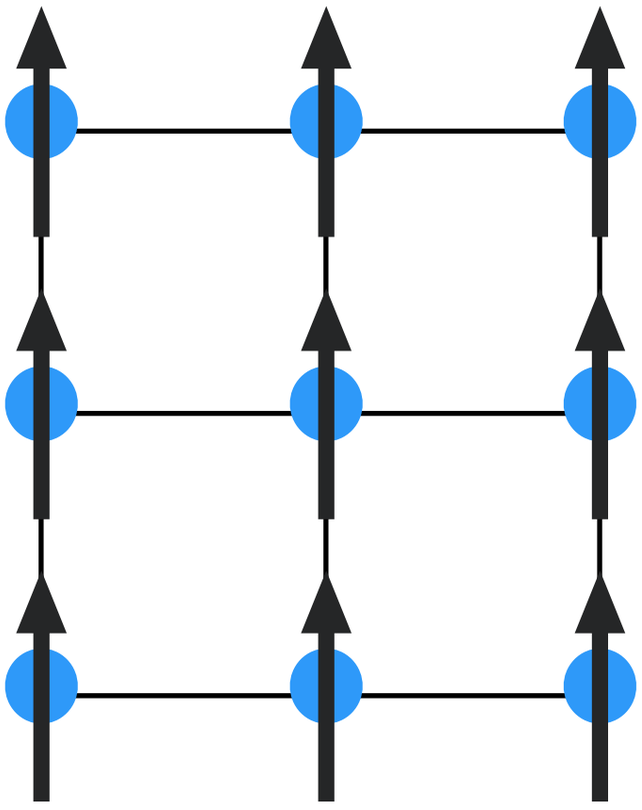

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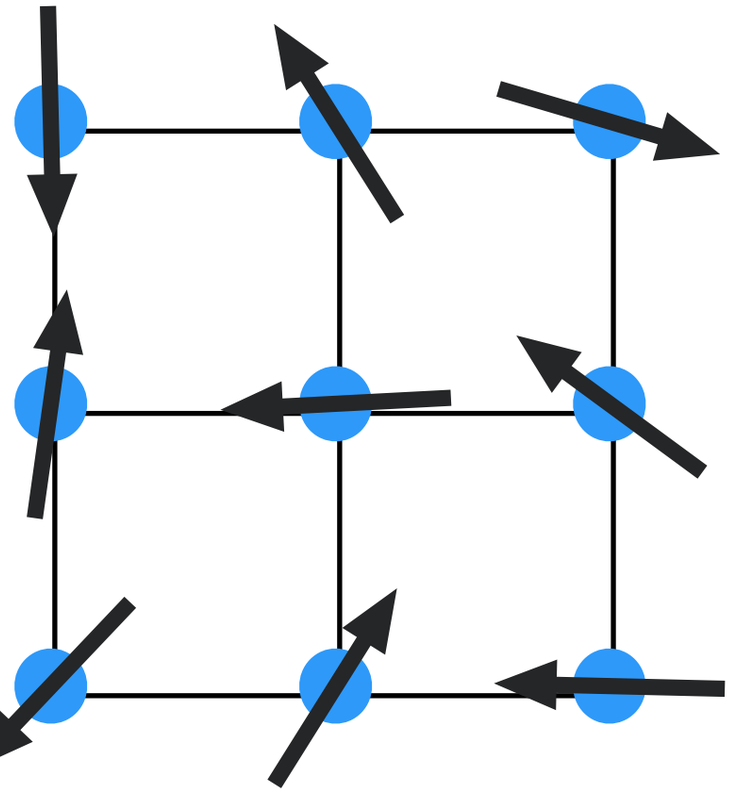

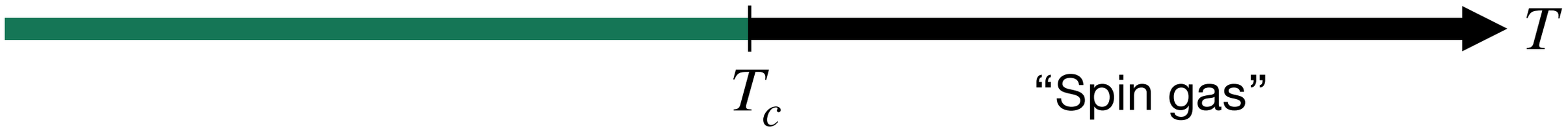

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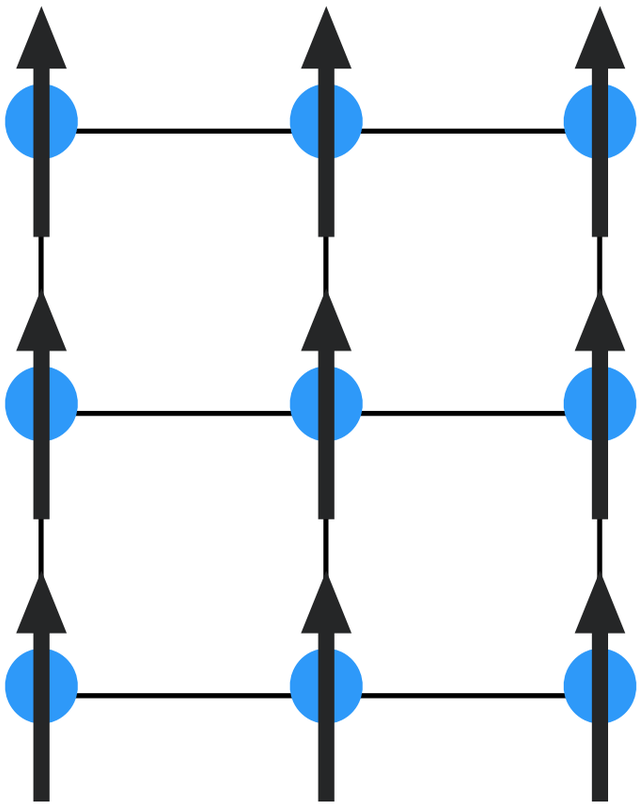

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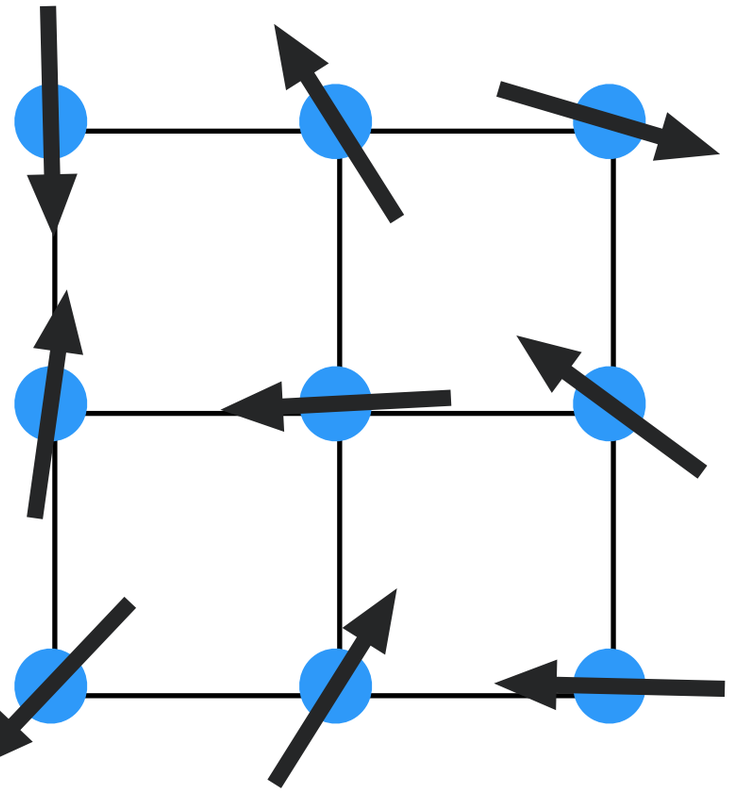
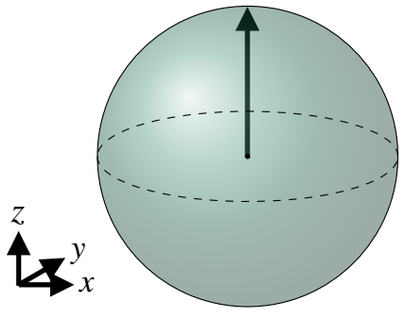
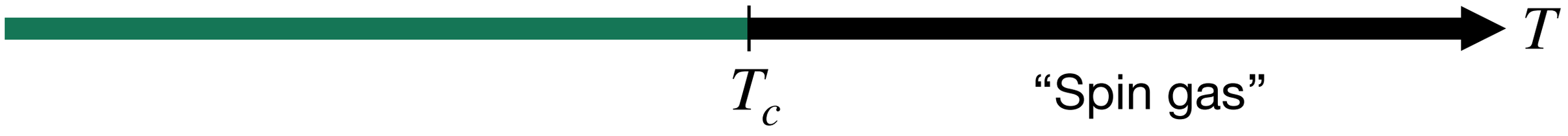




SYMMETRY BREAKING



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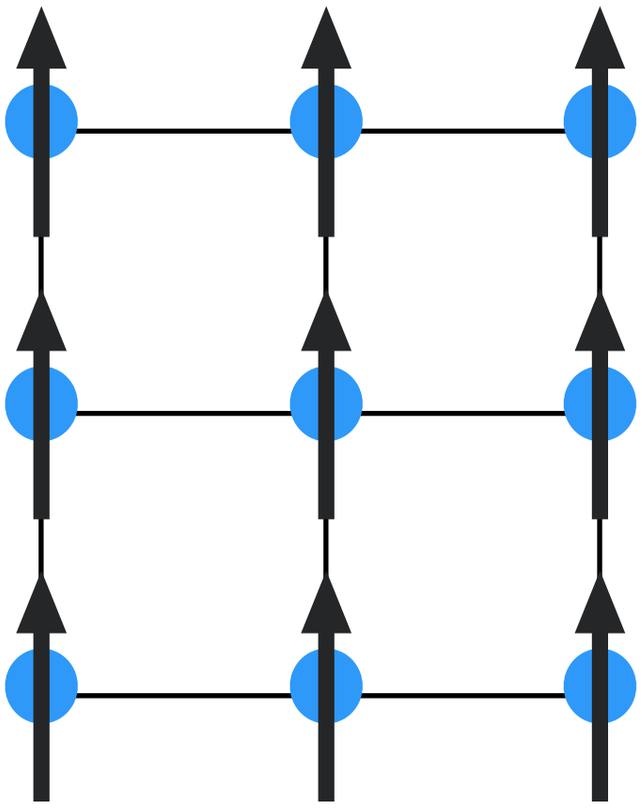

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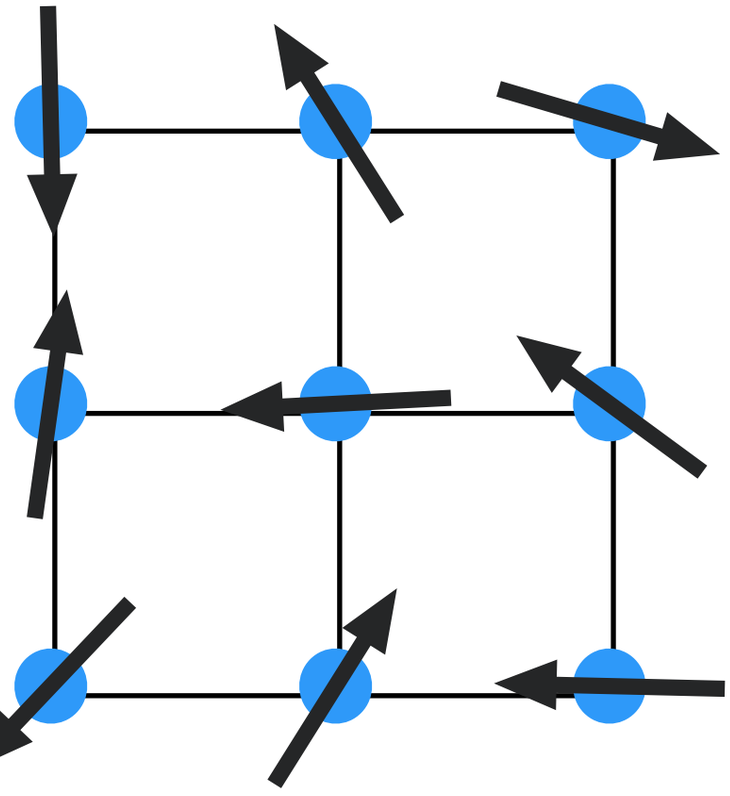

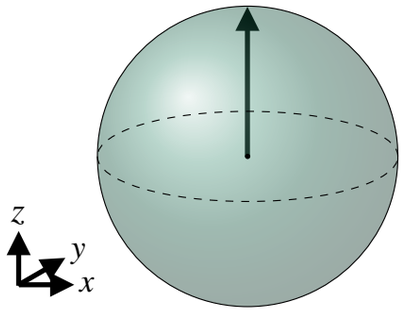

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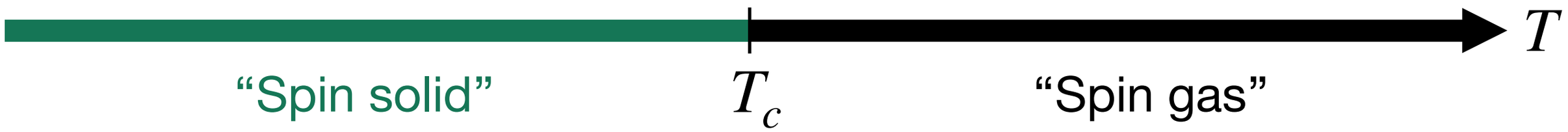
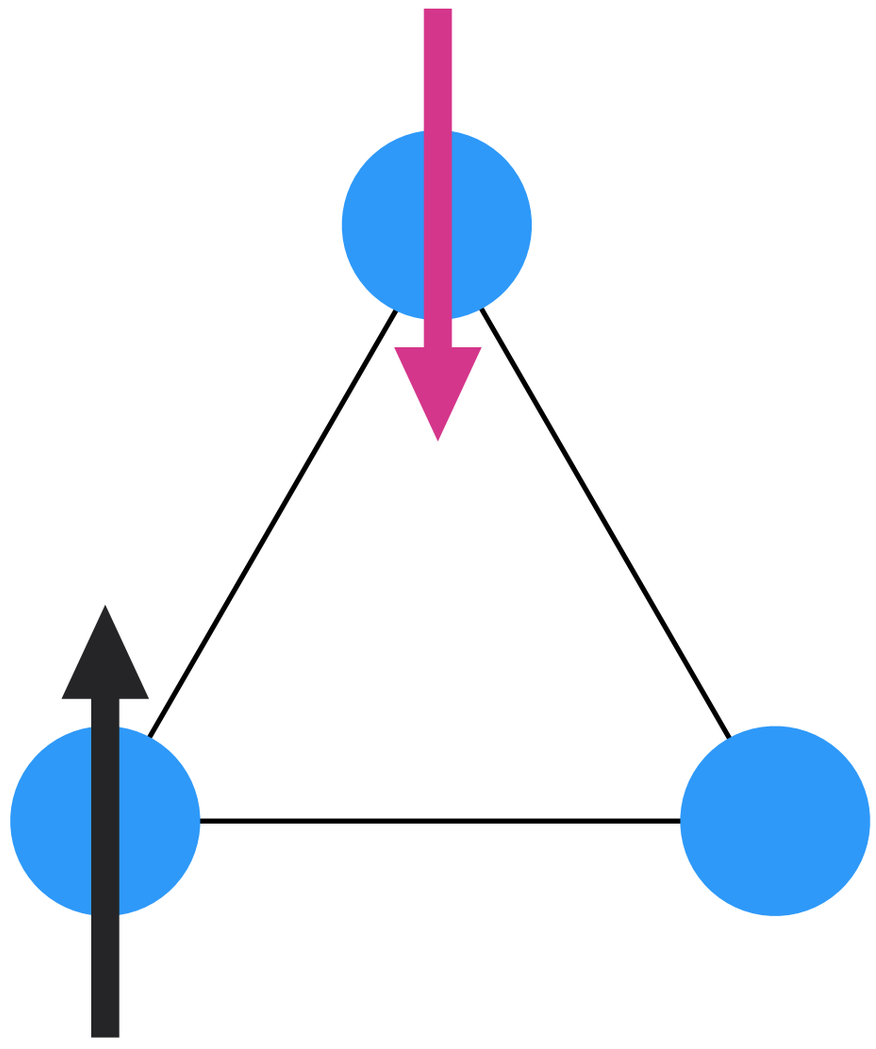


Frustrated magnets cannot satisfy all interactions simultaneously.

Simplest example: Ising antiferromagnet on a triangle



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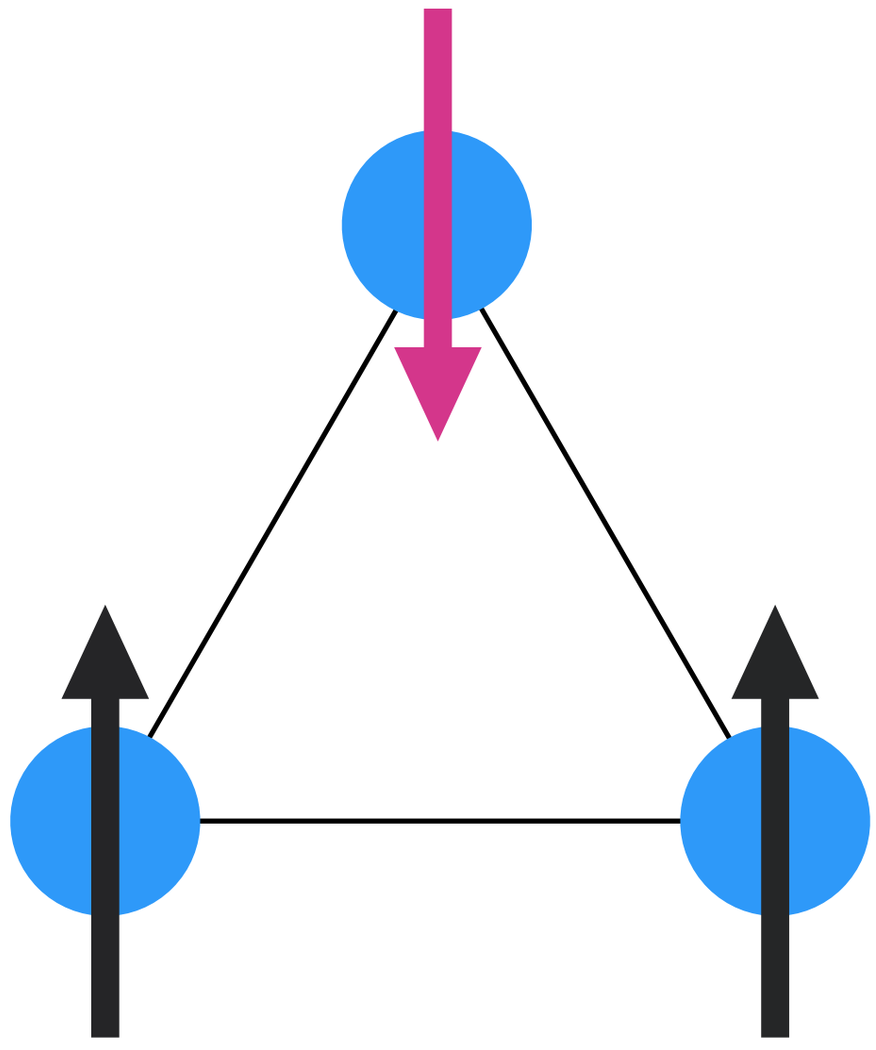

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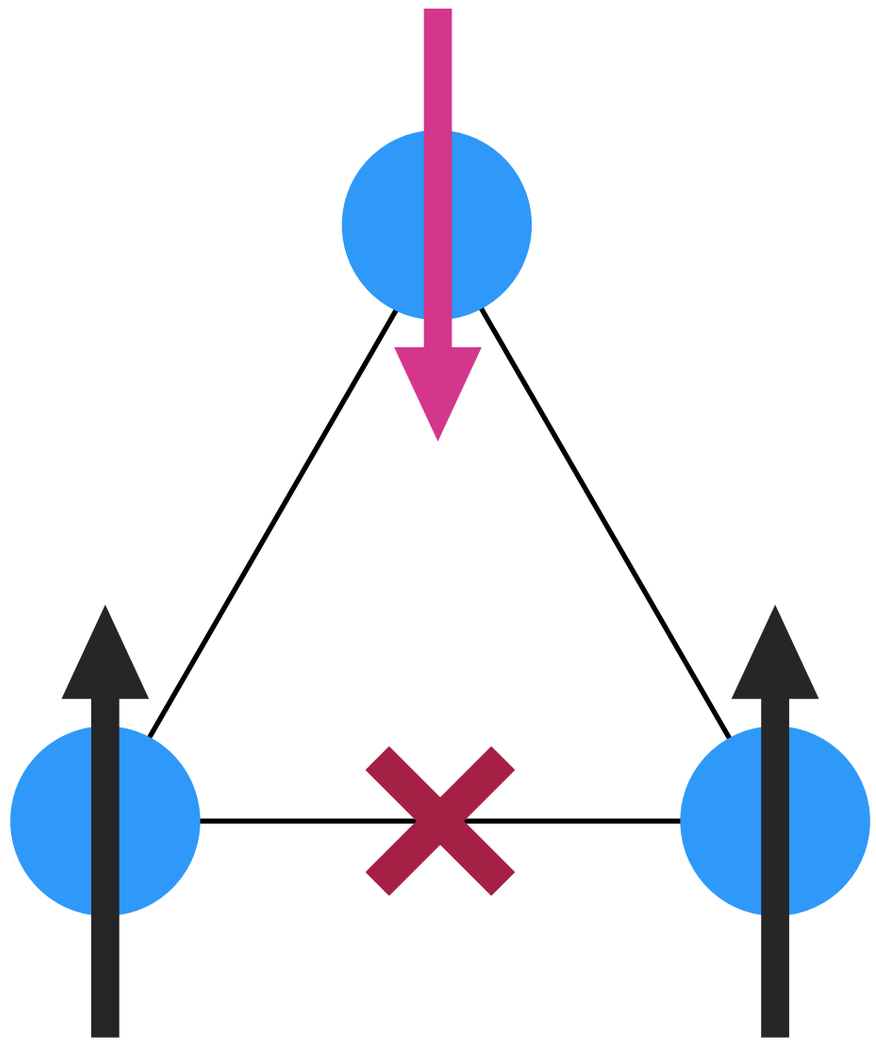

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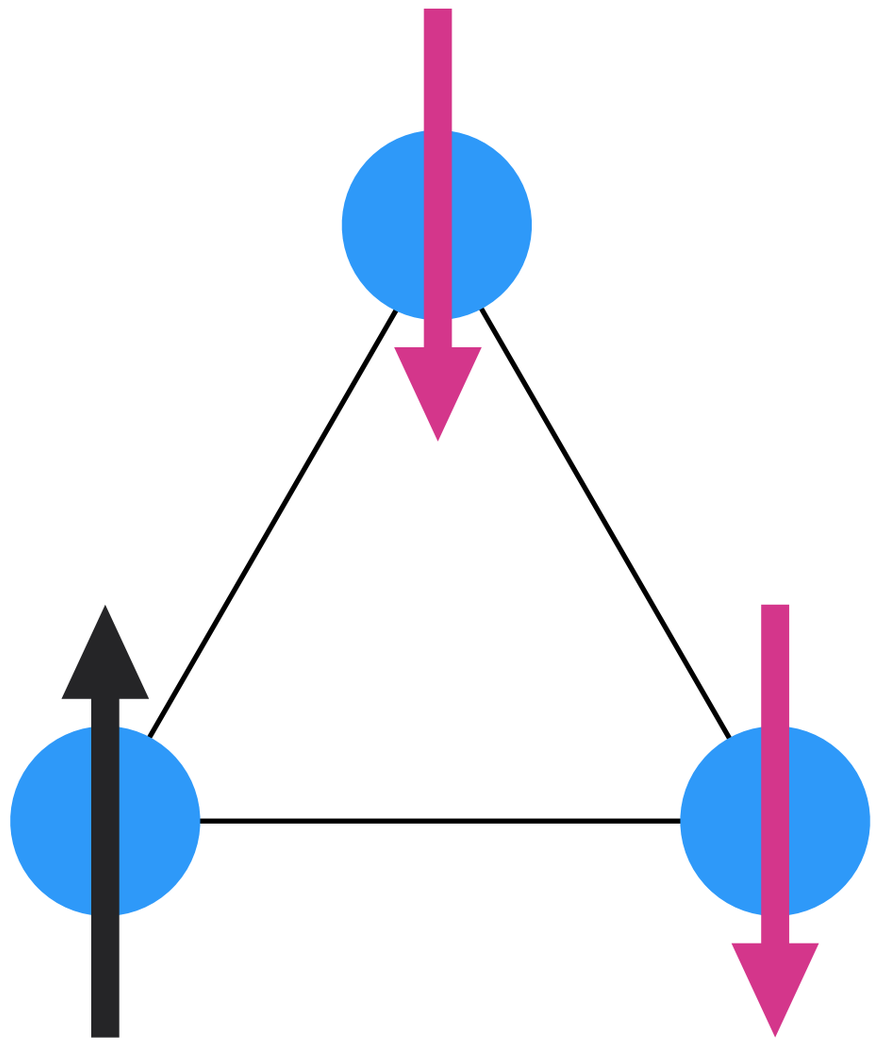

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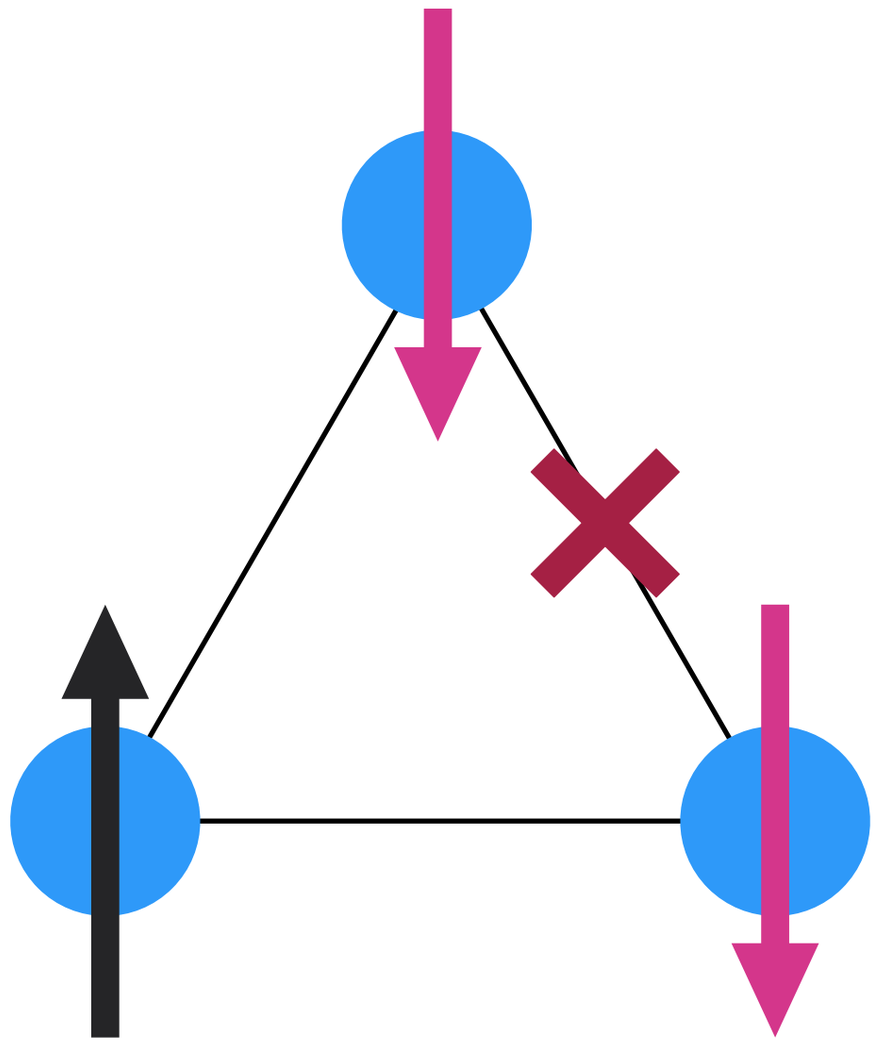

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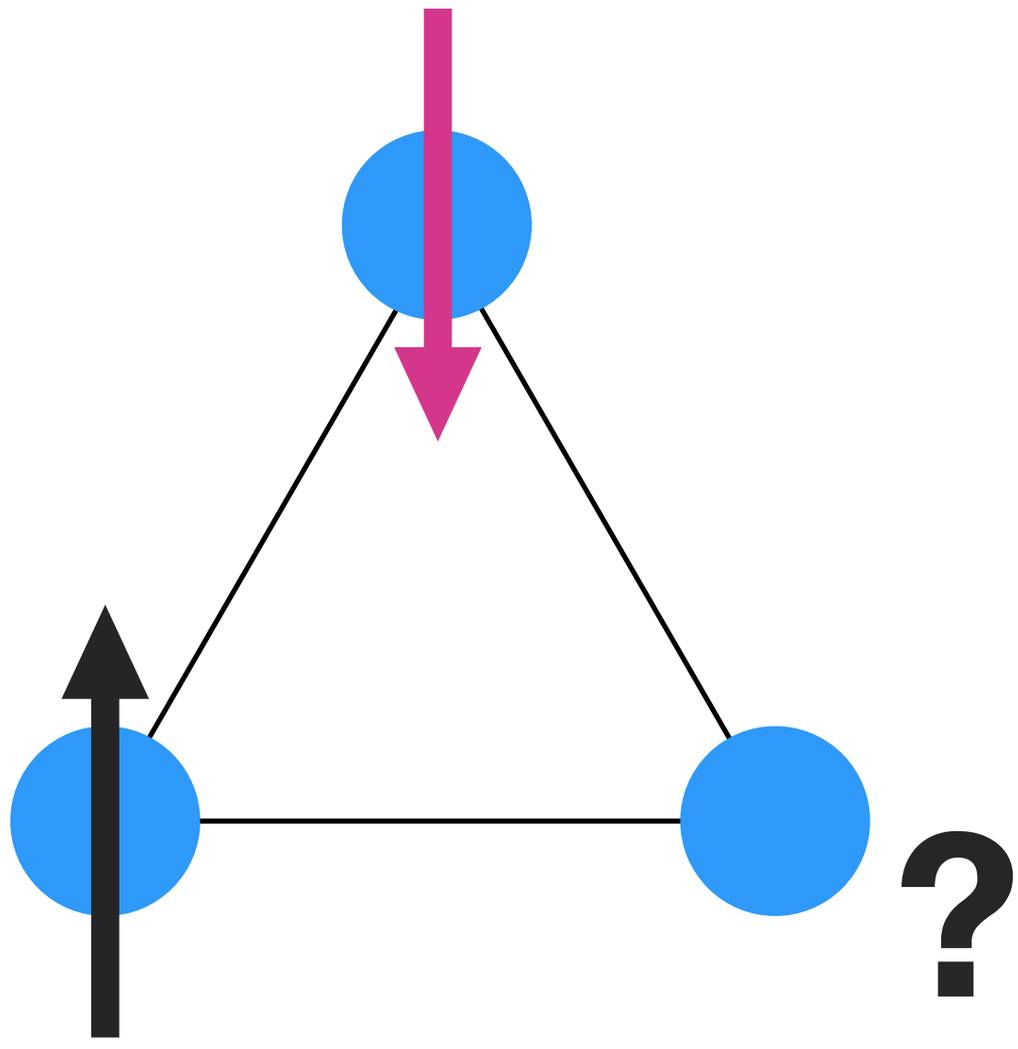
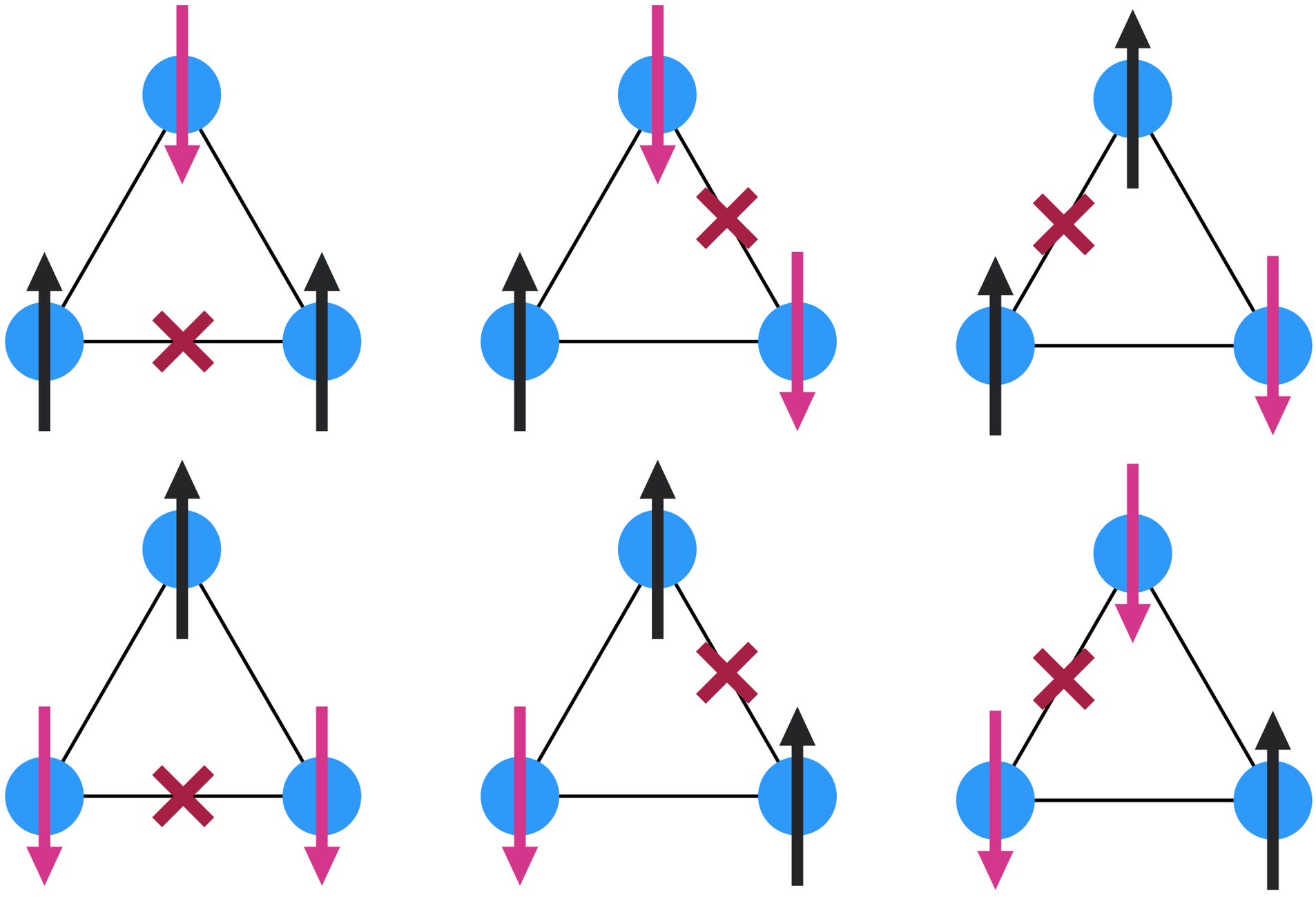
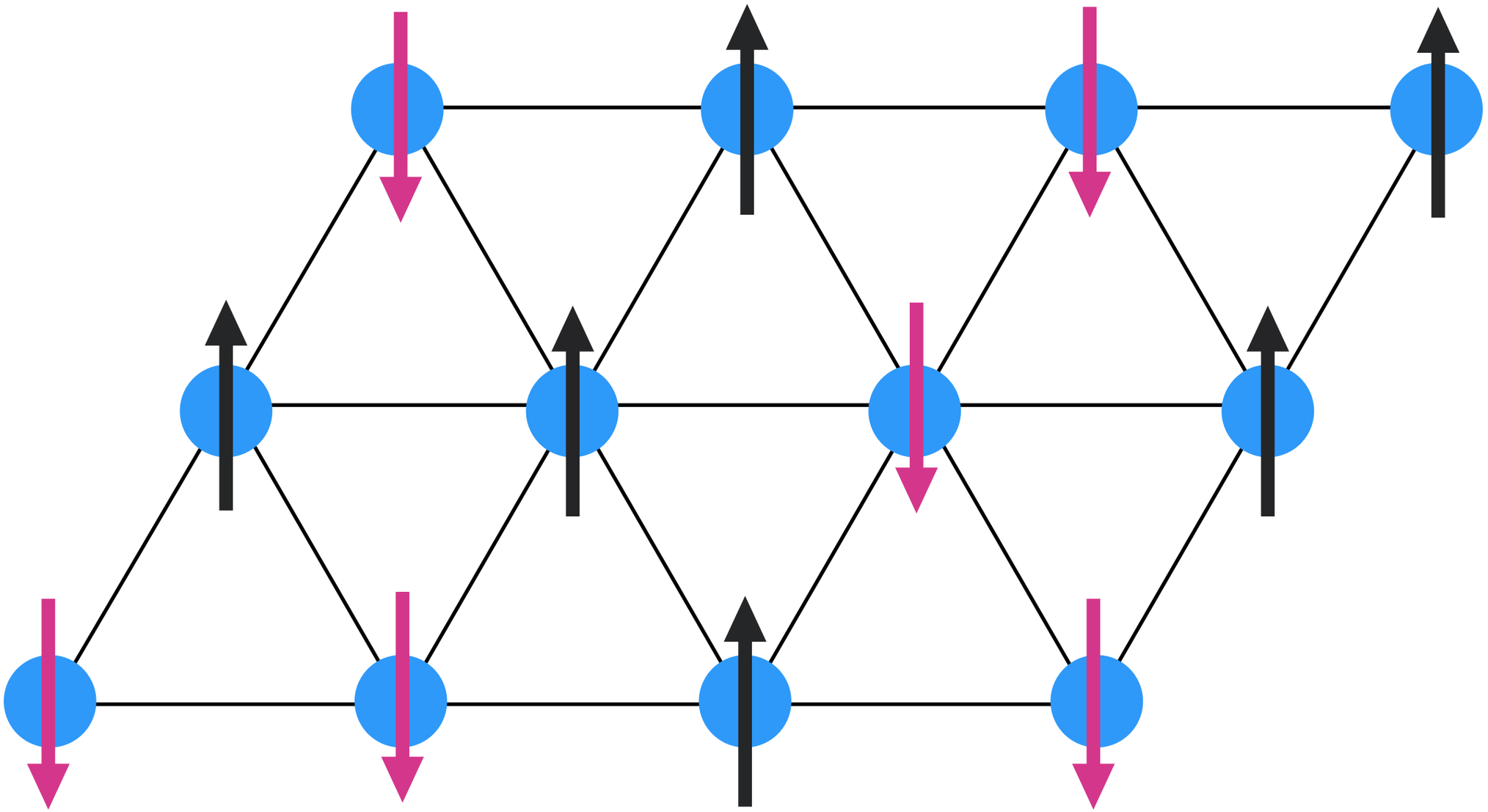


Frustrated magnets often have an extensive ground state degeneracy.



Ising model on triangular lattice…



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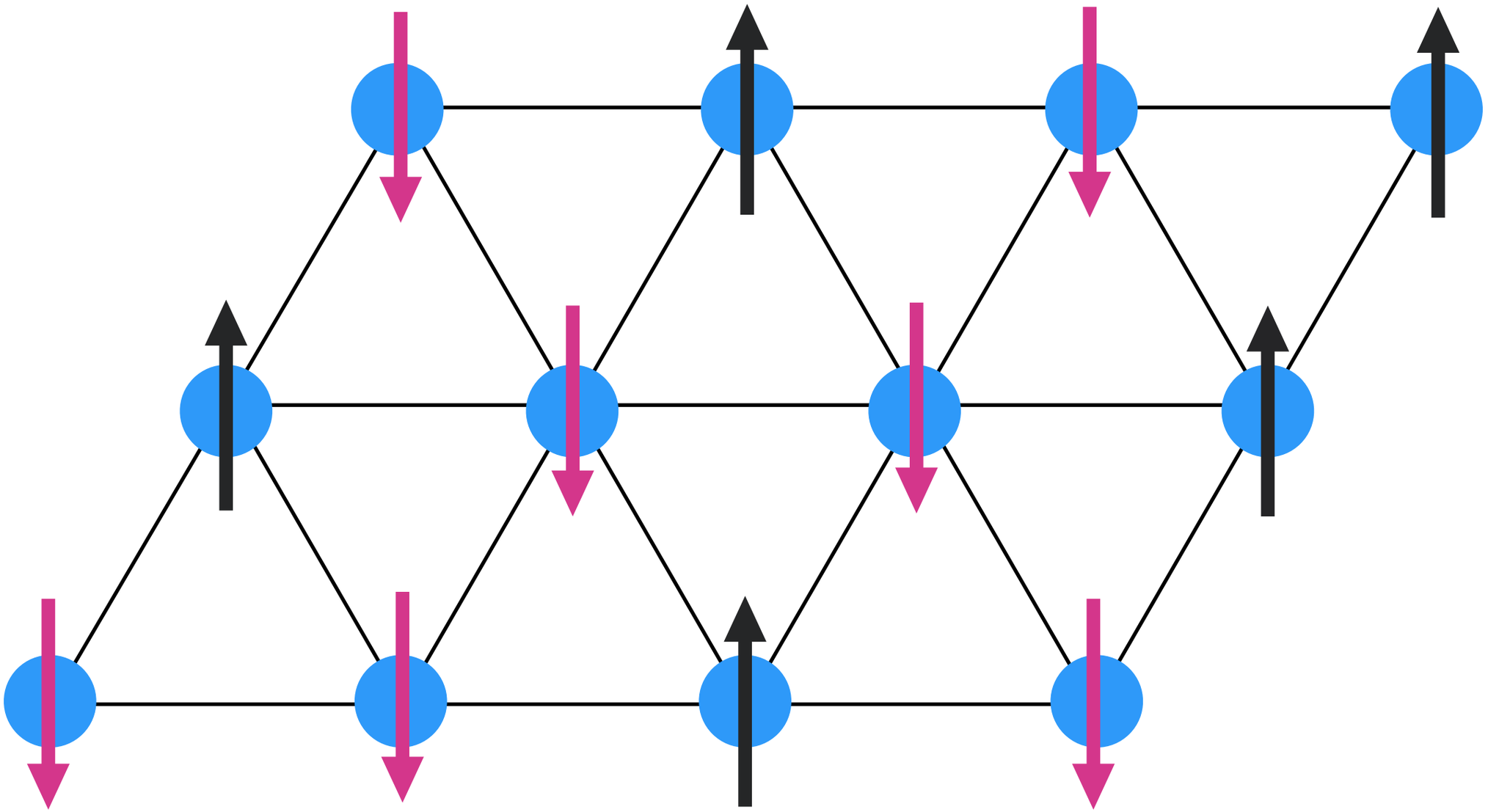

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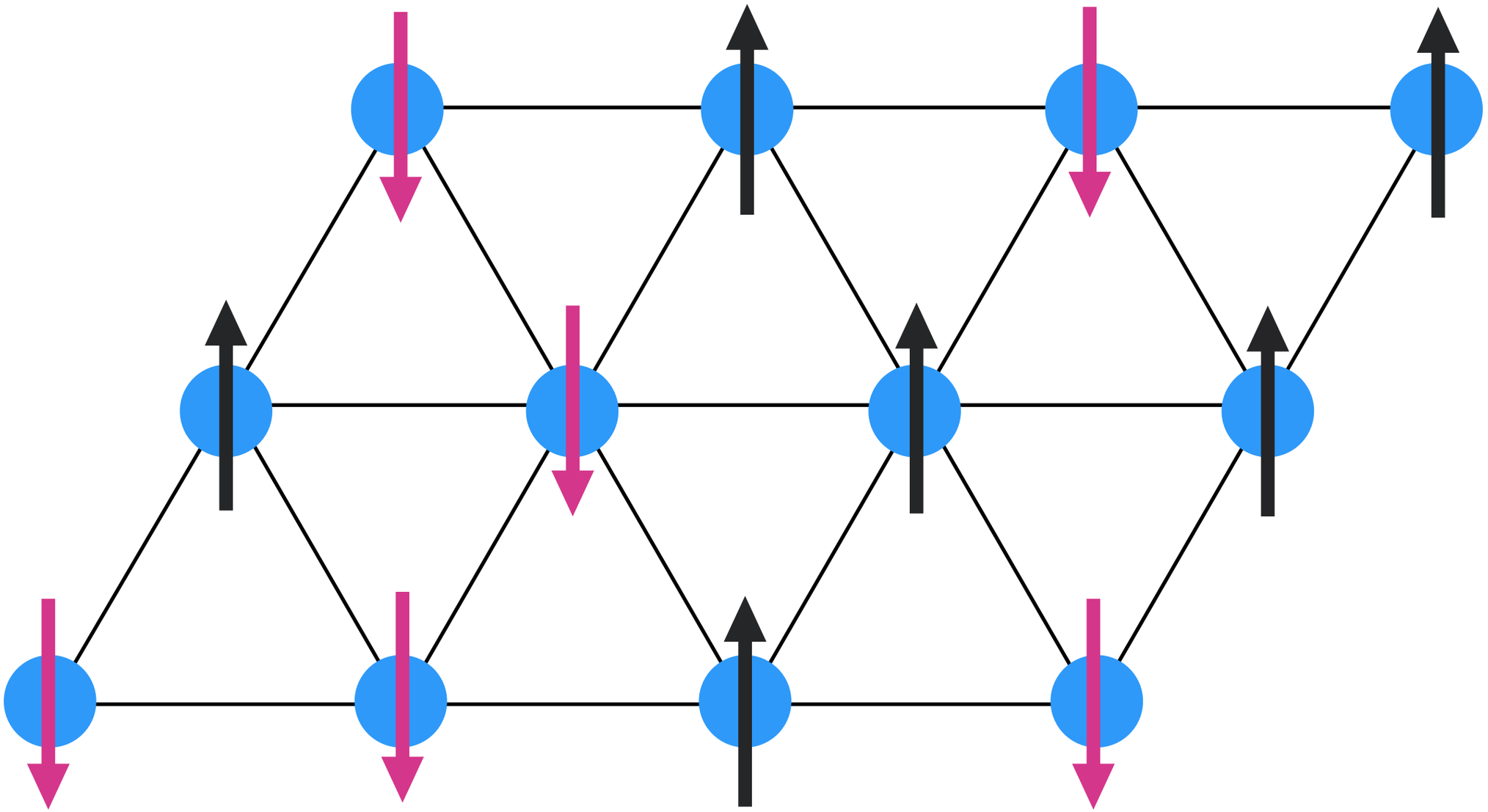

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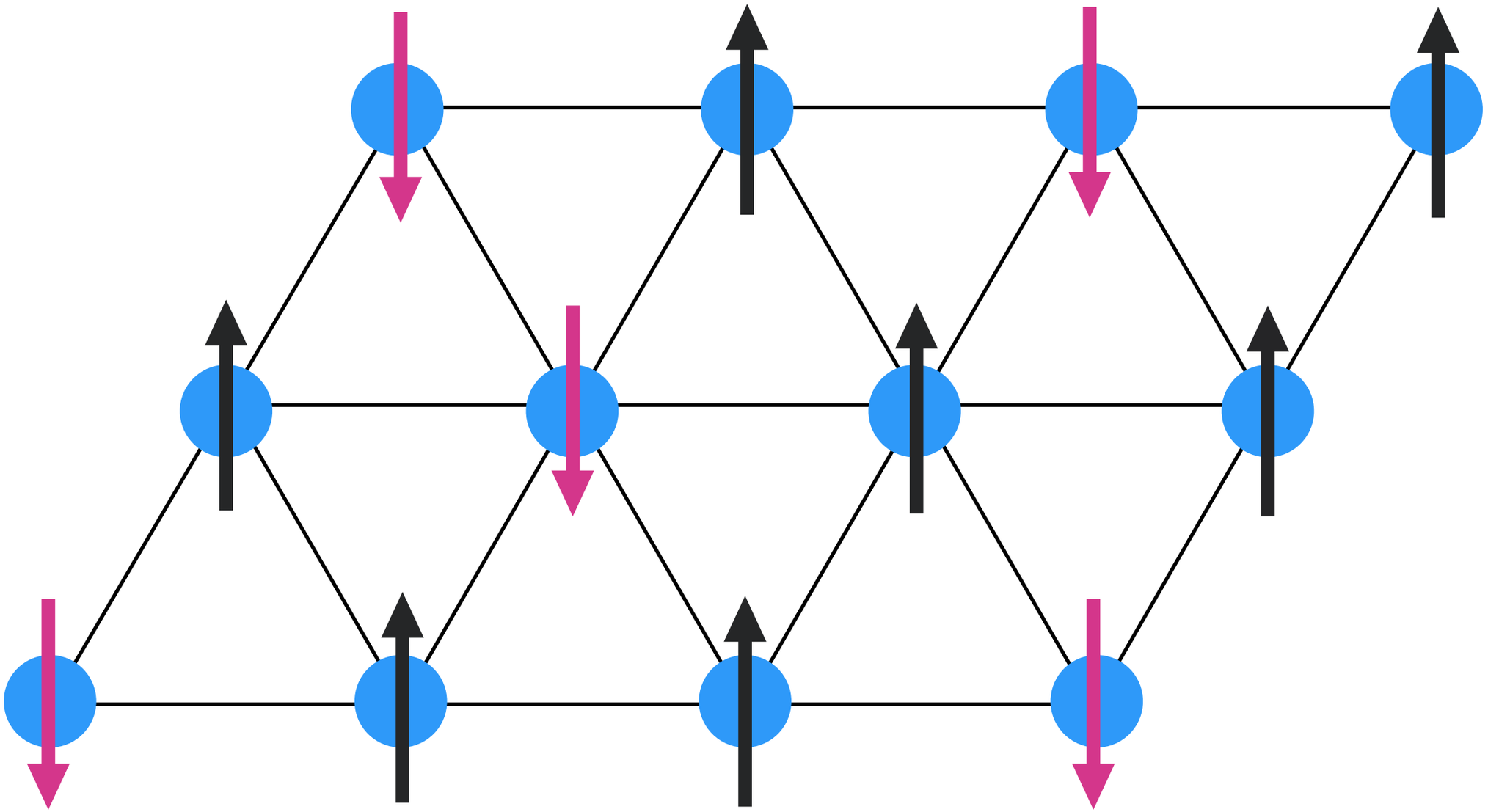

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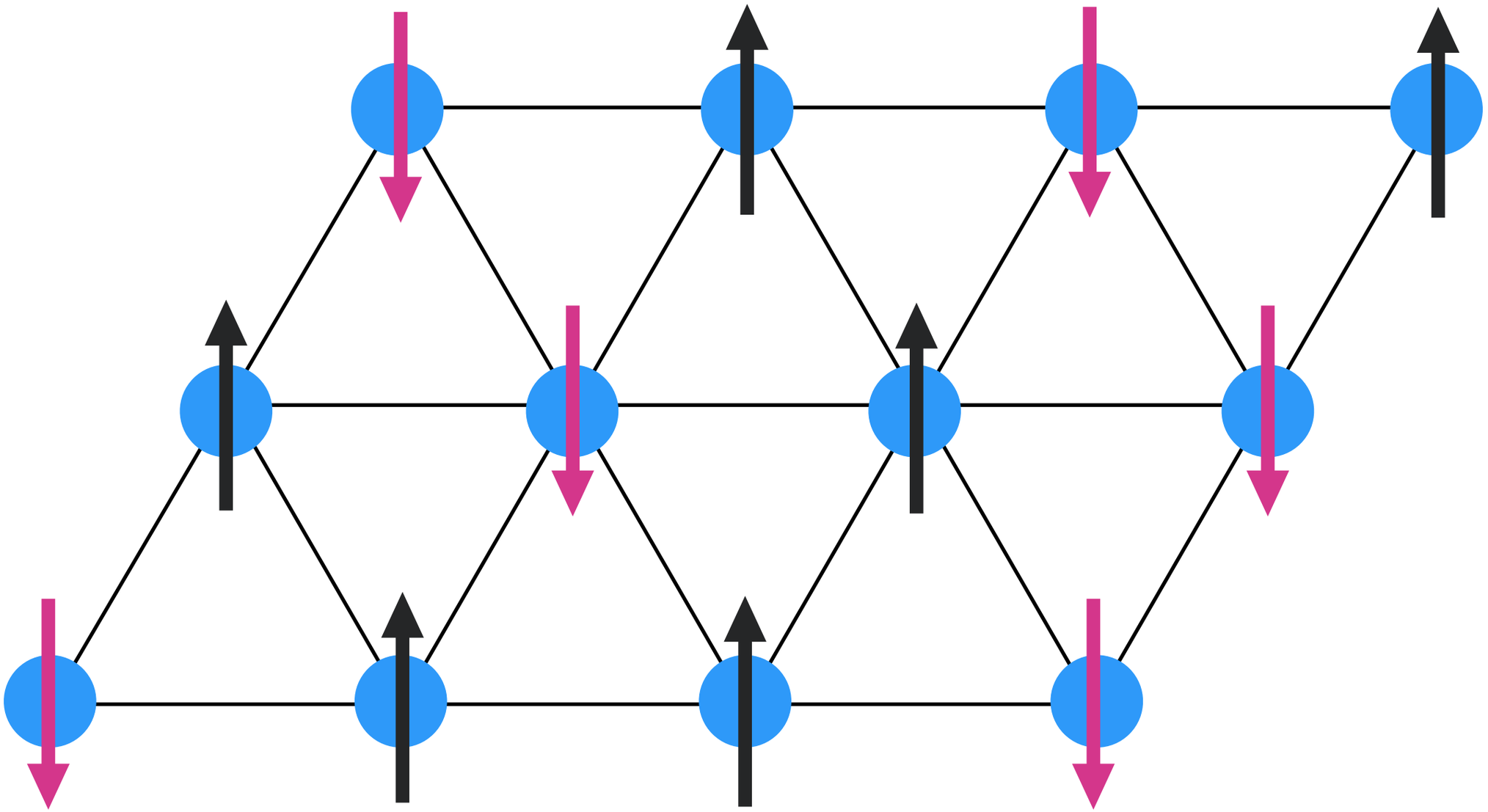

Lack of ordering leads to a strongly correlated spin liquid.

The single-$\vec{q}$ ground states of the classical Heisenberg model are spiral states.

$$H = \frac{1}{2}\sum_{\vec{r},\vec{r}'} J_{\vec{r},\vec{r}'}\vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} \qquad J_{\vec{q}} = \frac{1}{2}\sum_{\vec{r}} J_{\vec{r}}\, e^{i\vec{q}\cdot\vec{r}}\,; \quad S_{\vec{q}} = \frac{1}{\sqrt{V}}\sum_{\vec{r}} S_{\vec{r}}\, e^{-i\vec{q}\cdot\vec{r}}$$

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$$H = \sum_{\vec{q}} J_{\vec{q}} |\vec{S}_{\vec{q}}|^2$$

$$J_{\vec{q}} = \frac{1}{2} \sum_{\vec{r}} J_{\vec{r}}\, e^{i\vec{q}\cdot\vec{r}}\,; \quad S_{\vec{q}} = \frac{1}{\sqrt{V}} \sum_{\vec{r}} S_{\vec{r}}\, e^{-i\vec{q}\cdot\vec{r}}$$

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$$H = \sum_{\vec{q}} J_{\vec{q}} |\vec{S}_{\vec{q}}|^2 \qquad J_{\vec{q}} = \frac{1}{2} \sum_{\vec{r}} J_{\vec{r}}\, e^{i\vec{q}\cdot\vec{r}}\,; \quad S_{\vec{q}} = \frac{1}{\sqrt{V}} \sum_{\vec{r}} S_{\vec{r}}\, e^{-i\vec{q}\cdot\vec{r}}$$

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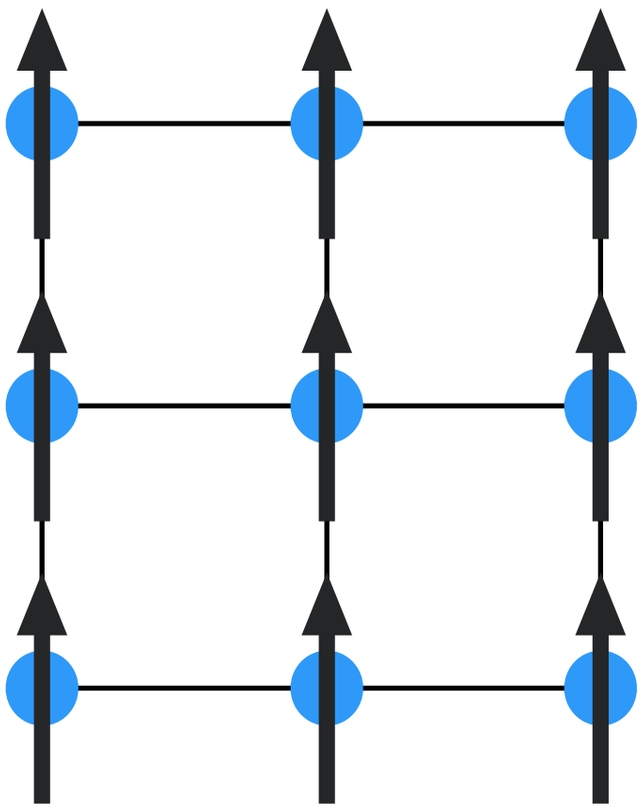
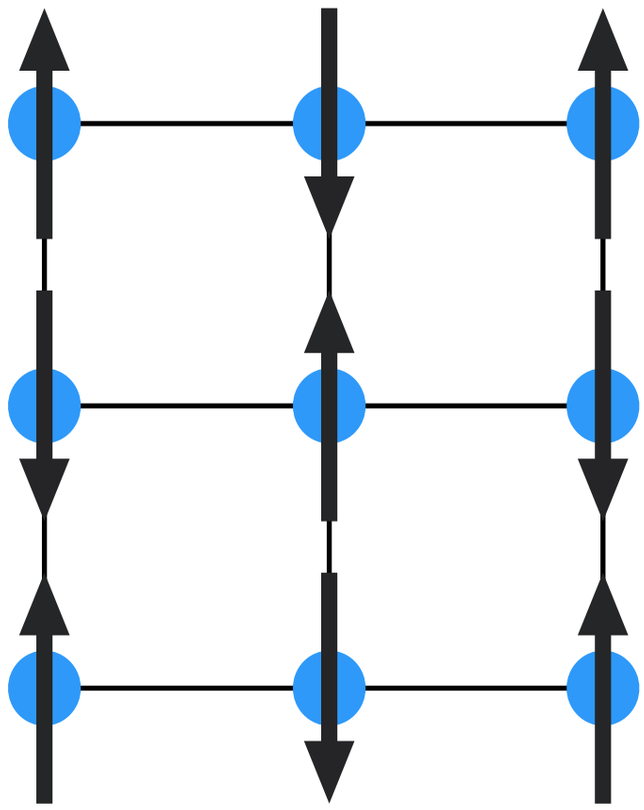
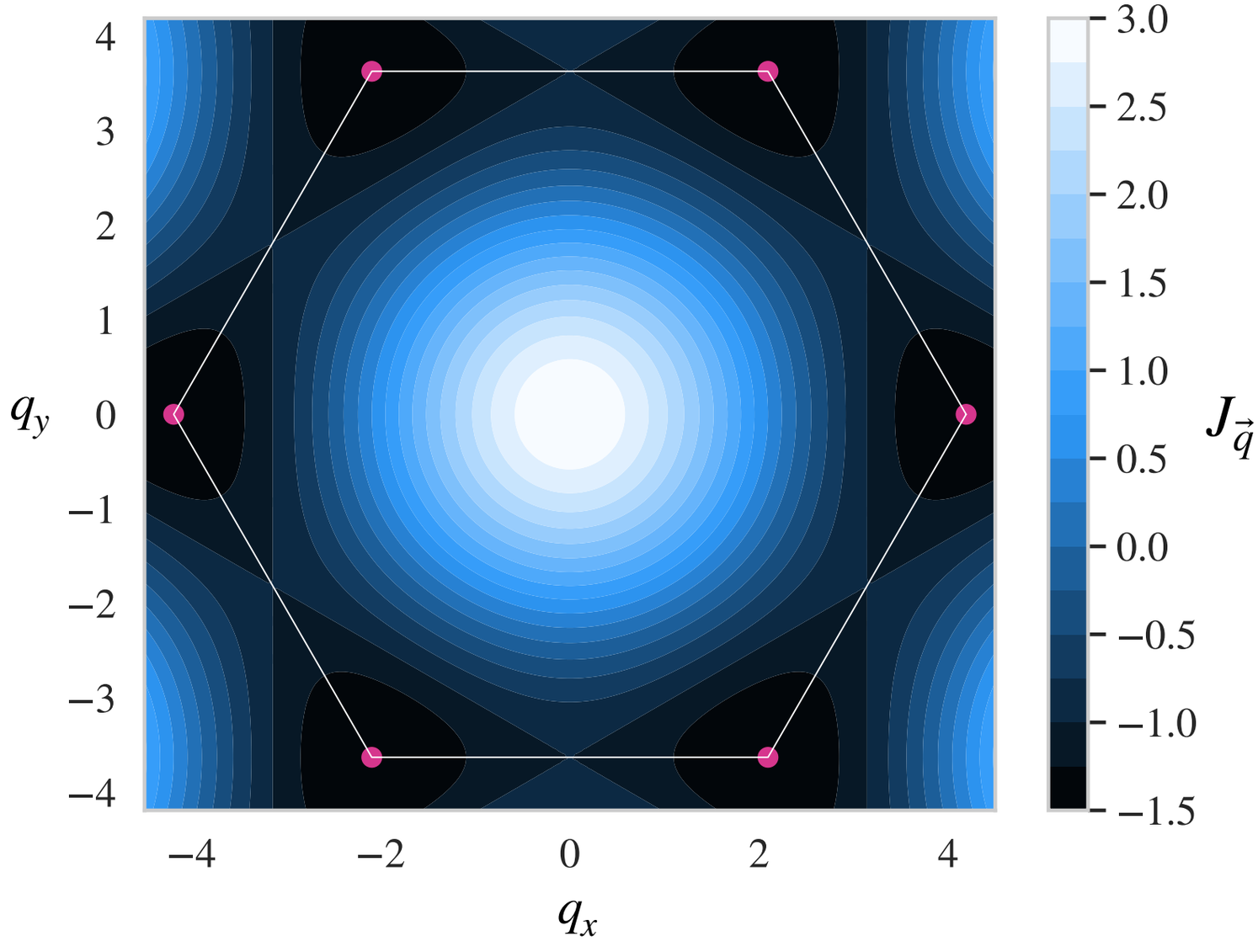


$\overrightarrow{Q} = (0, 0)$



$\overrightarrow{Q} = (\pi, \pi)$

The Heisenberg model on the triangular lattice orders in a 120 degree phase.



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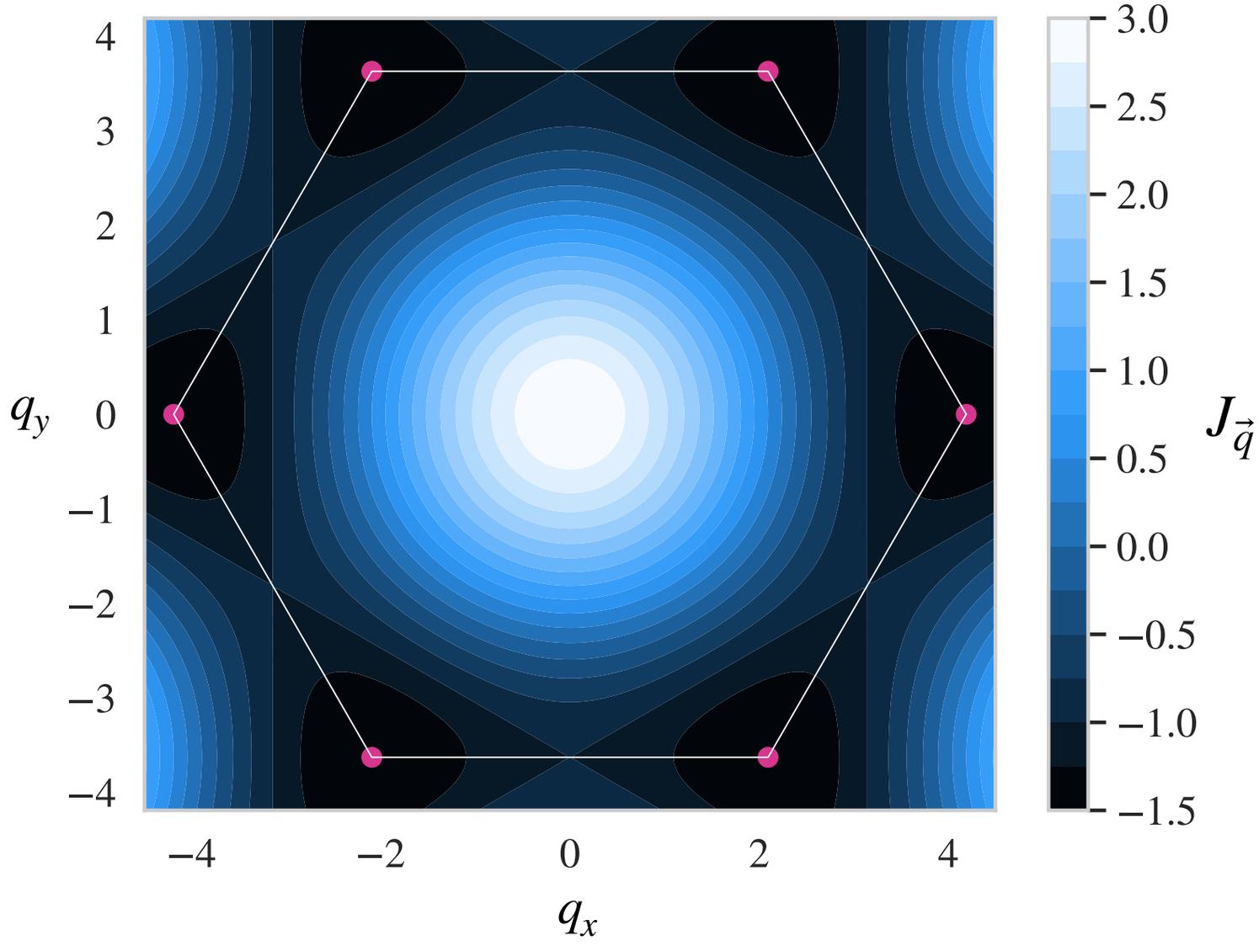

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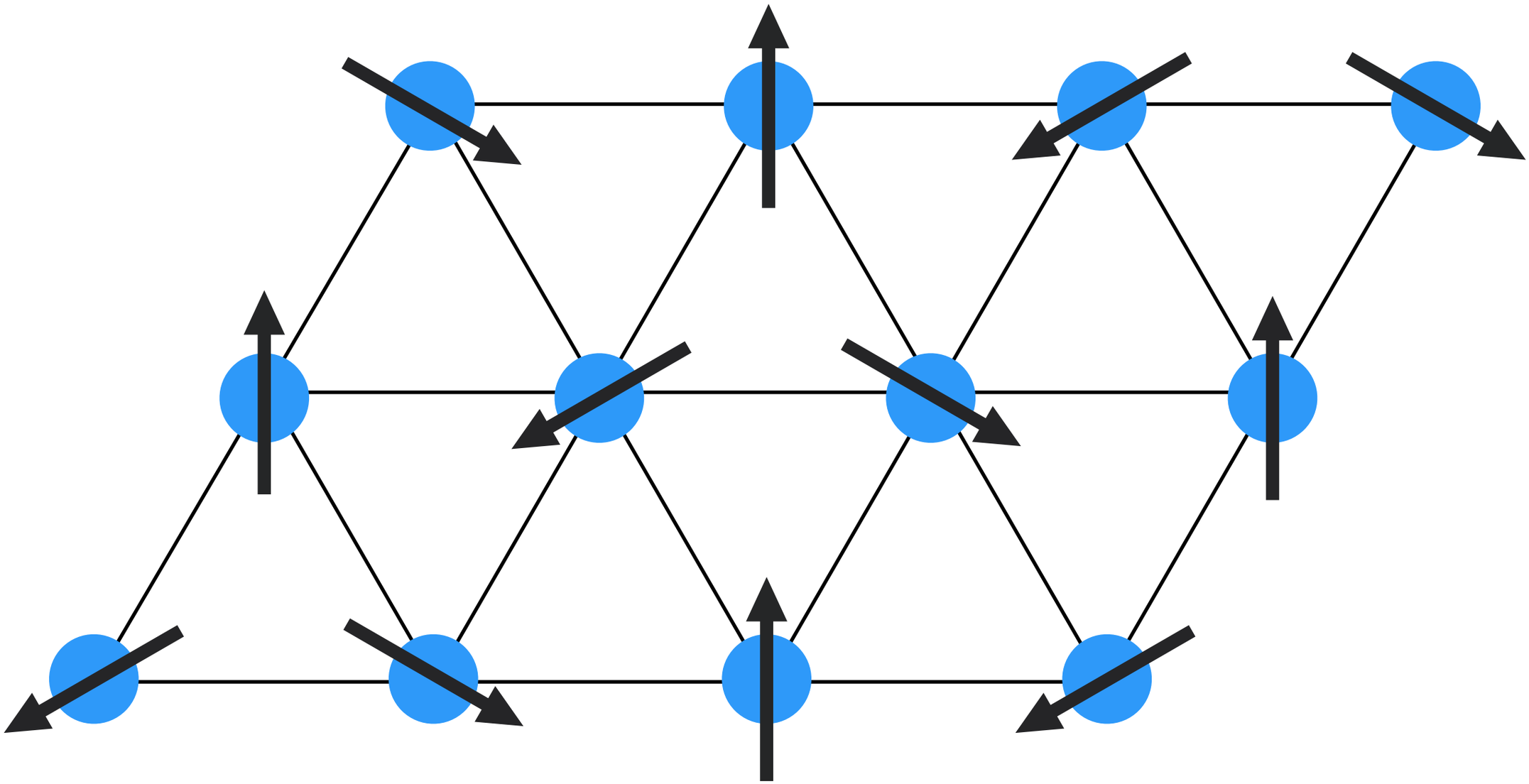

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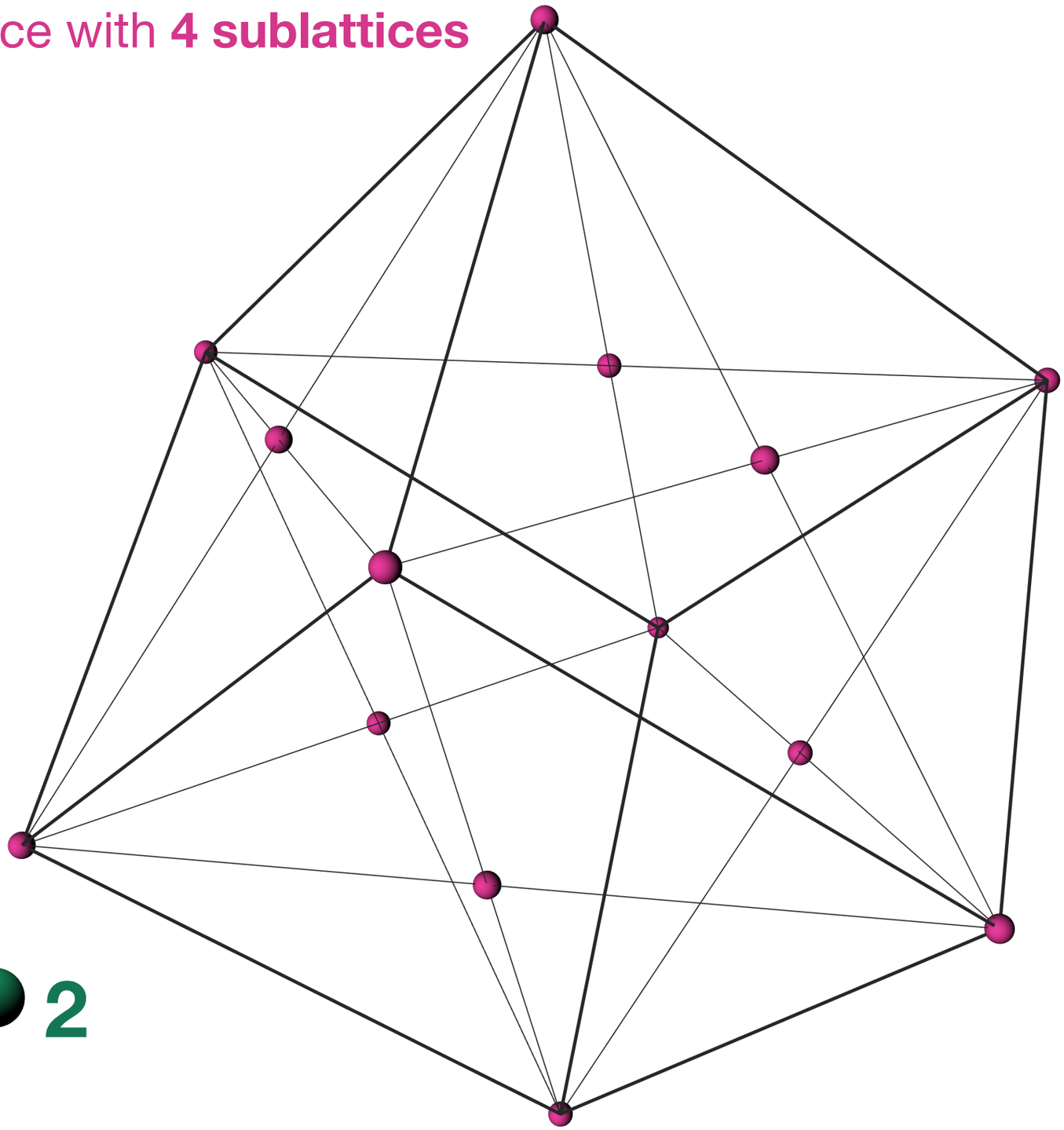
The highly frustrated pyrochlore lattice:

corner sharing tetrahedra

or equivalently

face centered cubic **(fcc)** lattice with **4 sublattices**



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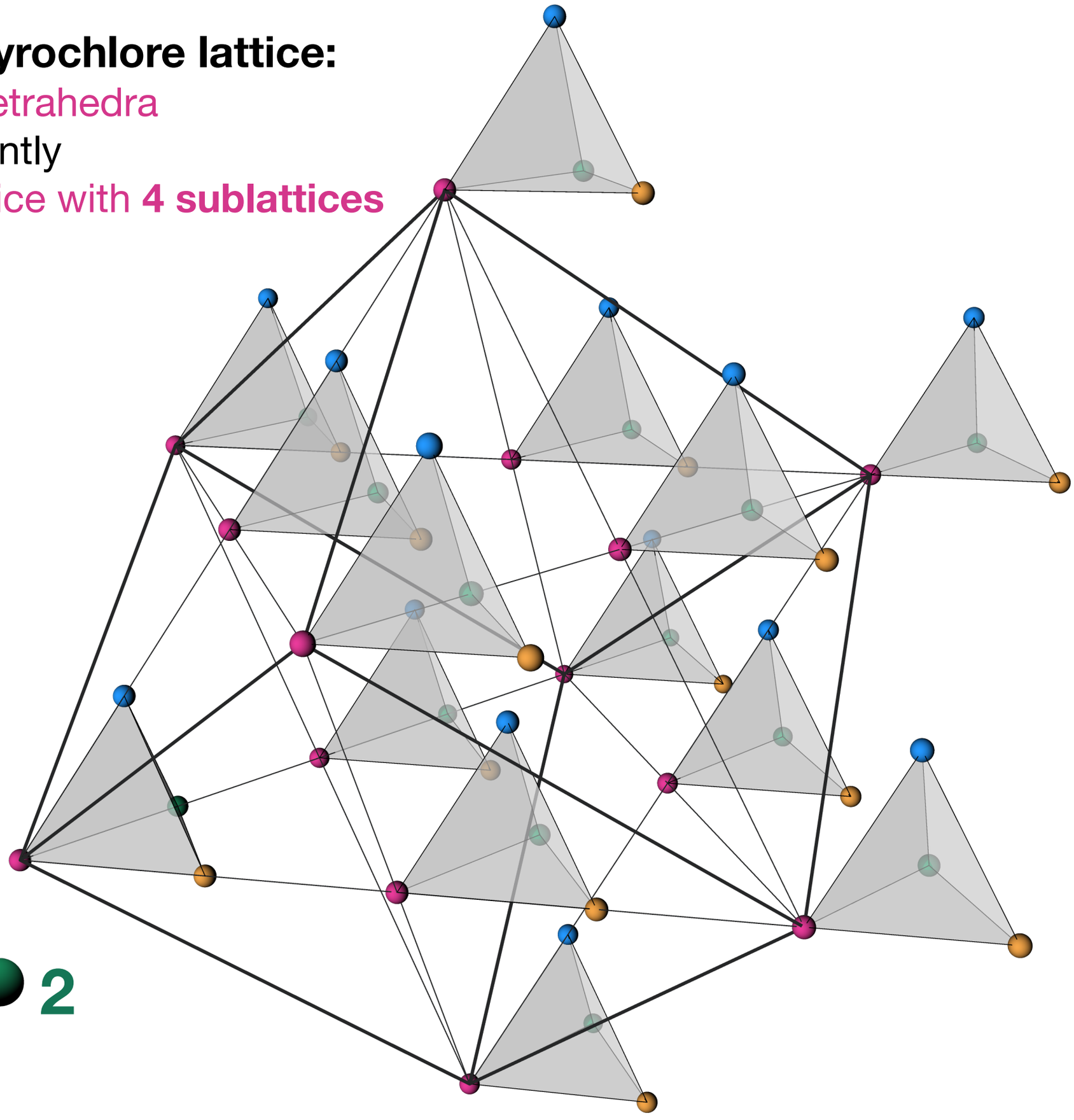

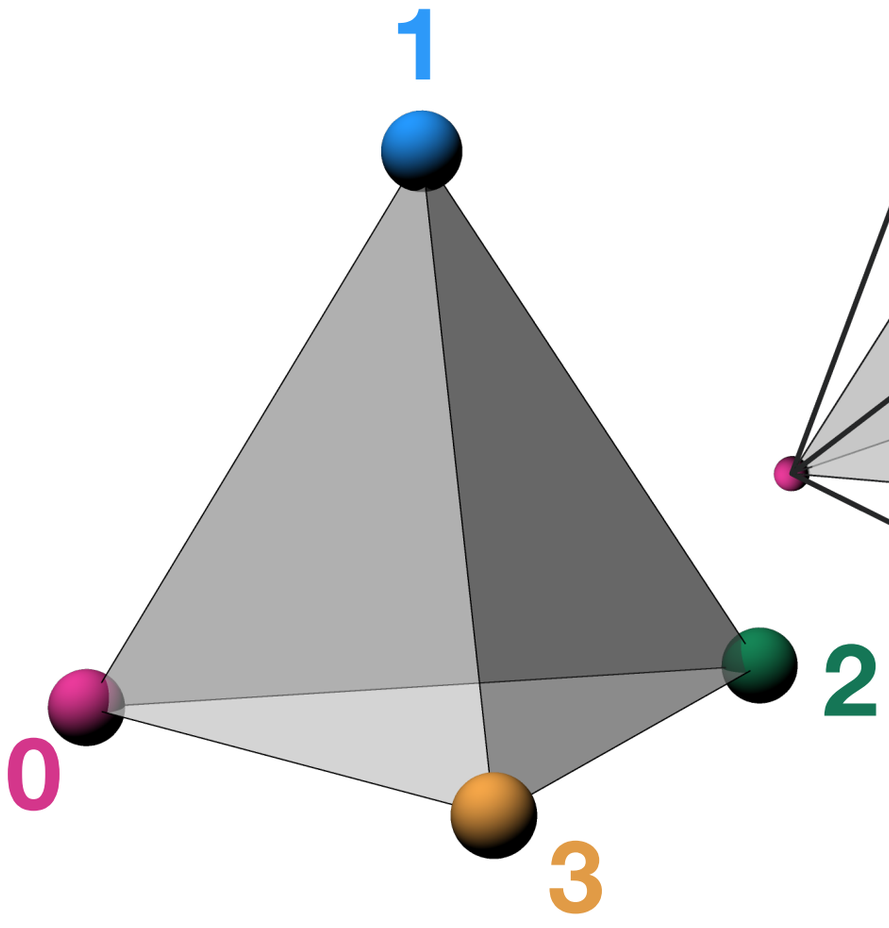

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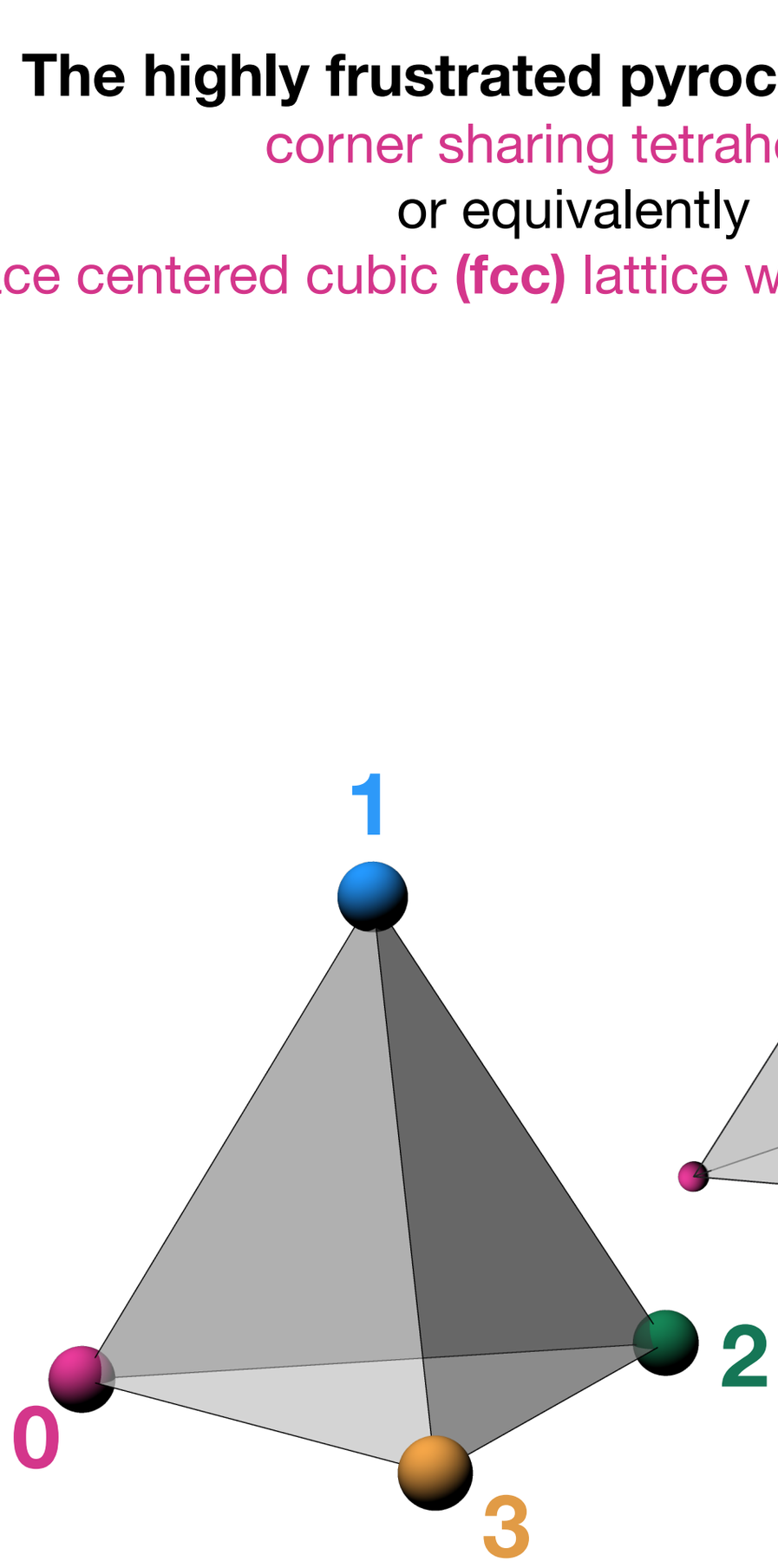

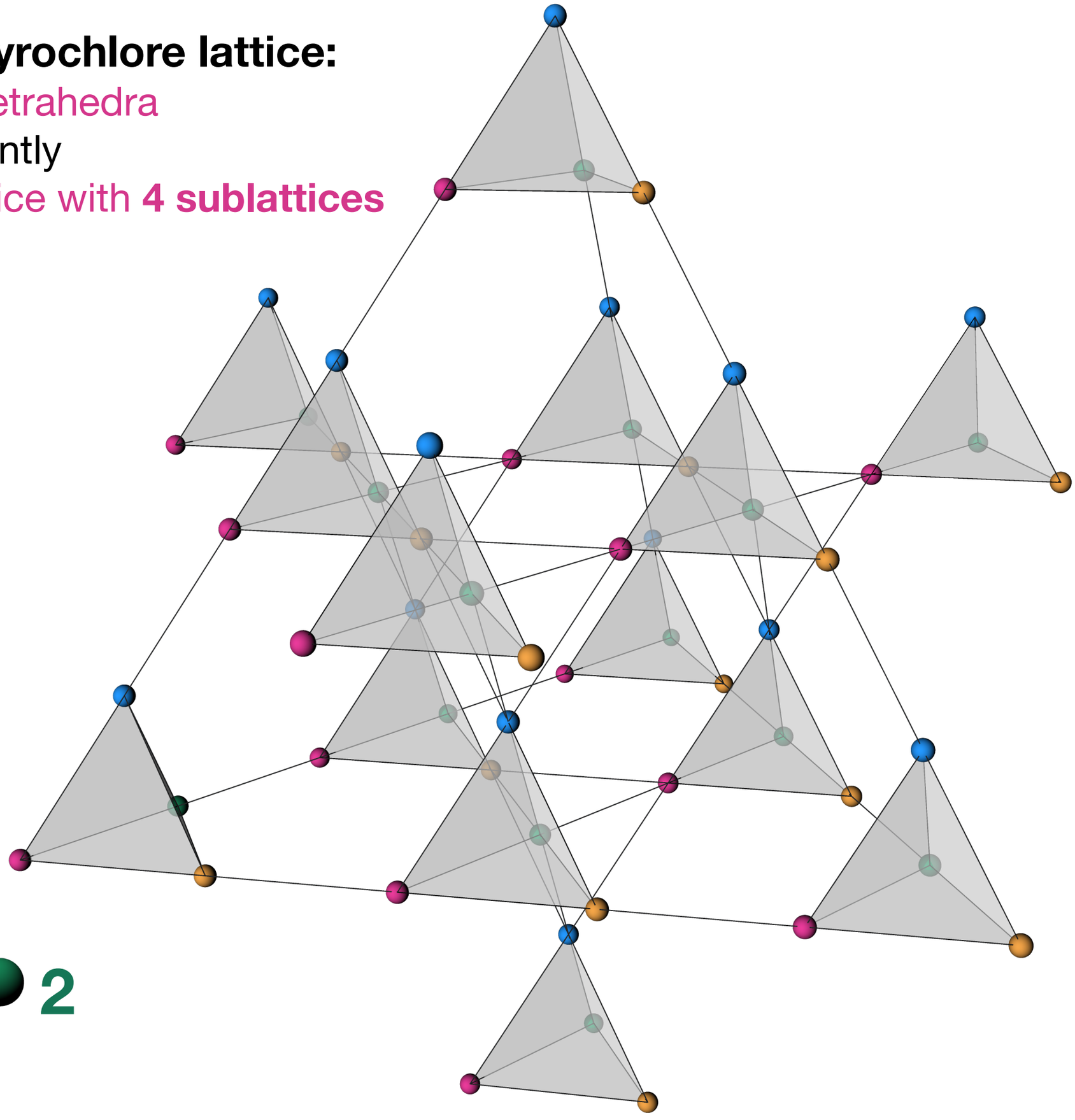

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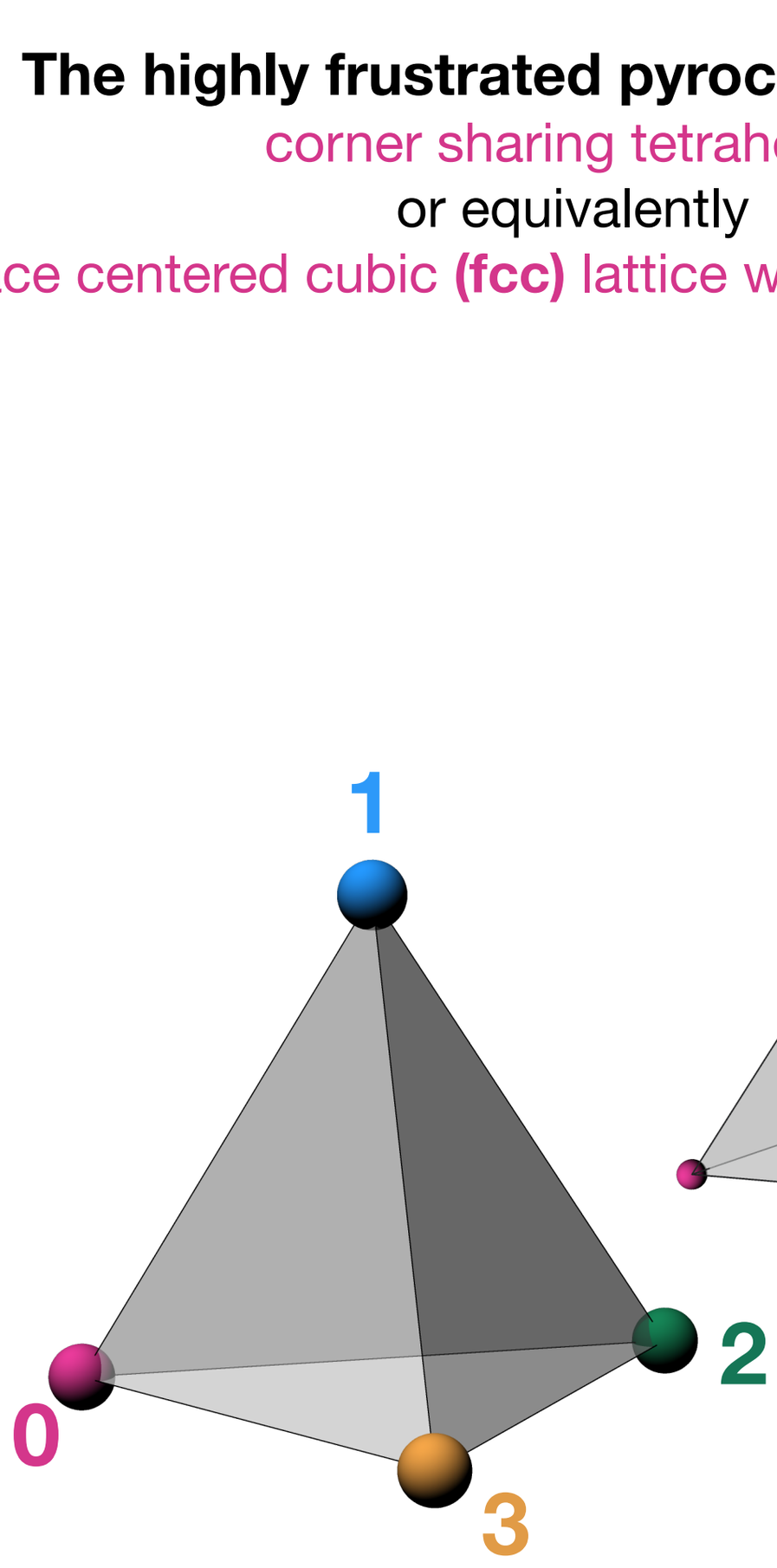

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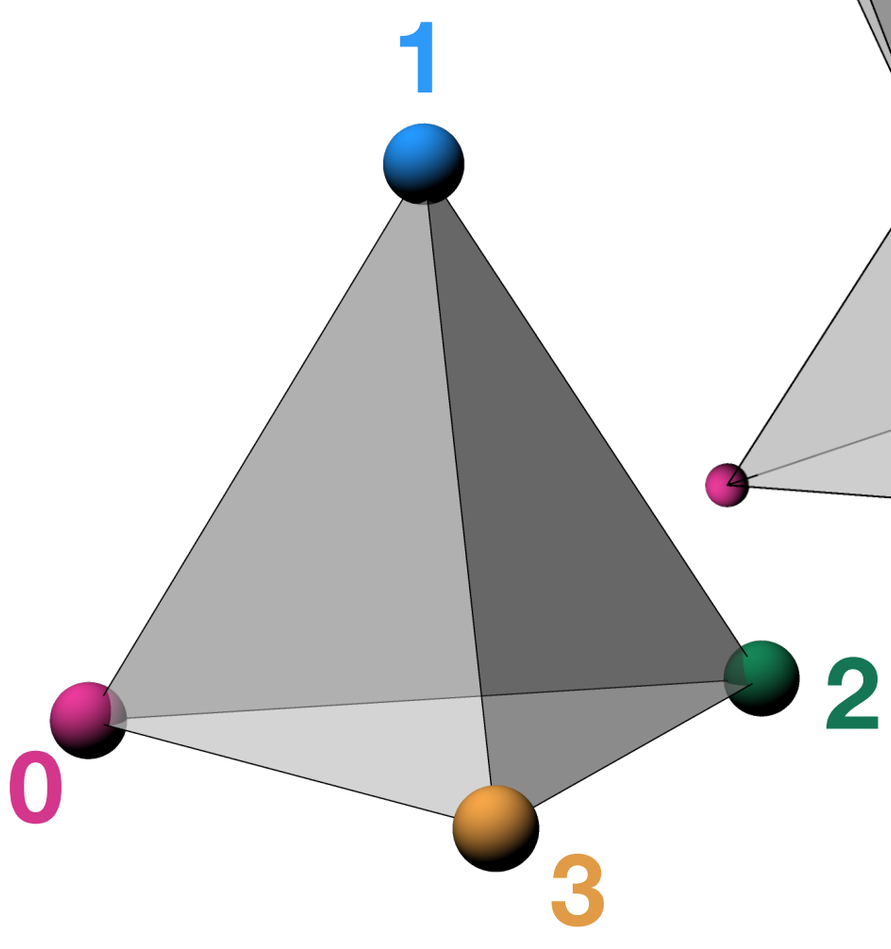

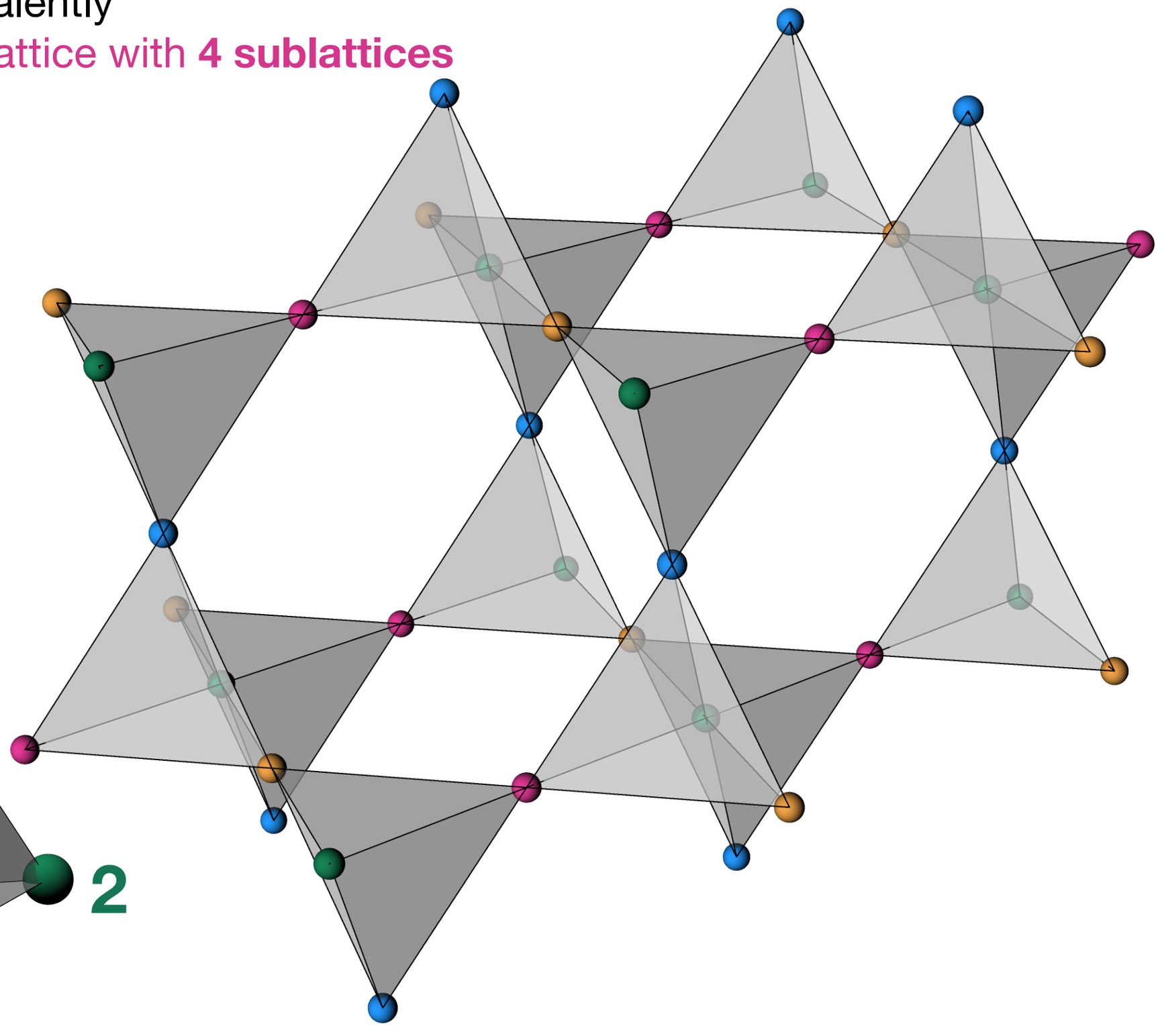

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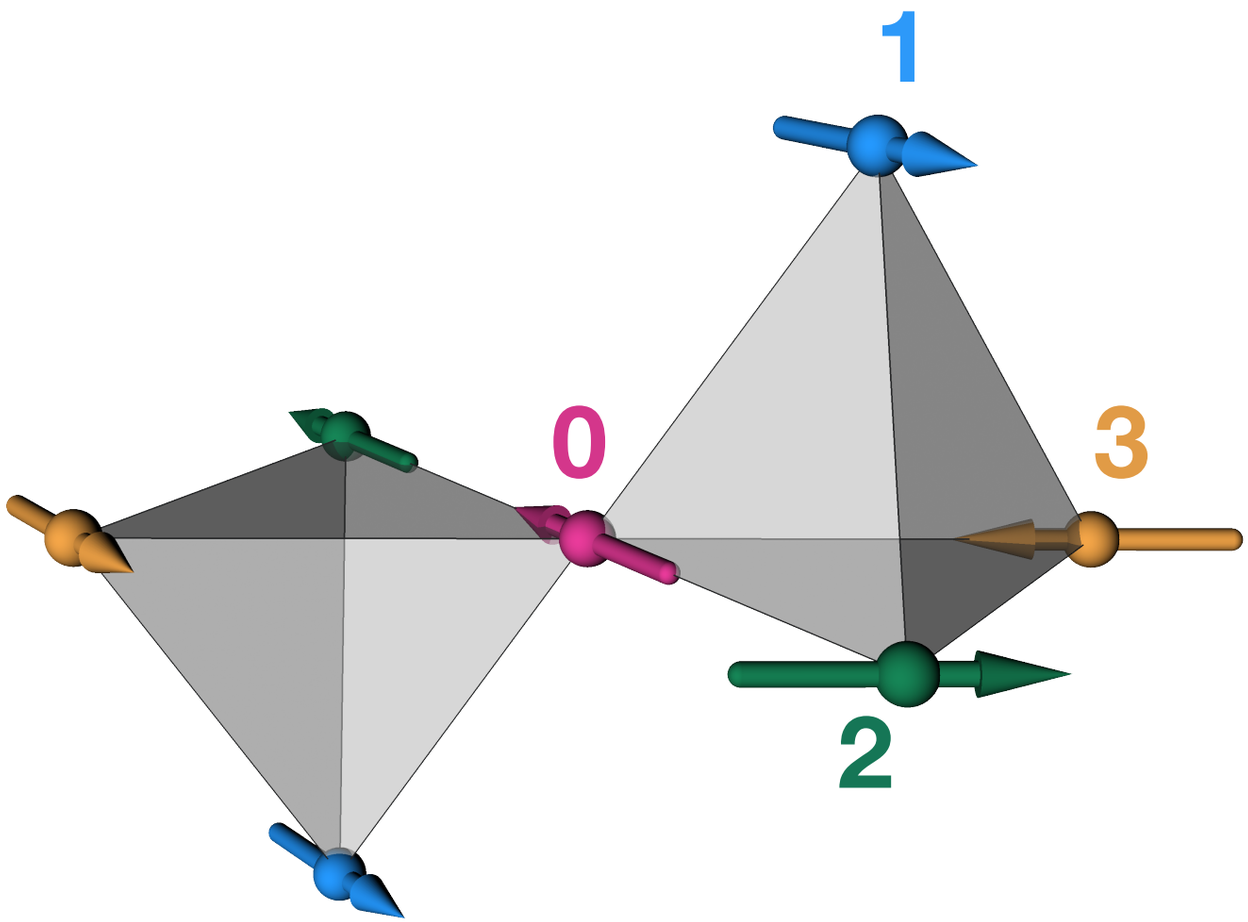

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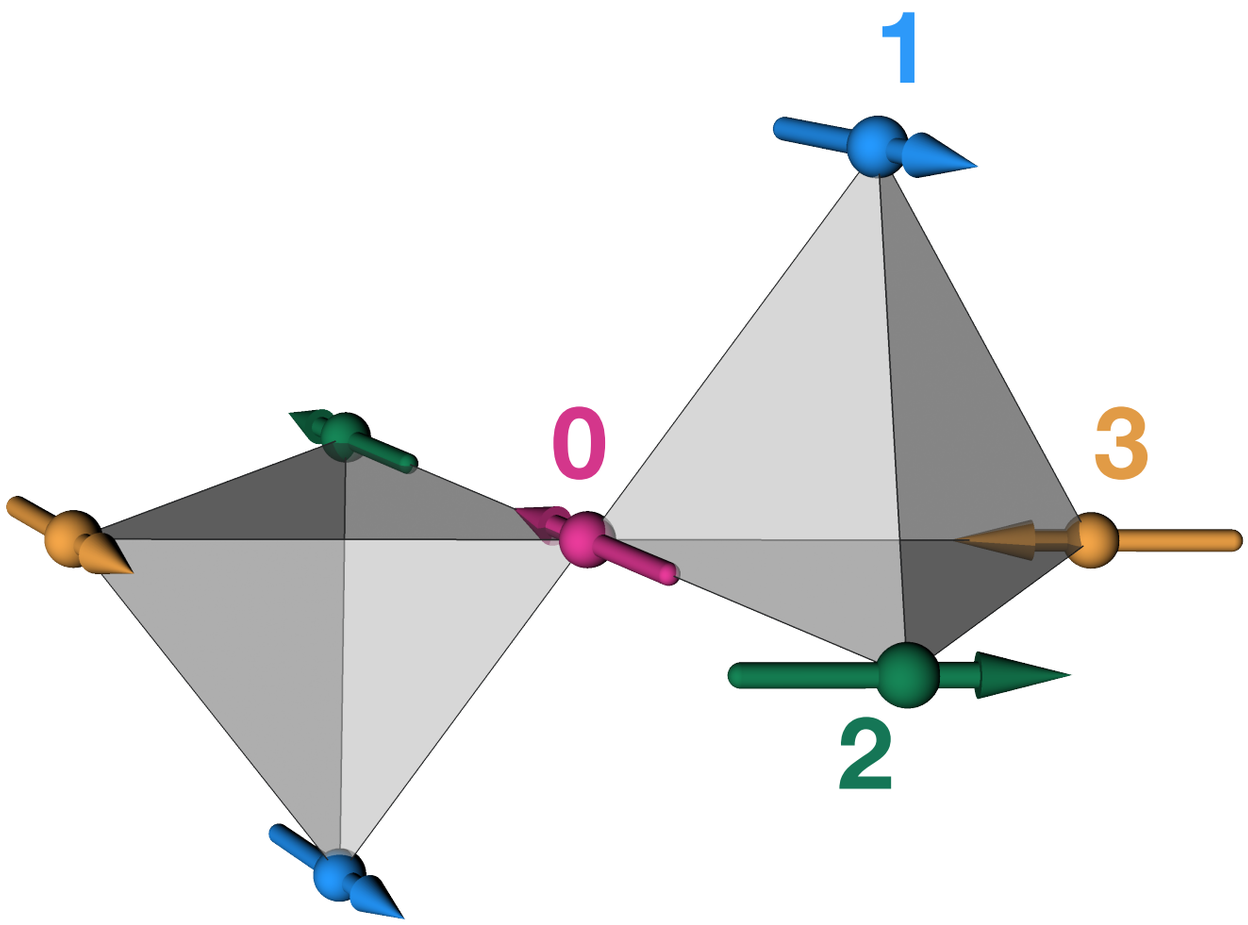

J. N. Reimers, Phys. Rev. B **45**, 7287 (1992).
R. Moessner and J. T. Chalker, Phys. Rev. Lett. **80**, 2929 (1998).

Spin liquid

Paramagnet

T

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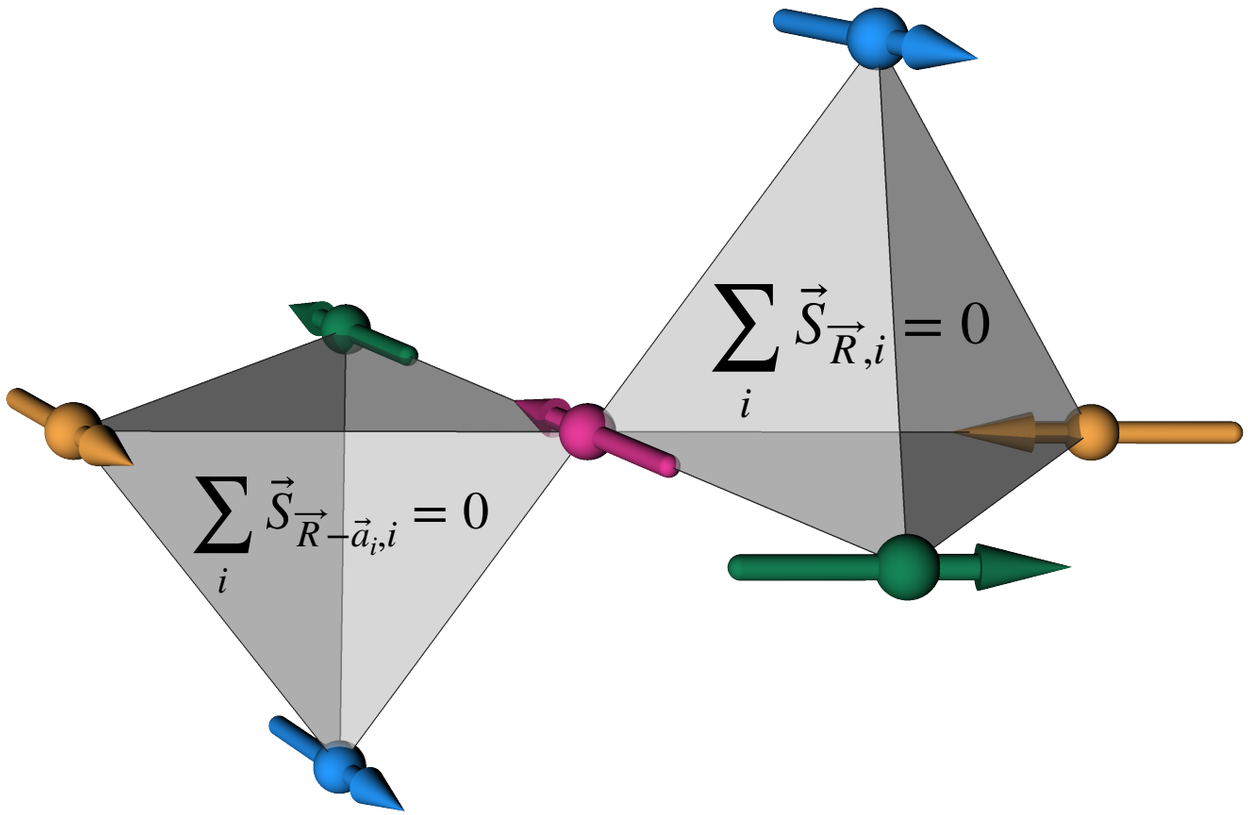

Phys. Rev. B 108, 014413 (2023)

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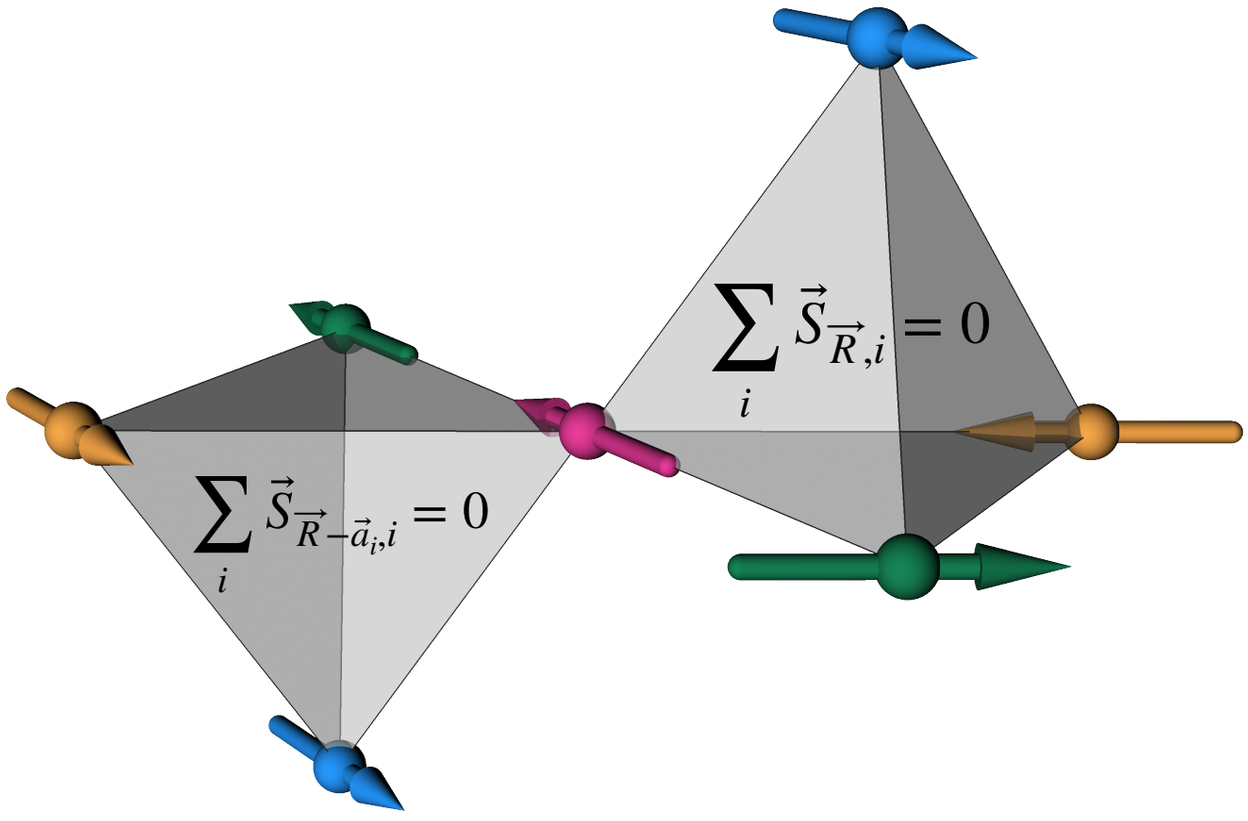

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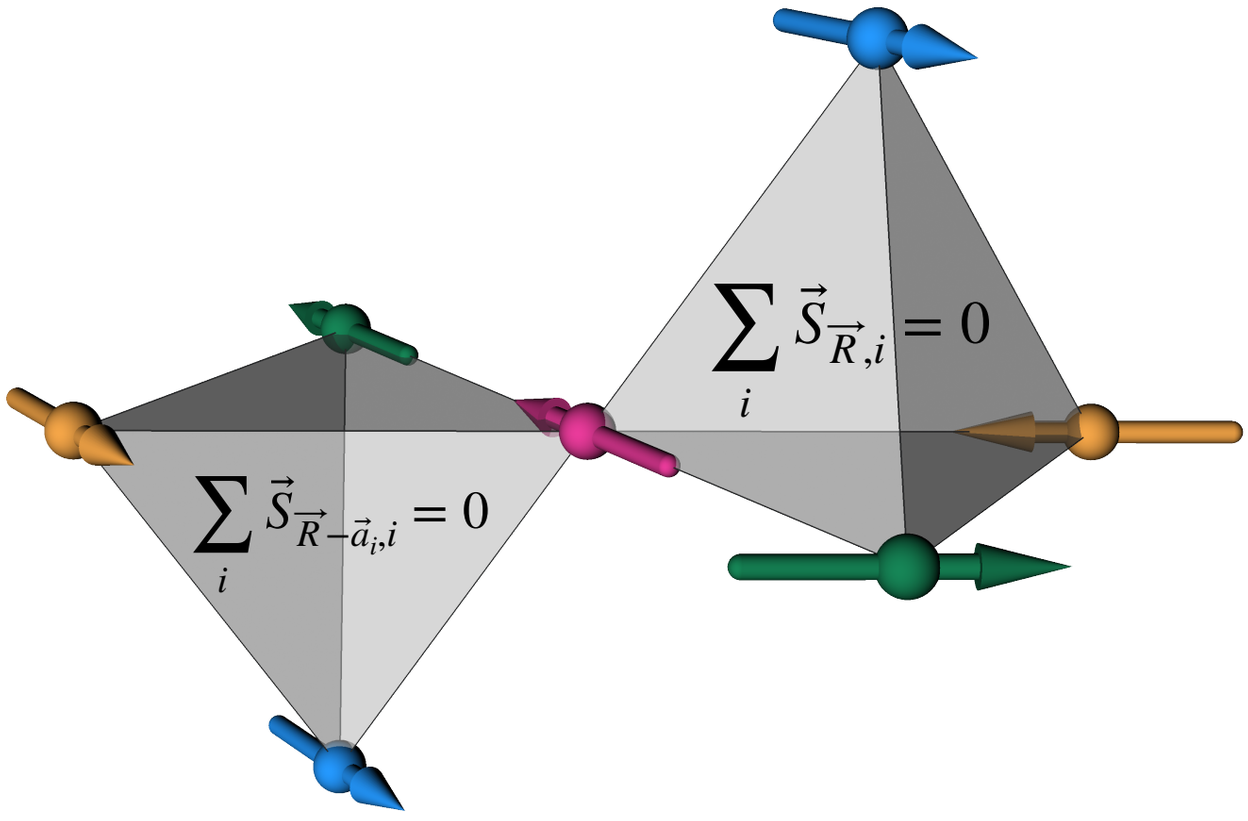

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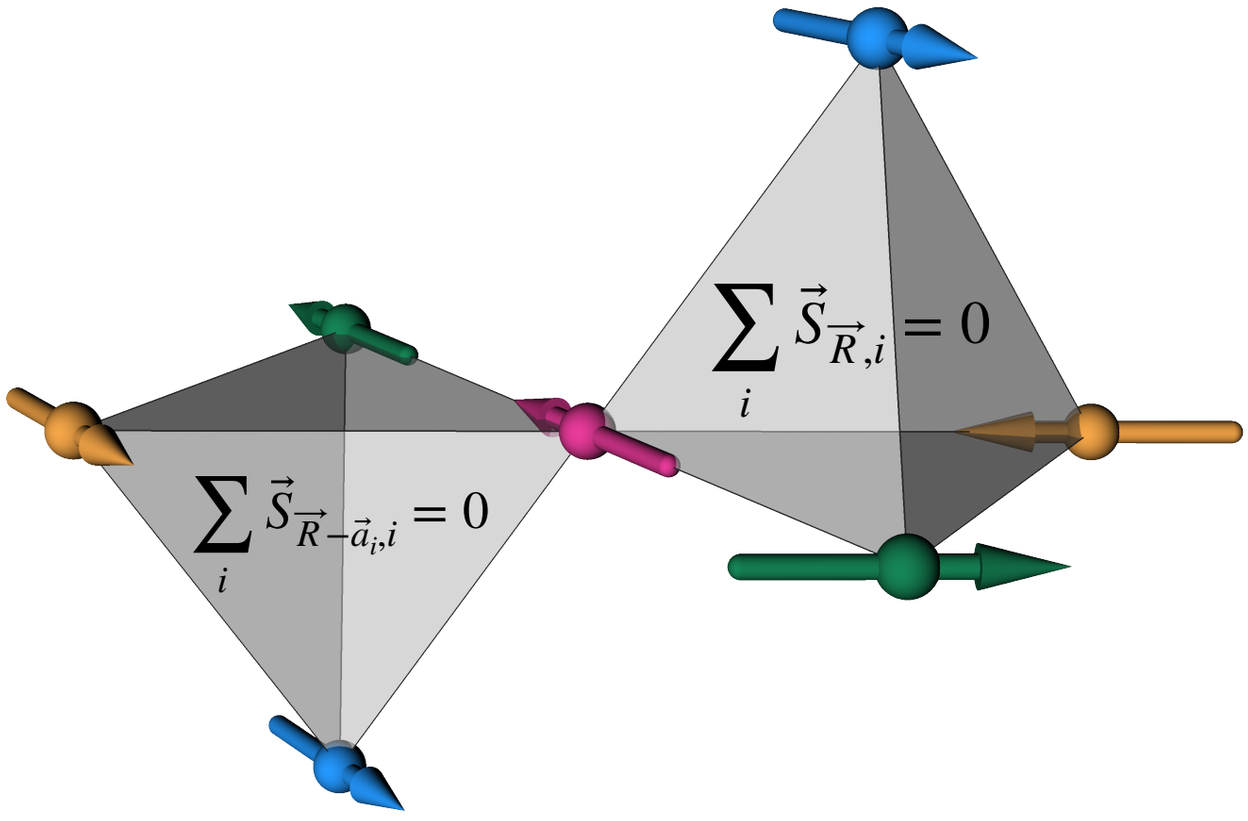

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Sublattice pairing states: two and two sublattices form antiparallel spirals

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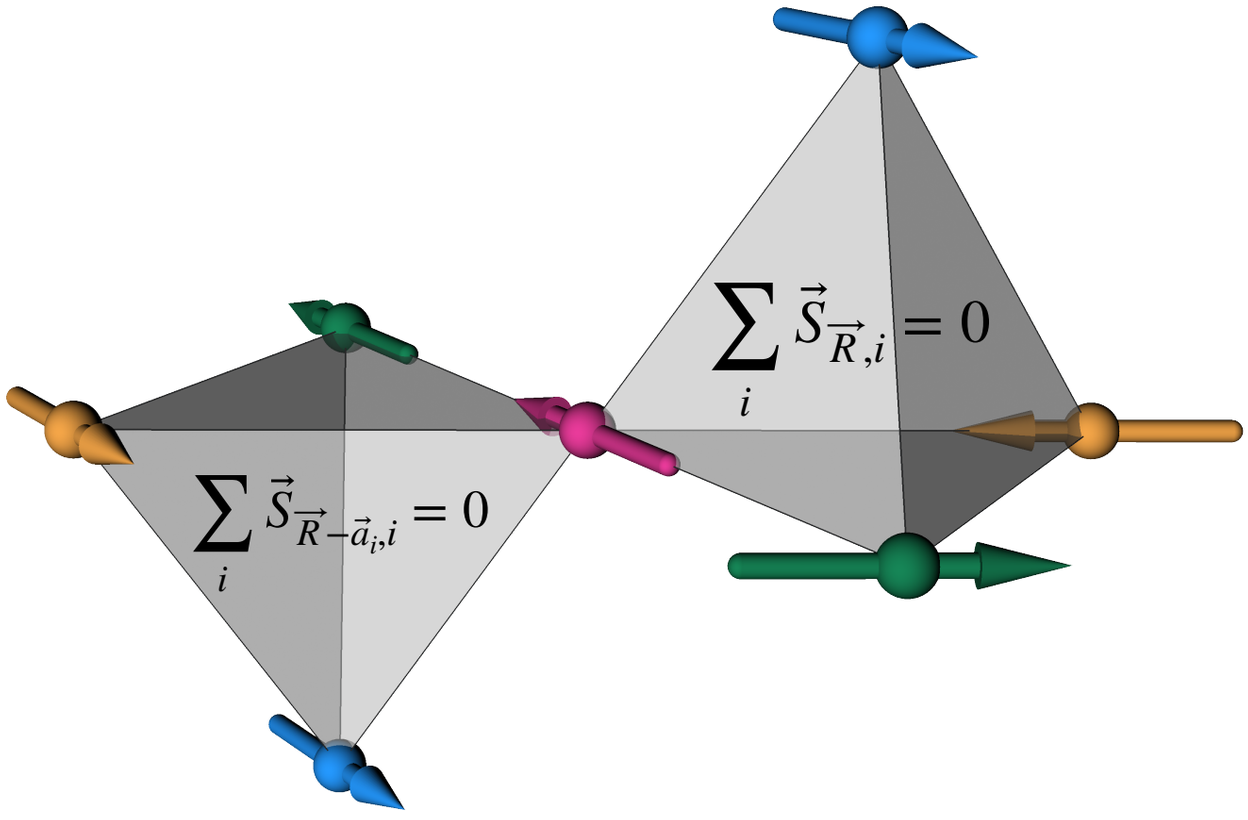

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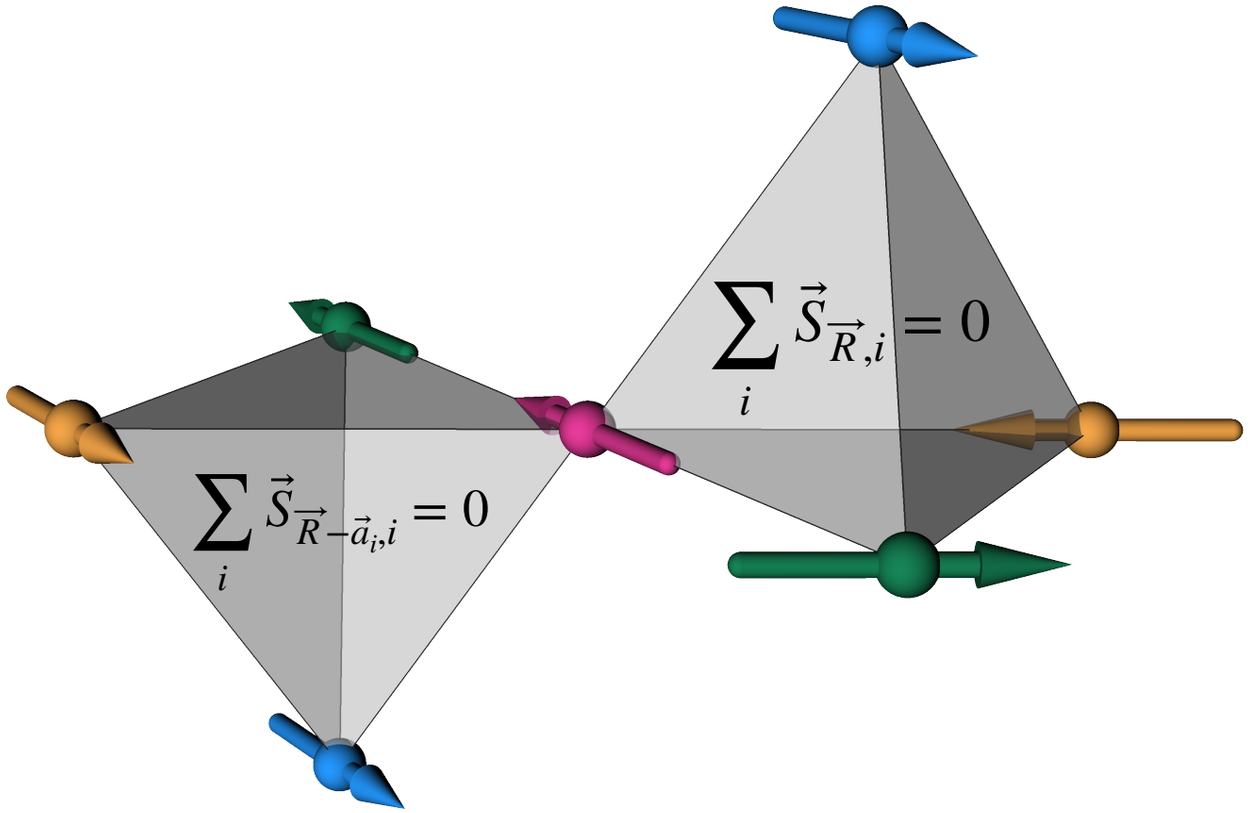

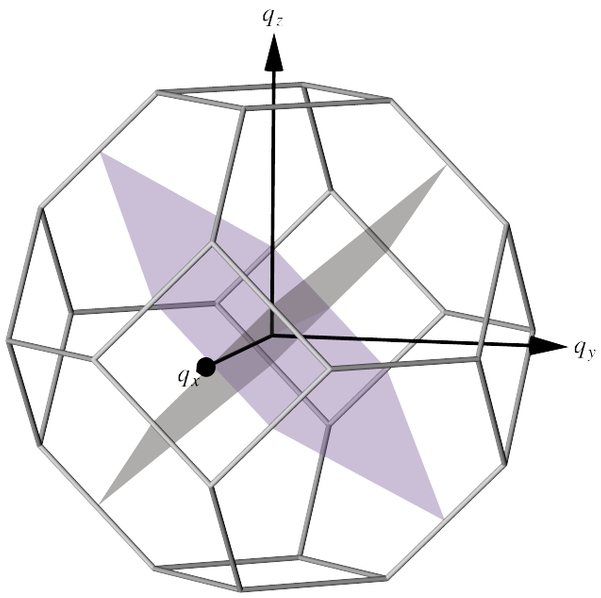

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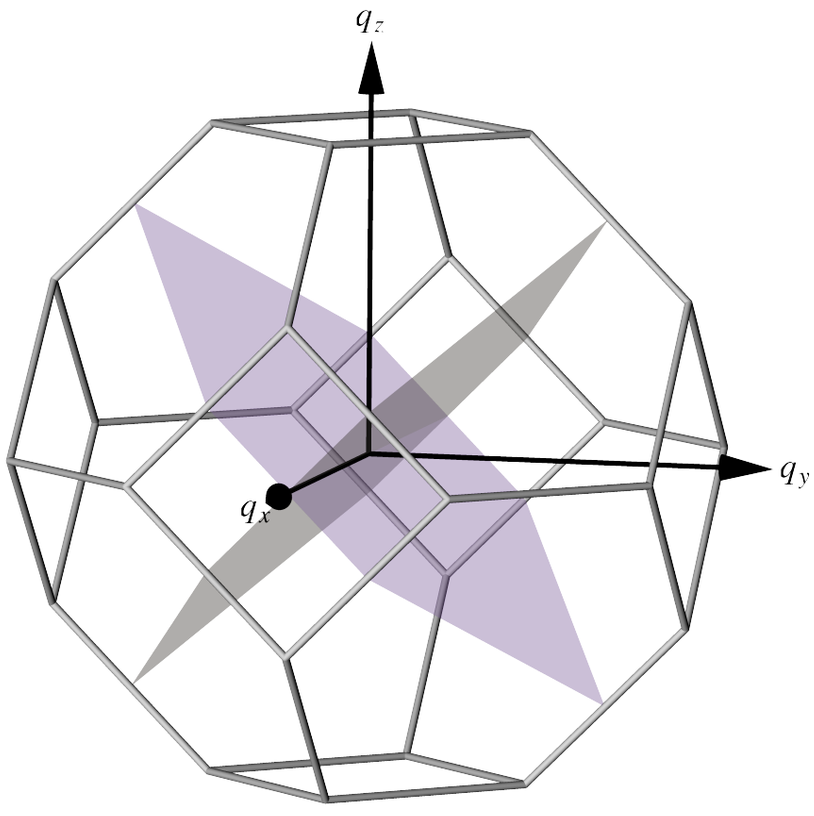

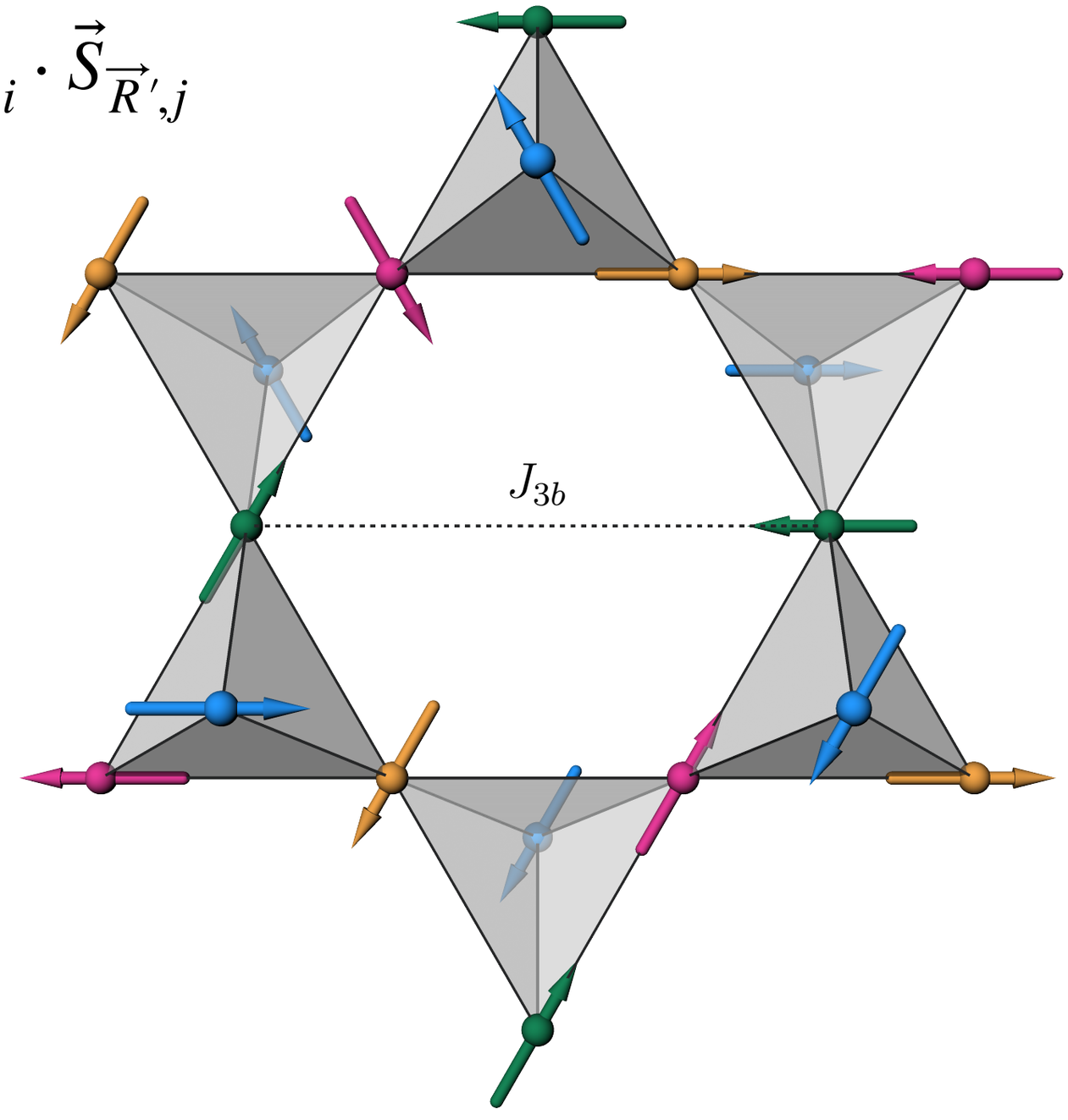

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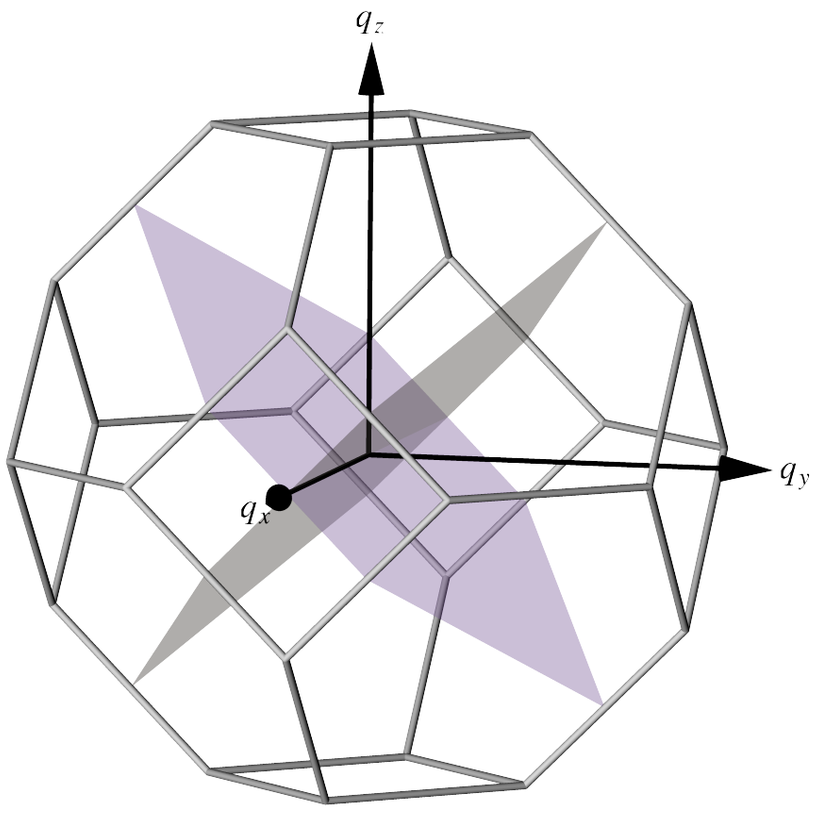

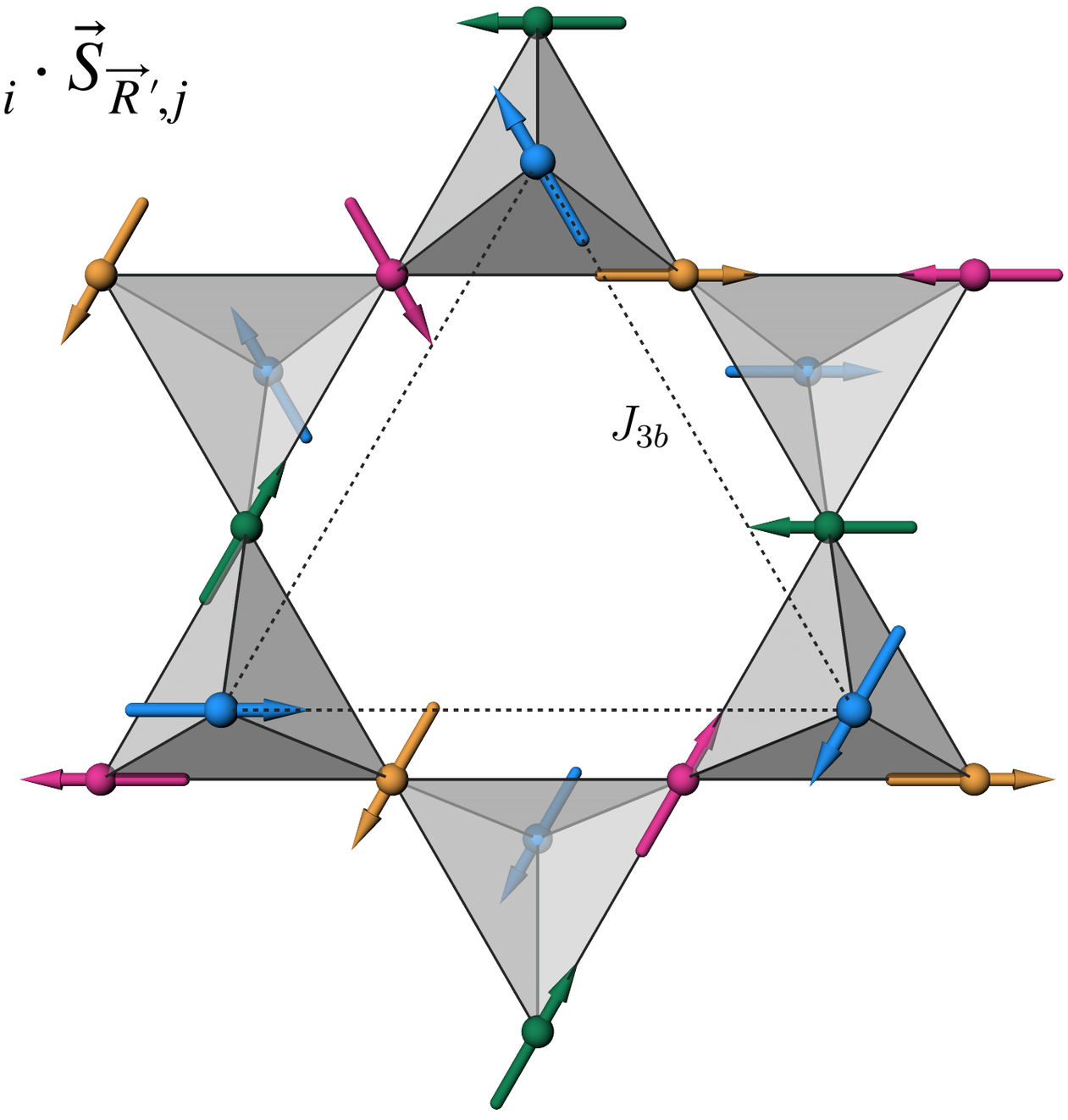

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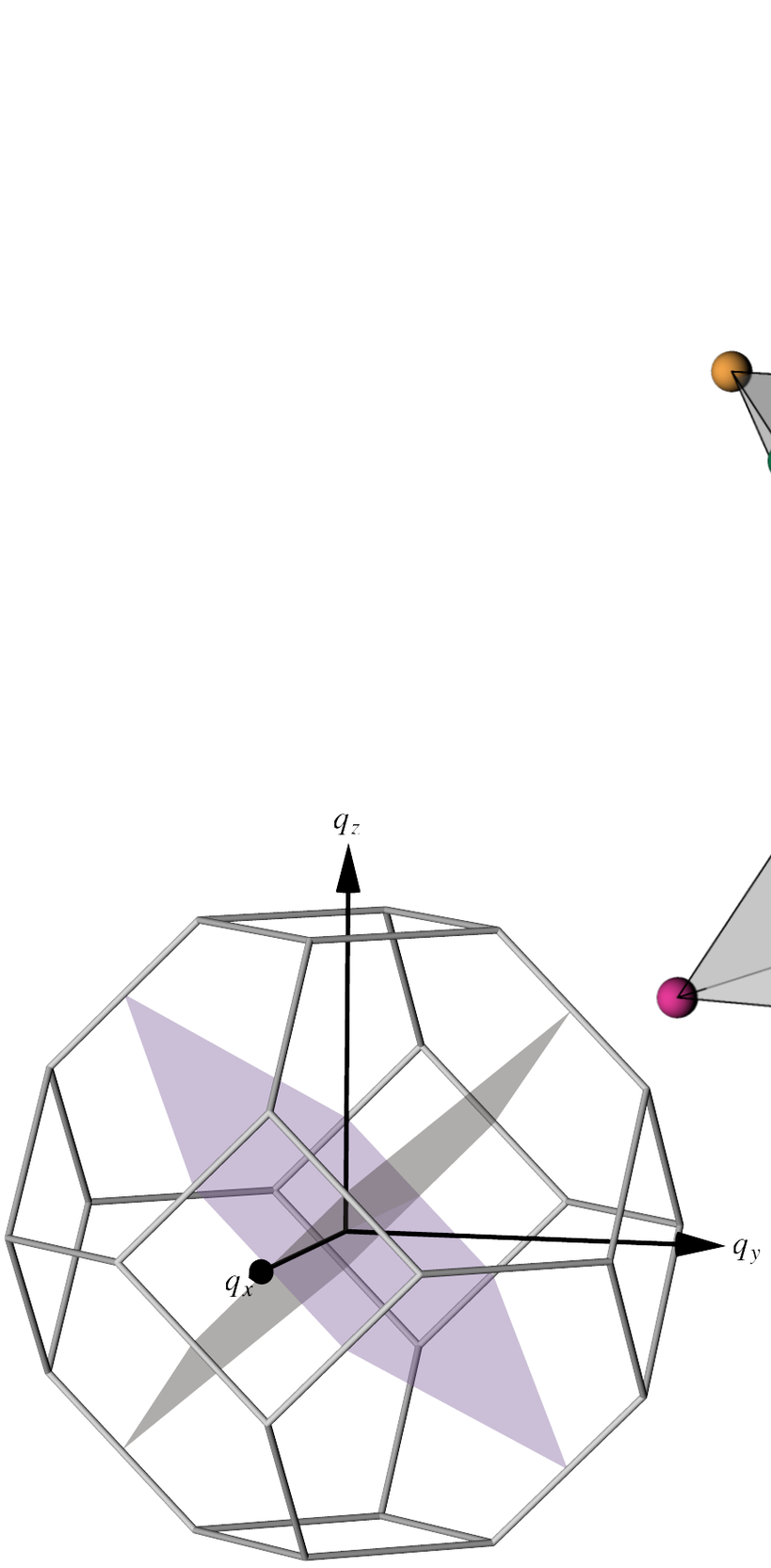

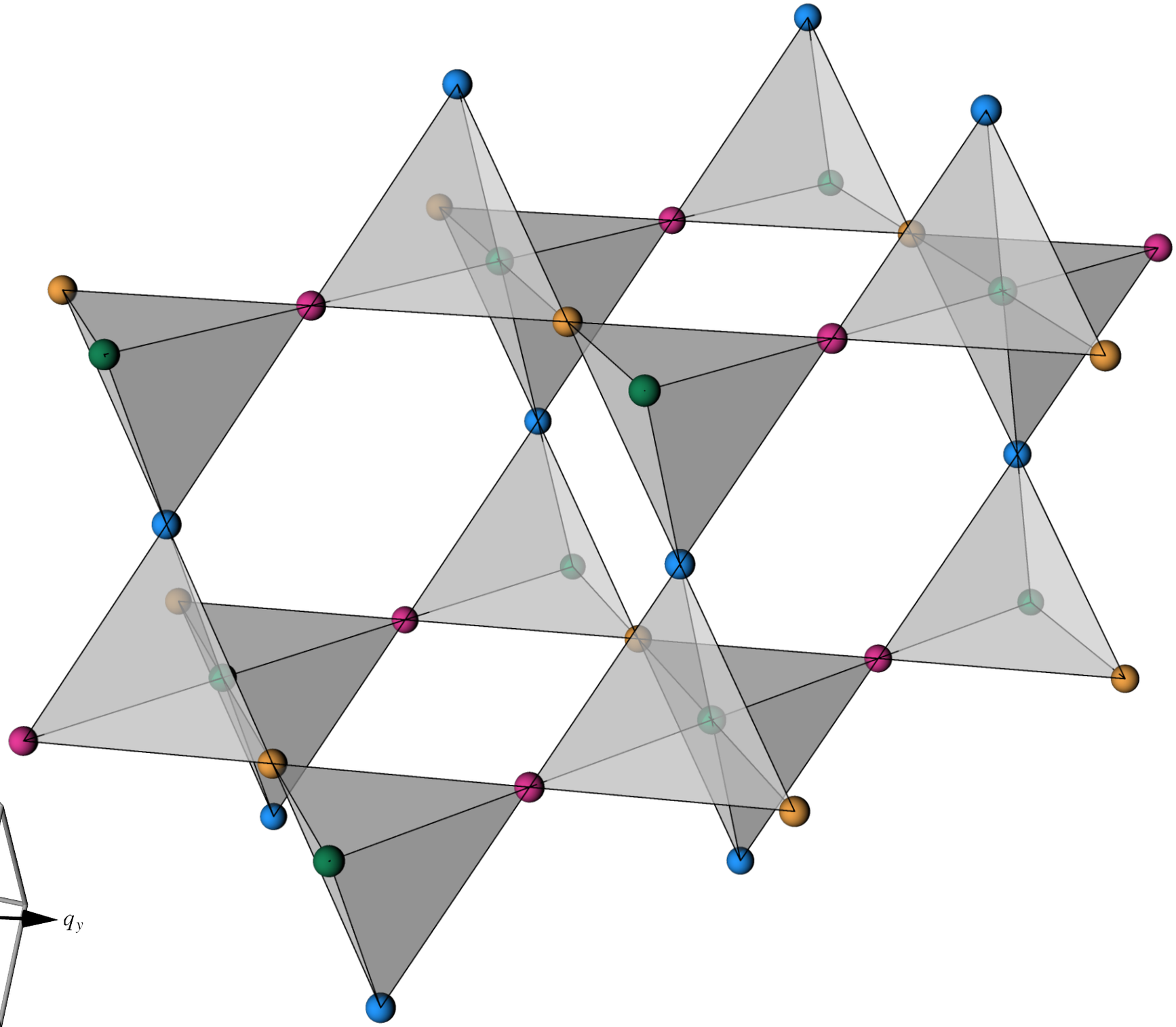

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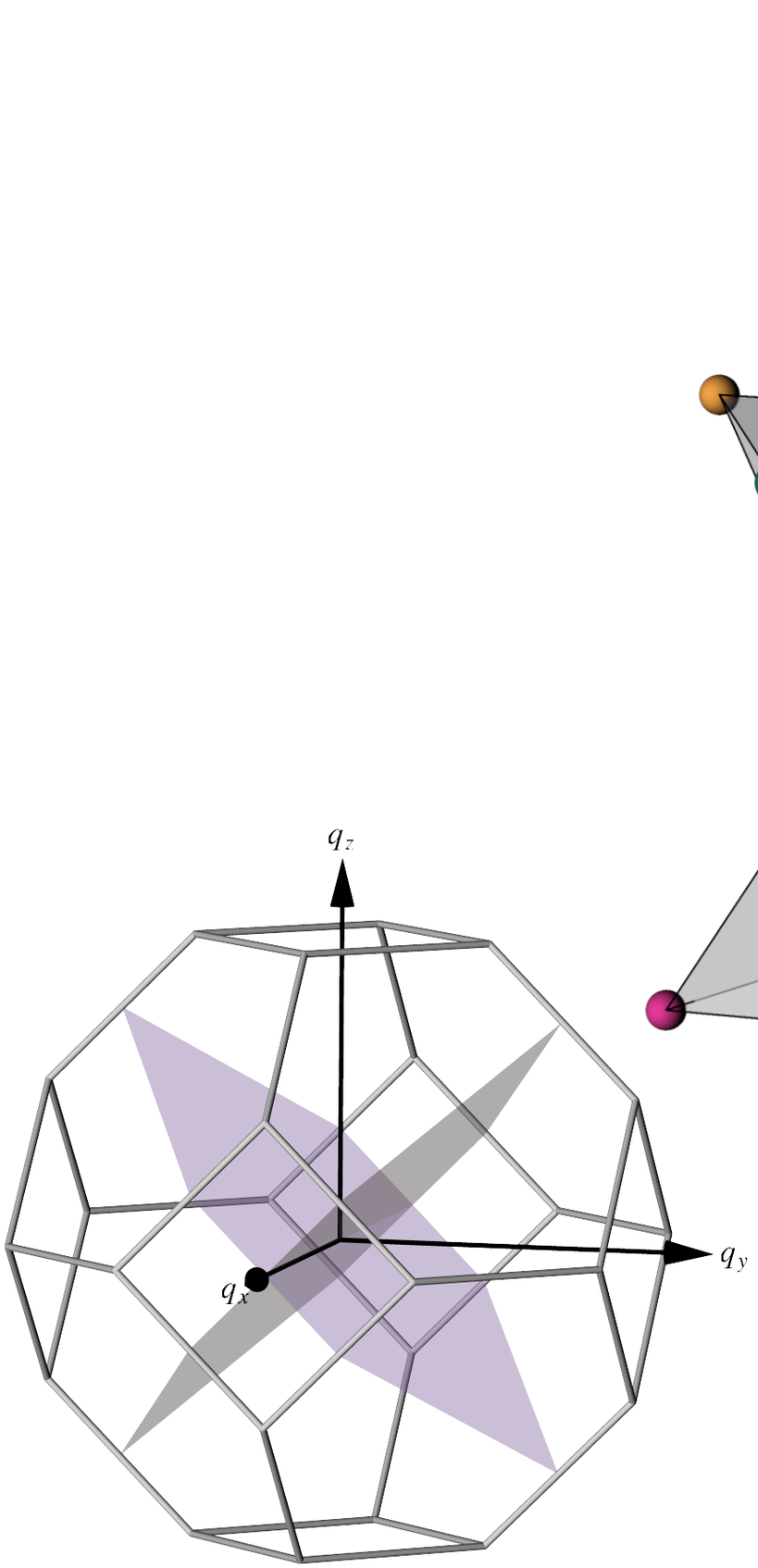

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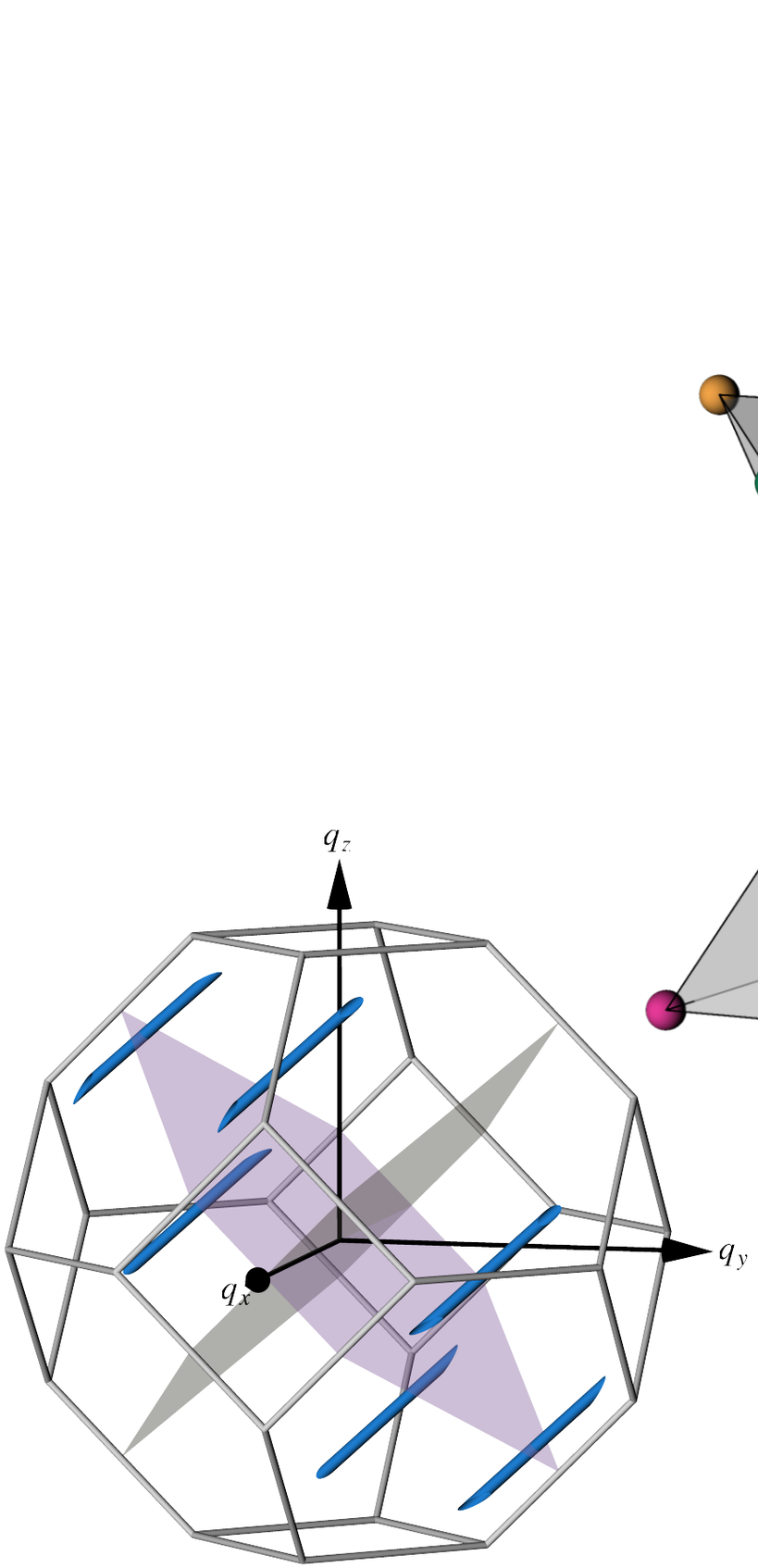

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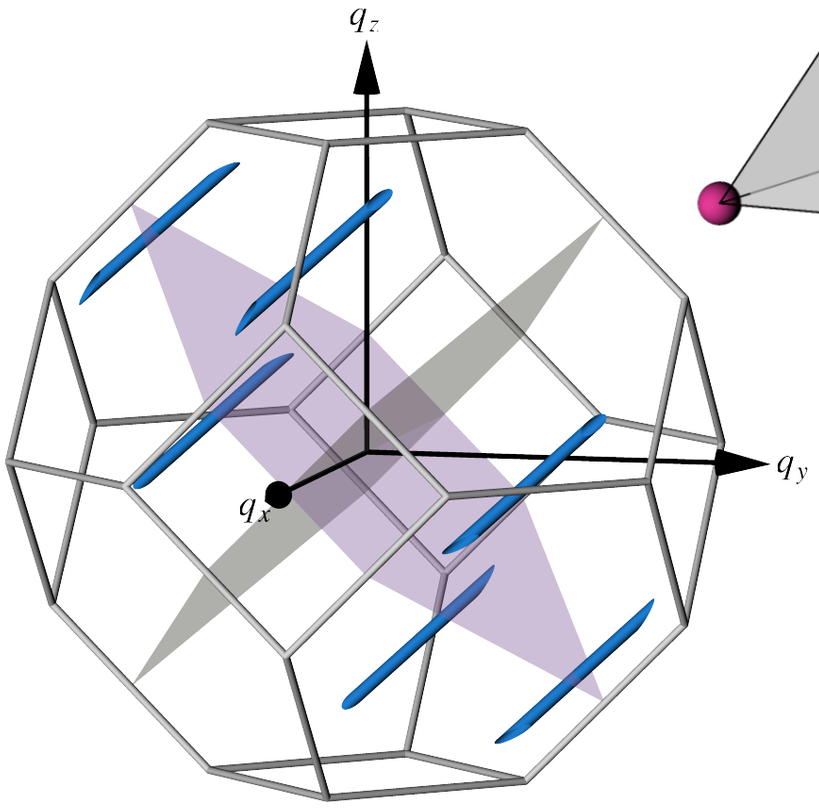

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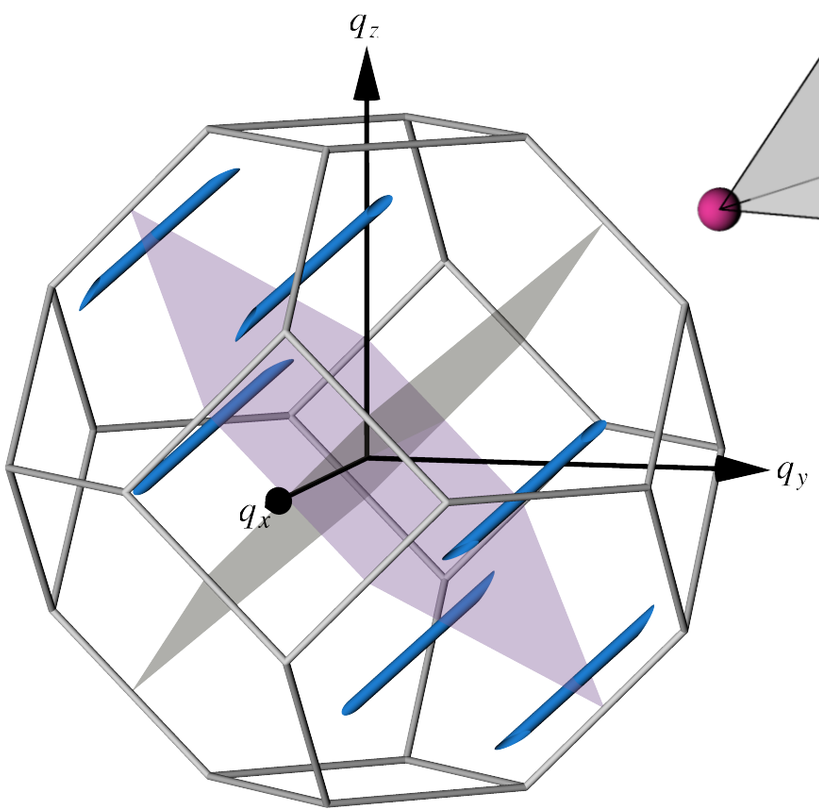

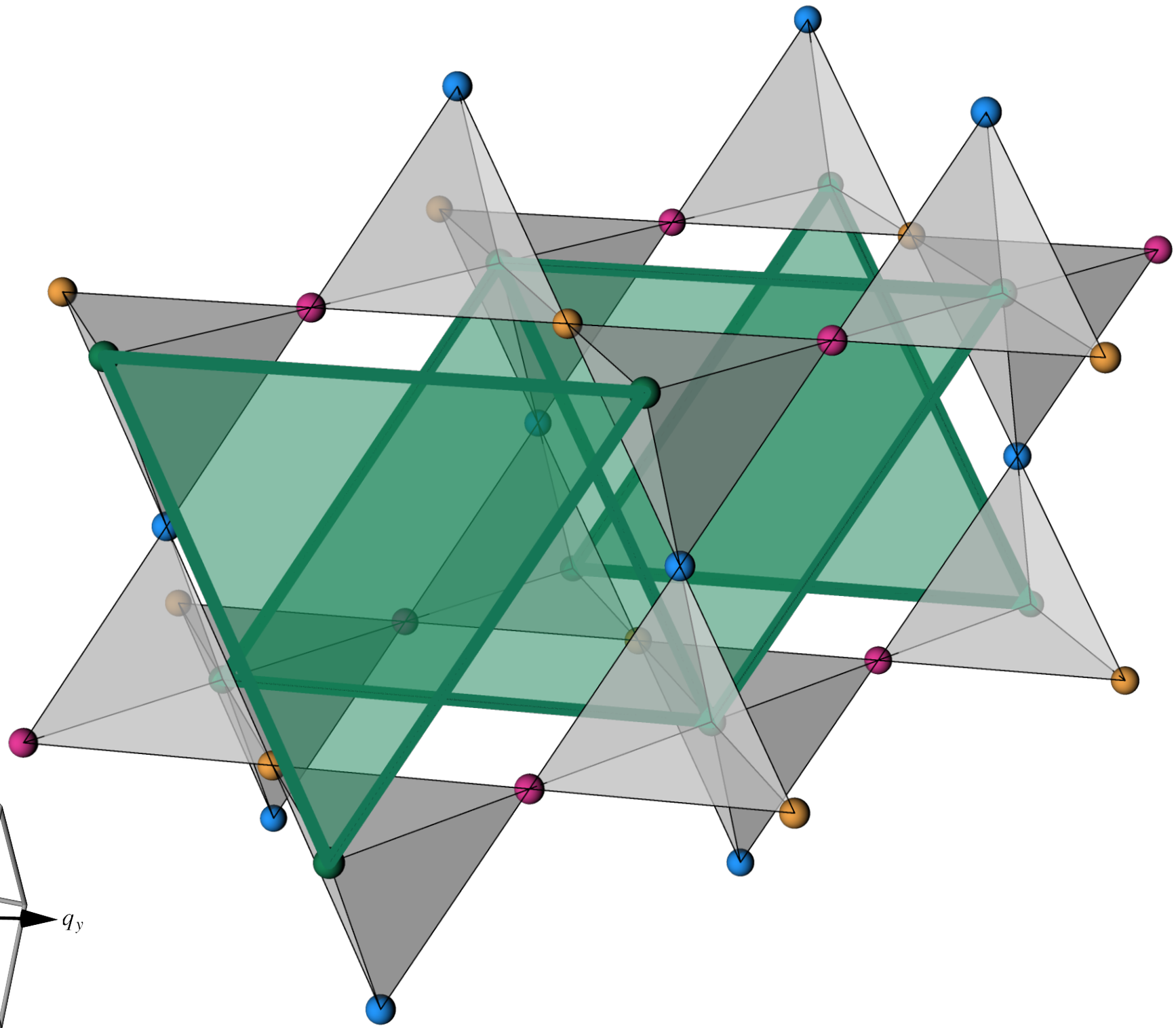

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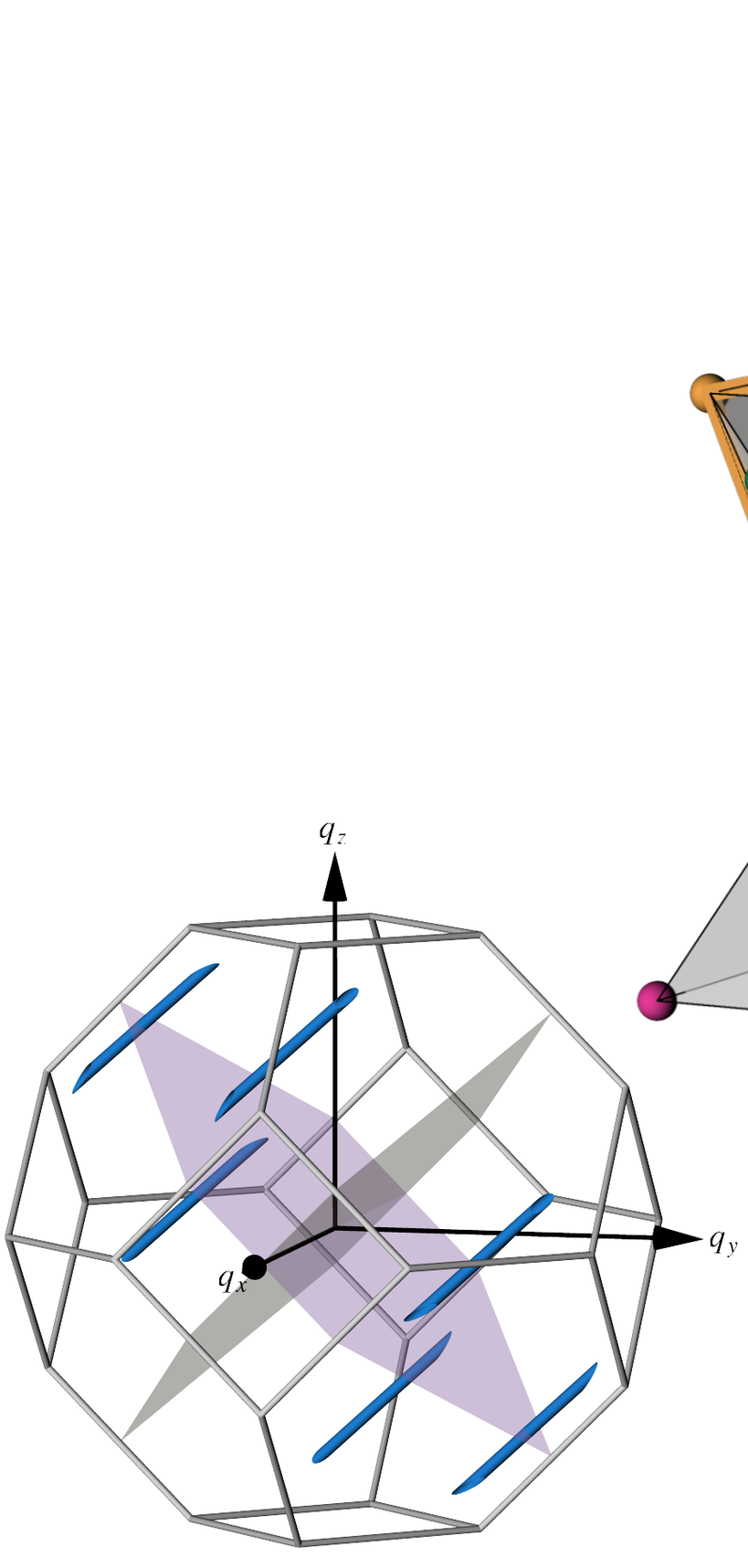

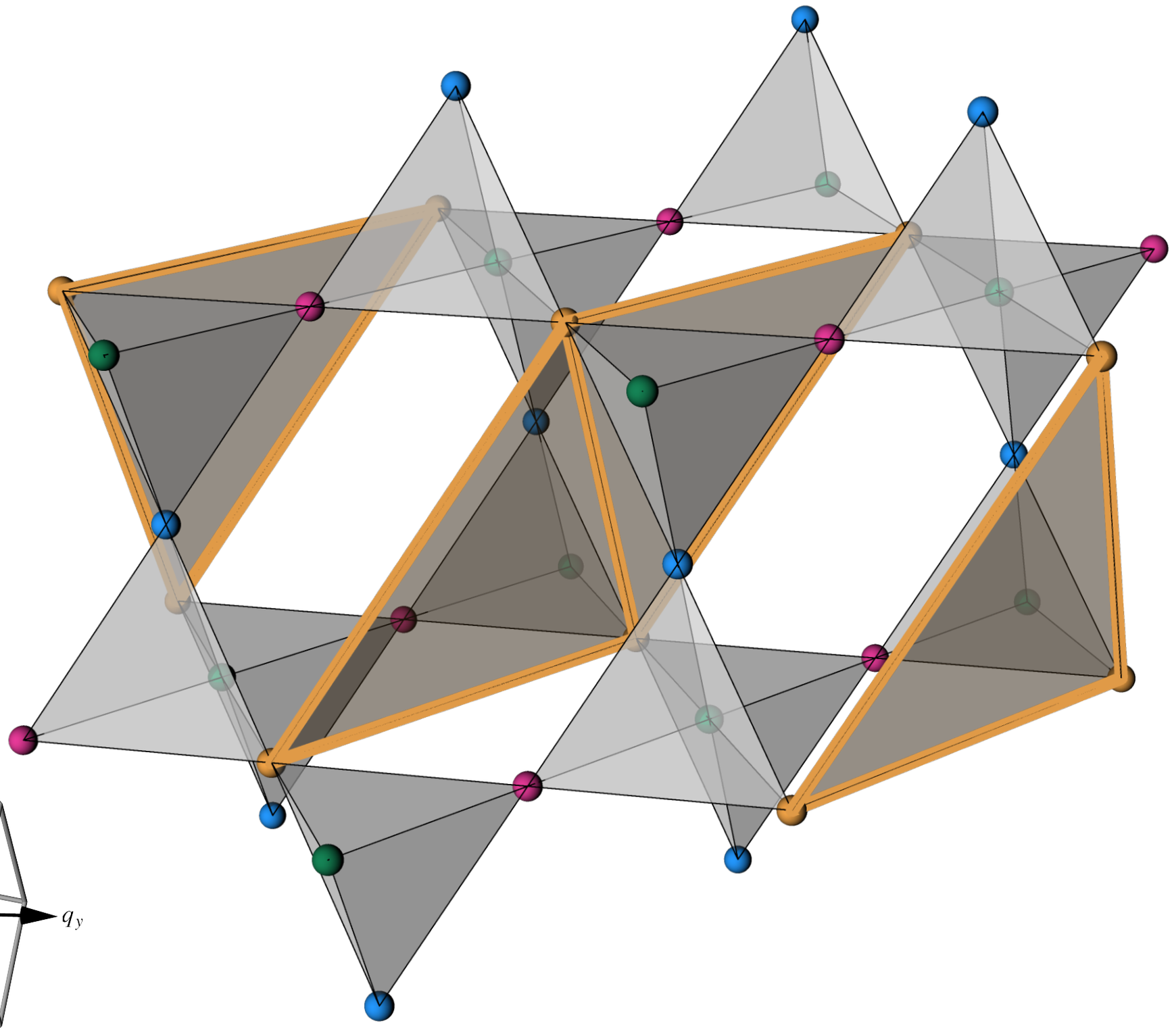

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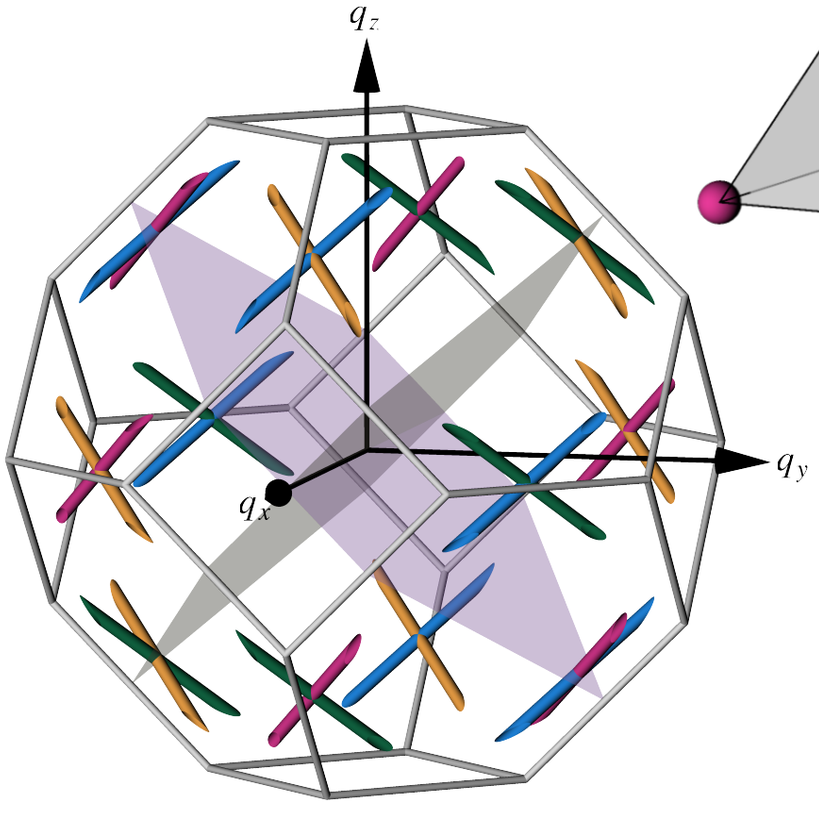

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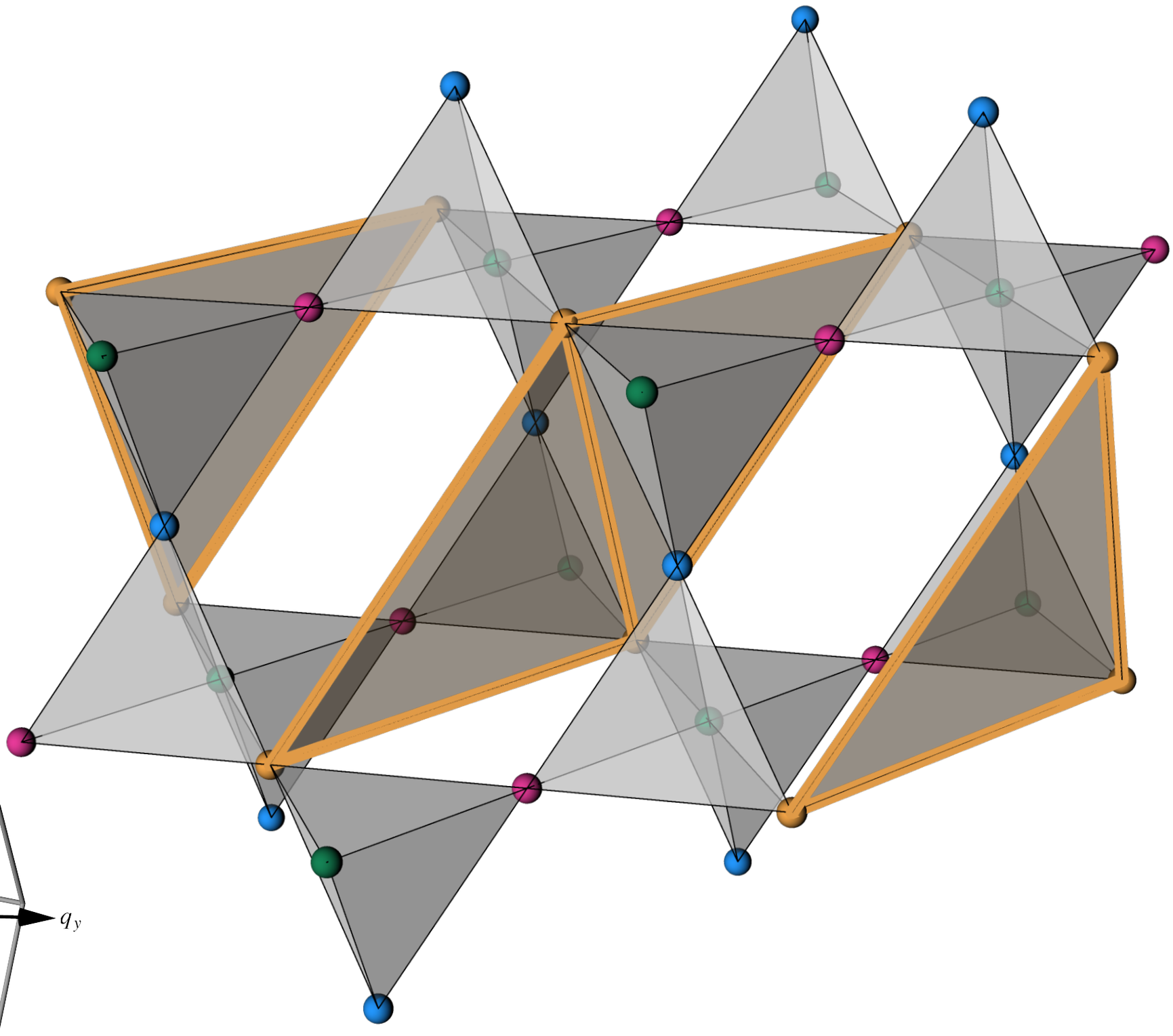
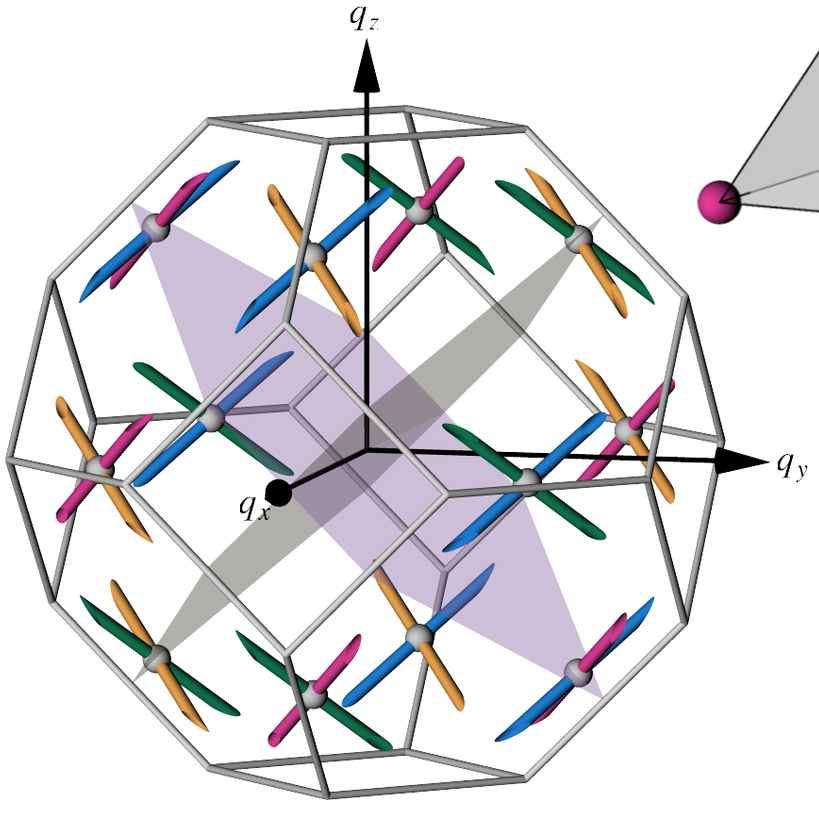
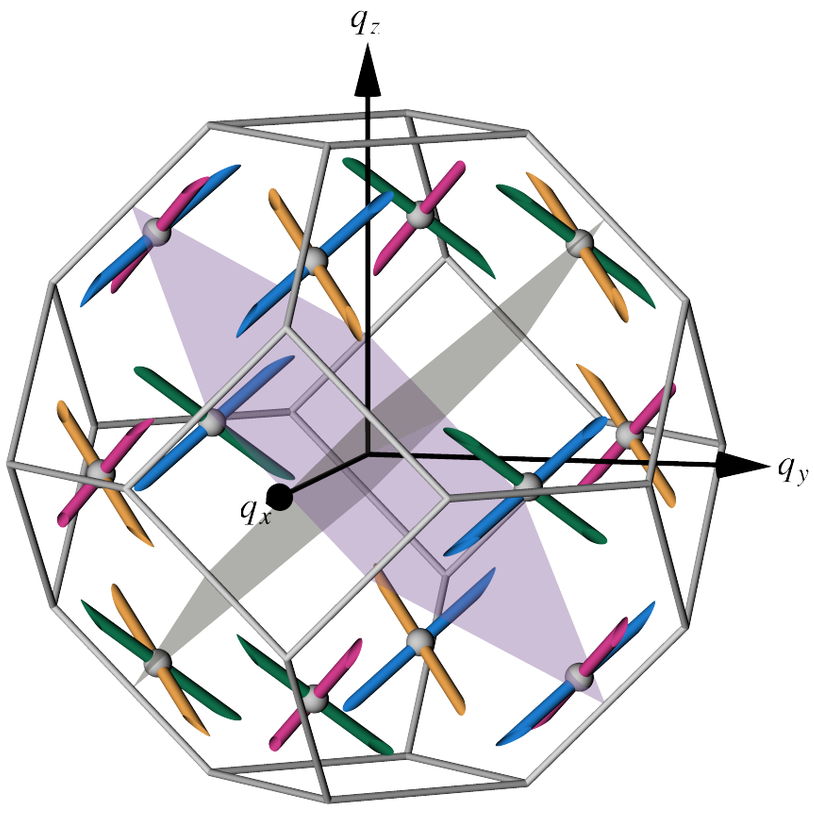


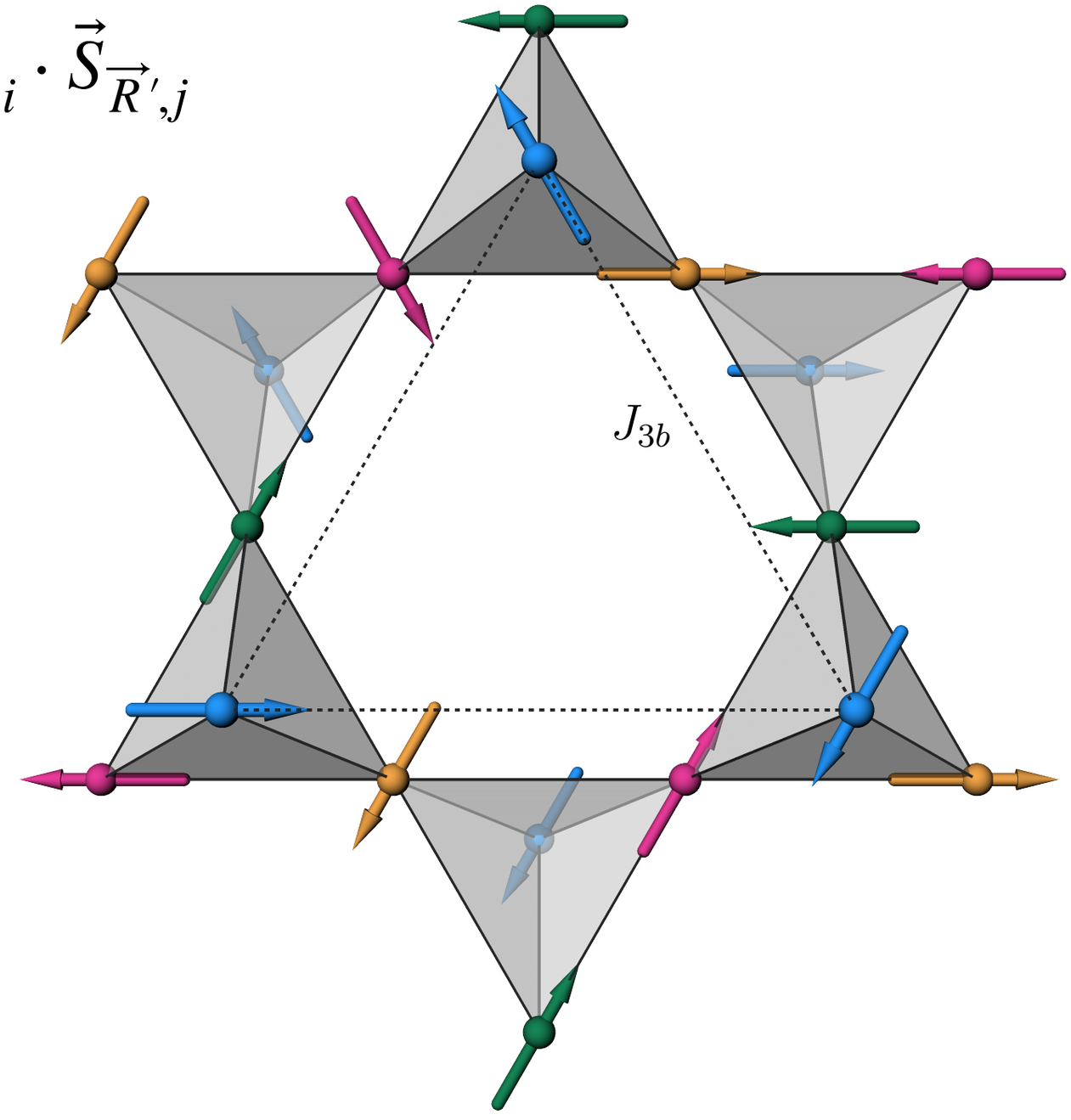


$$\vec{S}_{\vec{R},i} = \vec{u}_i \cos(\vec{Q}_i \cdot \vec{R}) + \vec{v}_i \sin(\vec{Q}_i \cdot \vec{R})$$

Sublattice pairing states minimise the J_1 and J_{3b} couplings simultaneously.

$$H = \frac{1}{2} \sum_{\vec{R},\vec{R}'} \sum_{i,j} J_{ij}(\vec{R}' - \vec{R}) \vec{S}_{\vec{R},i} \cdot \vec{S}_{\vec{R}',j}$$





Phys. Rev. B 108, 014413 (2023)

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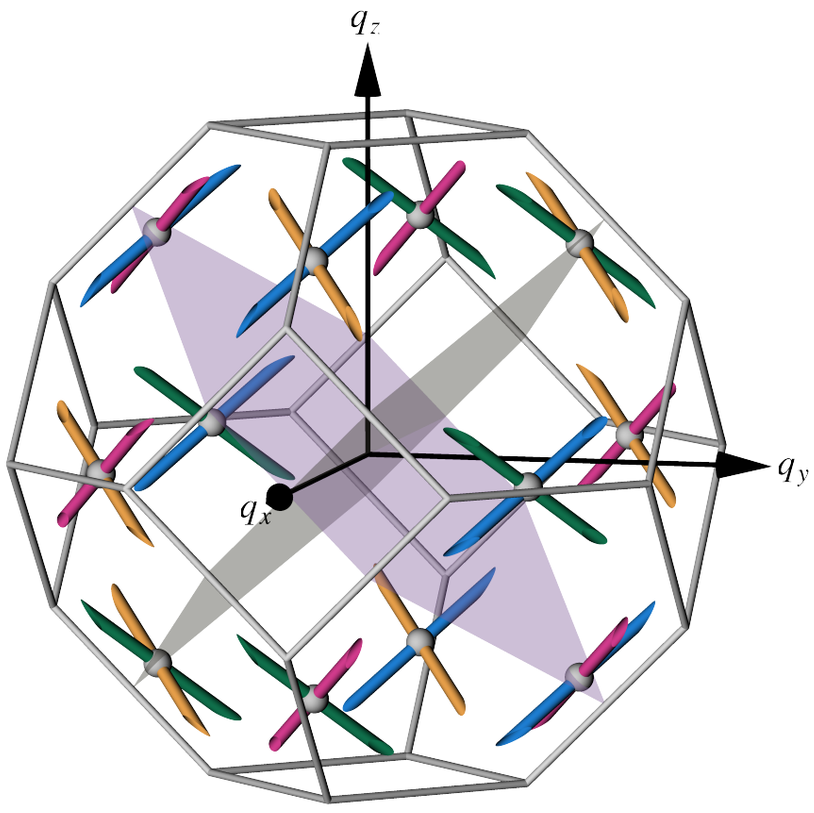
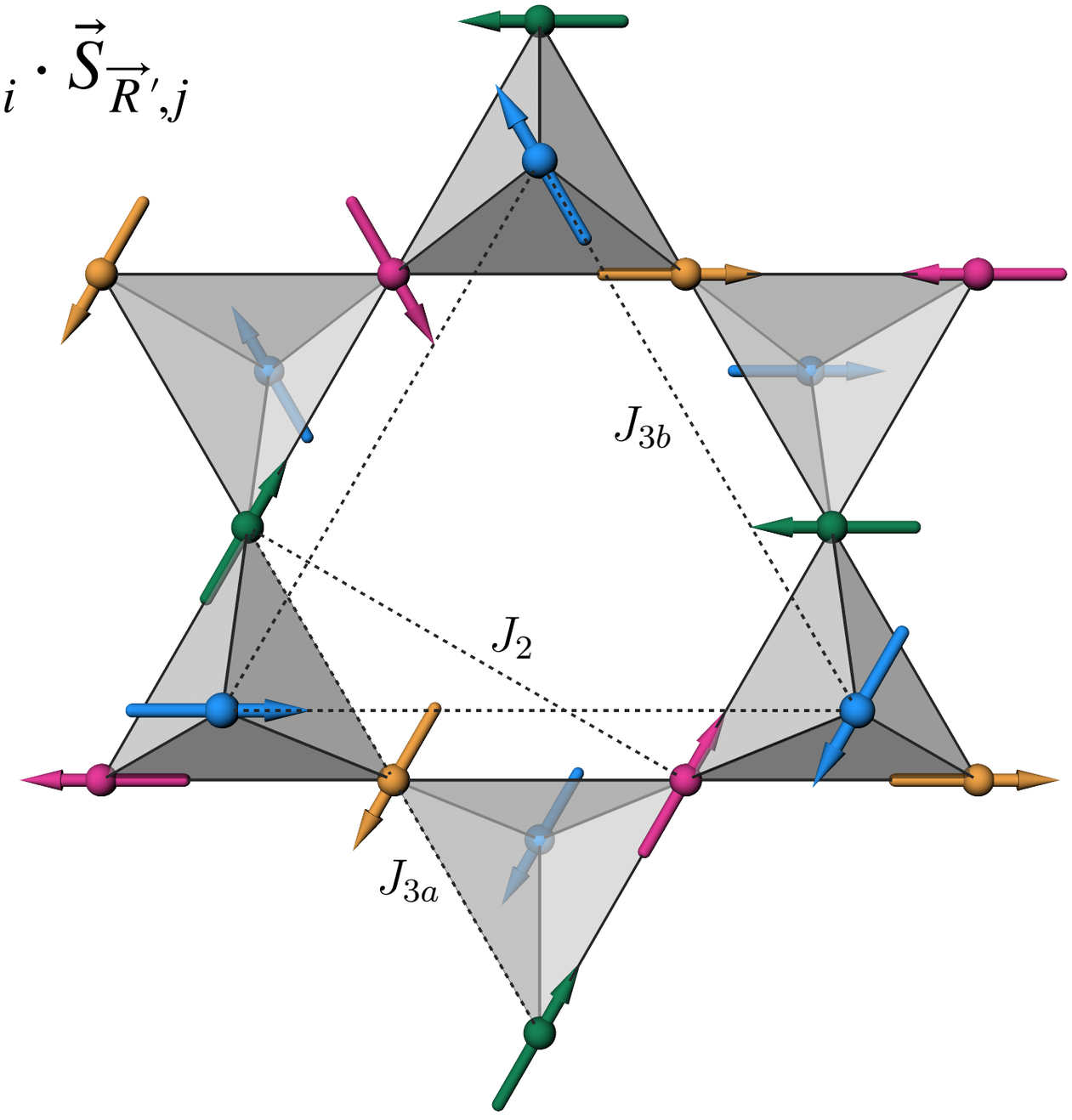
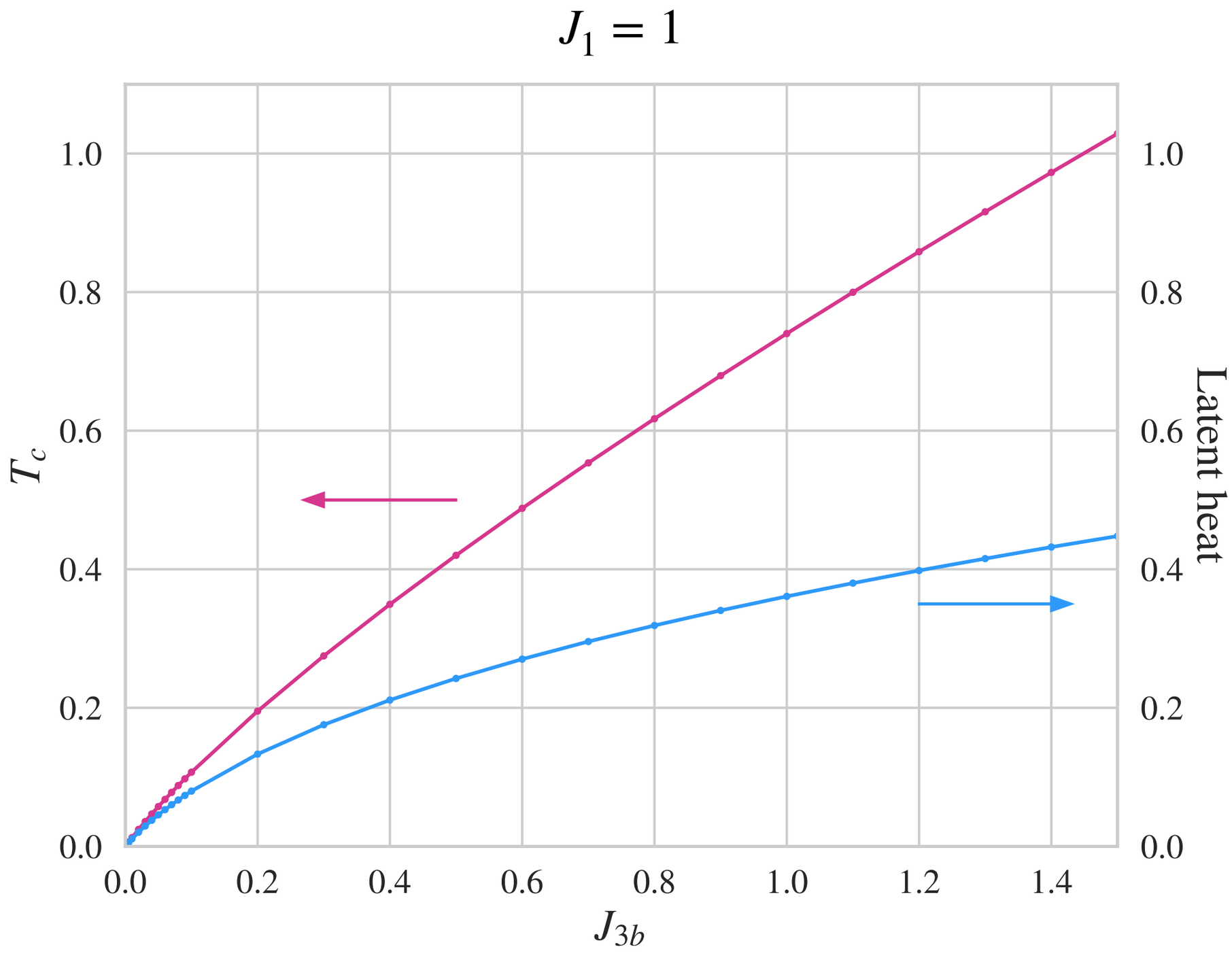




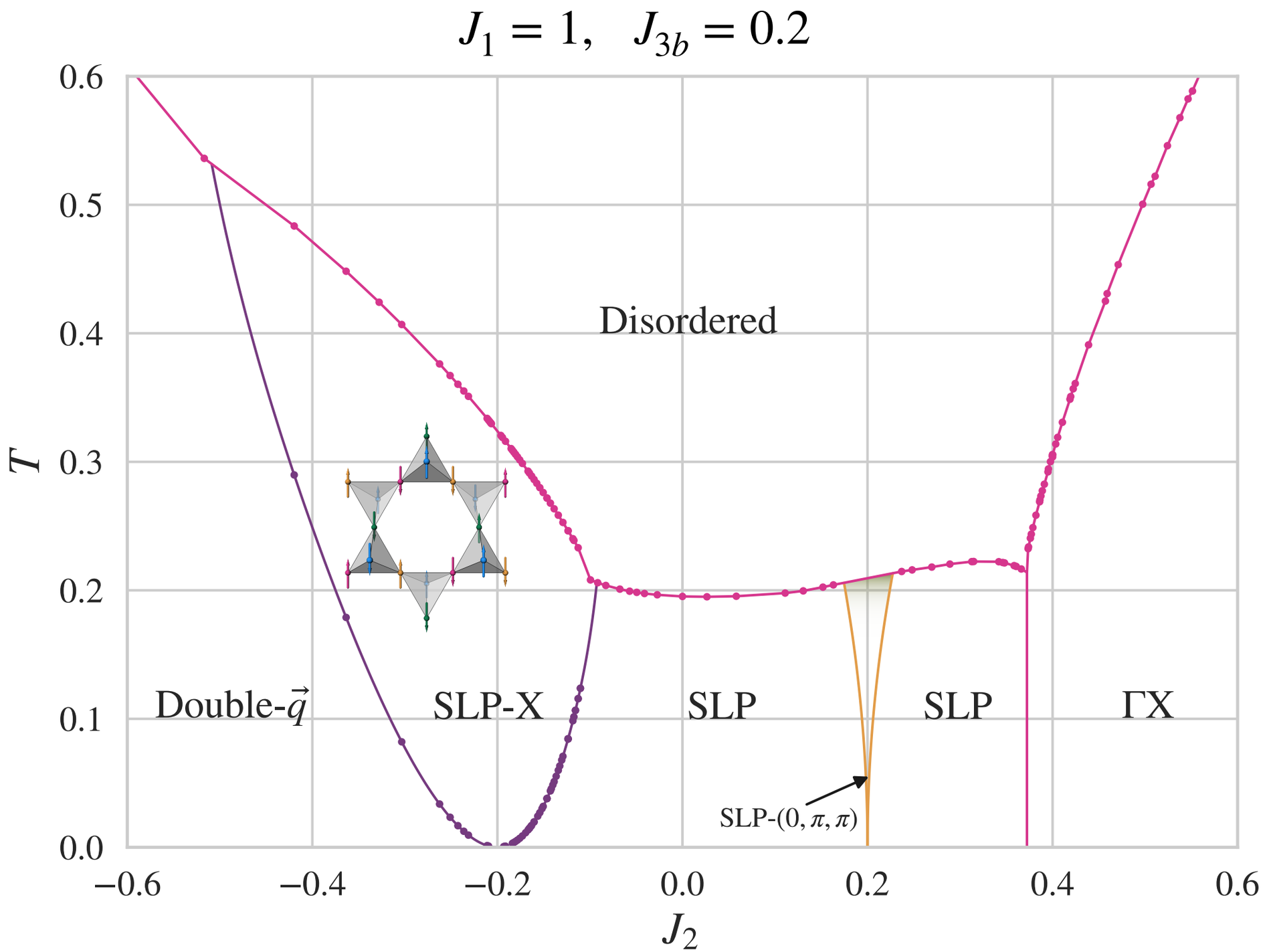
Phys. Rev. B 108, 014413 (2023)

The J_1- J_{3b} model orders in sublattice pairing states (SLP).



Phys. Rev. B 108, 014413 (2023)

Sublattice pairing states (SLP) are stable when adding small J_2.



Phys. Rev. B 108, 014413 (2023)

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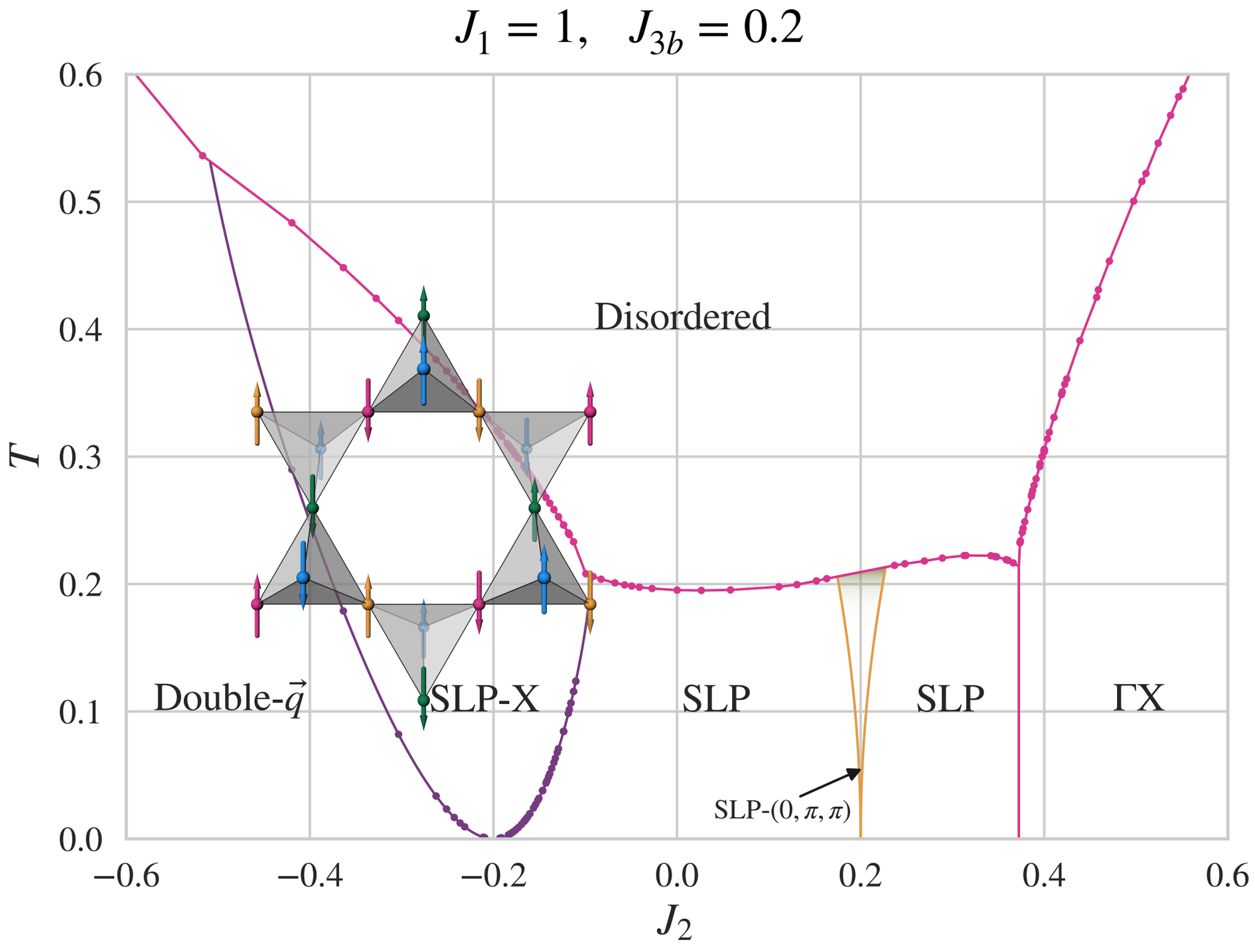

Phys. Rev. B 108, 014413 (2023)

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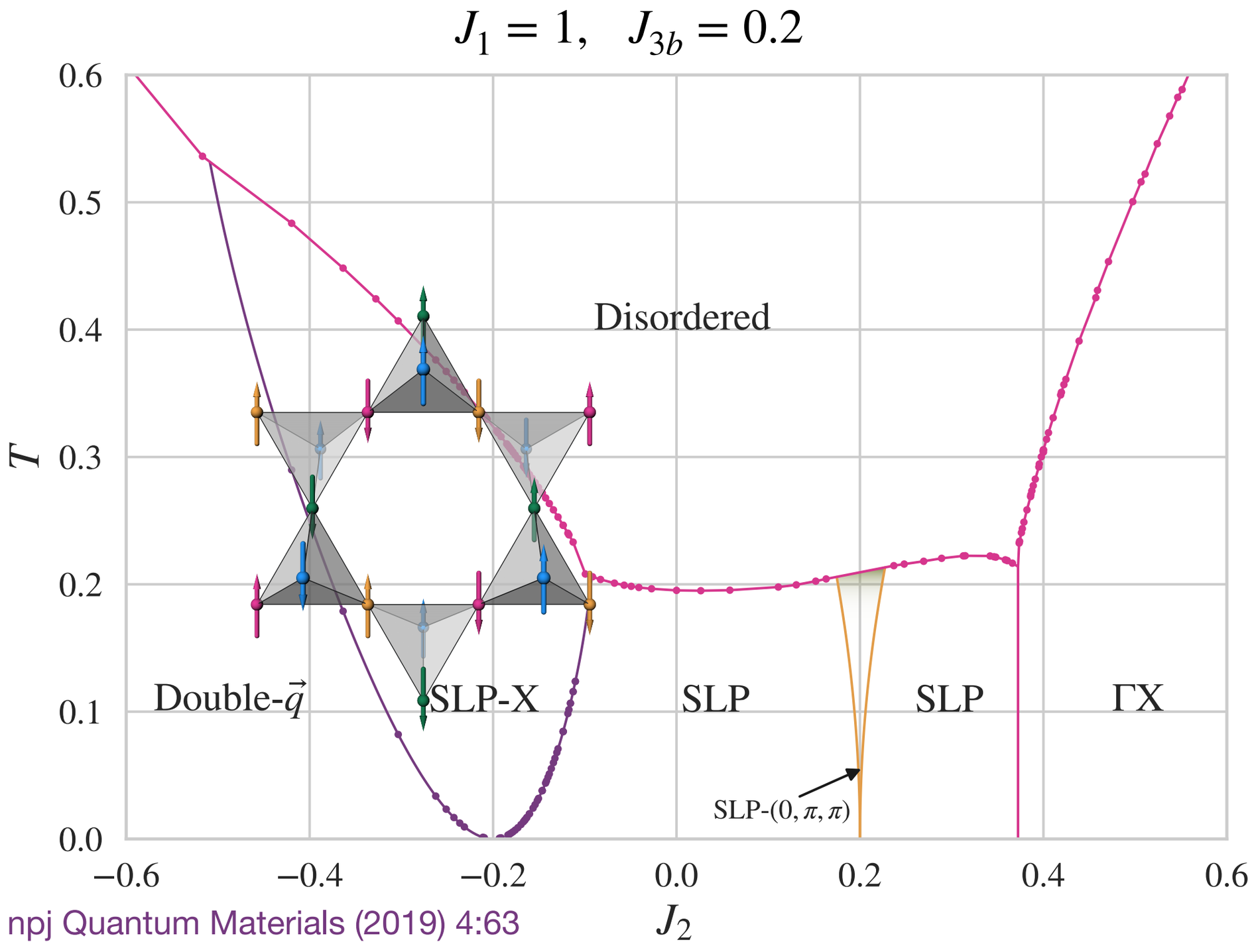
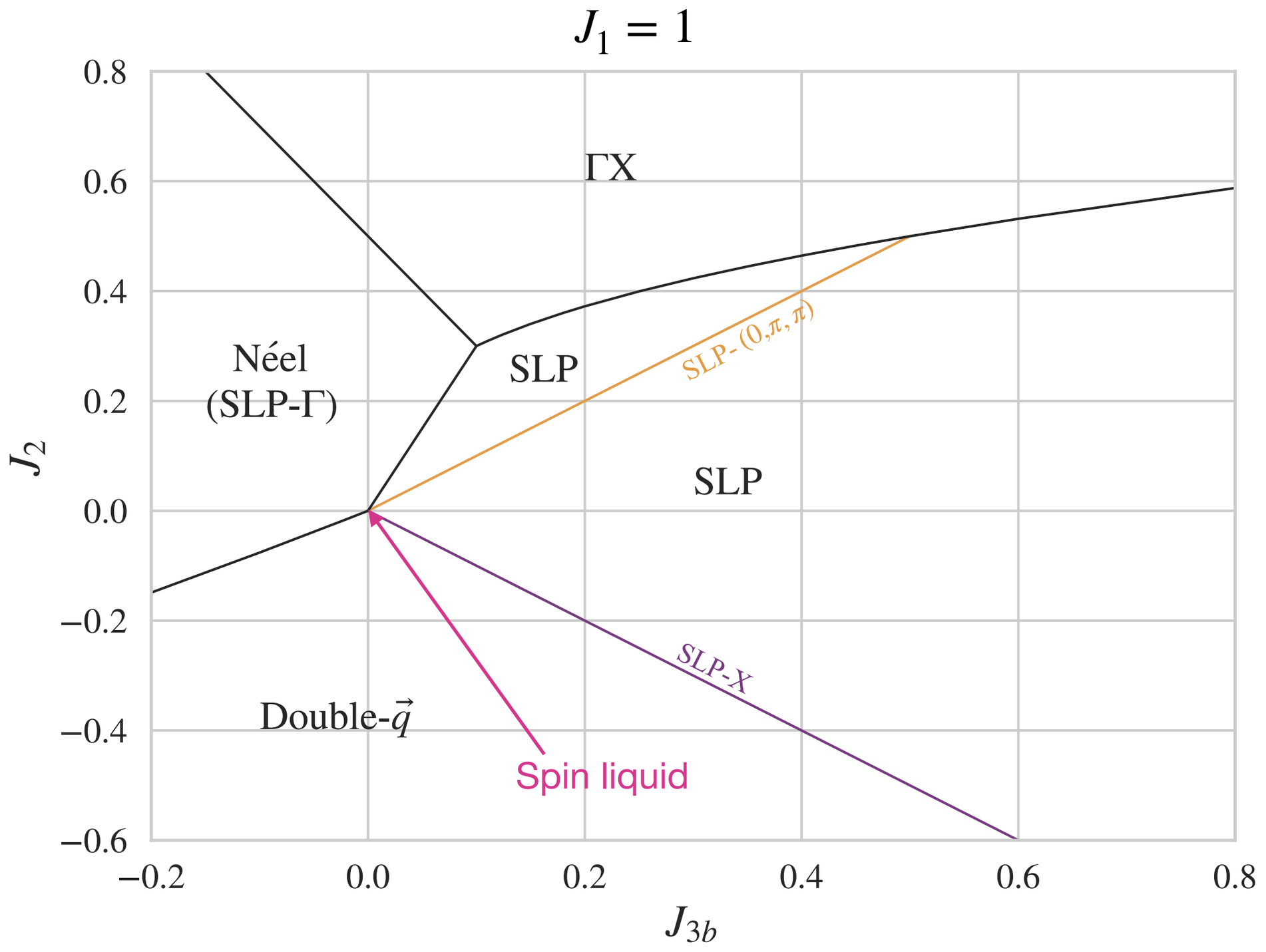


Ghosh et al., npj Quantum Materials (2019) 4:63

Phys. Rev. B 108, 014413 (2023)

The sublattice pairing state (SLP) is realised at low temperatures in a large region of exchange coupling space.



Phys. Rev. B 108, 014413 (2023)

SMALL FURTHER-NEIGHBOUR COUPLINGS DESTABILISE THE SPIN LIQUID ON THE CLASSICAL PYROCHLORE HEISENBERG MODEL

J_{3b} → **SUBLATTICE PAIRING STATES**

$$\vec{S}_{\vec{R},0} = \vec{u}\cos(\vec{Q}_{(0,1)}\cdot\vec{R}) + \vec{v}\sin(\vec{Q}_{(0,1)}\cdot\vec{R}) \qquad \vec{S}_{\vec{R},1} = -\vec{S}_{\vec{R},0}$$

$$\vec{S}_{\vec{R},2} = \vec{w}\cos(\vec{Q}_{(2,3)}\cdot\vec{R}) + \vec{z}\sin(\vec{Q}_{(2,3)}\cdot\vec{R}) \qquad \vec{S}_{\vec{R},3} = -\vec{S}_{\vec{R},2}$$

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Phys. Rev. B 108, 014413 (2023)

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THANK YOU FOR YOUR ATTENTION!

AKER SCHOLARSHIP

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