Orbital ordering in e_g orbital systems

Ground states and thermodynamic of the 120º model

IFW Dresden June 2010

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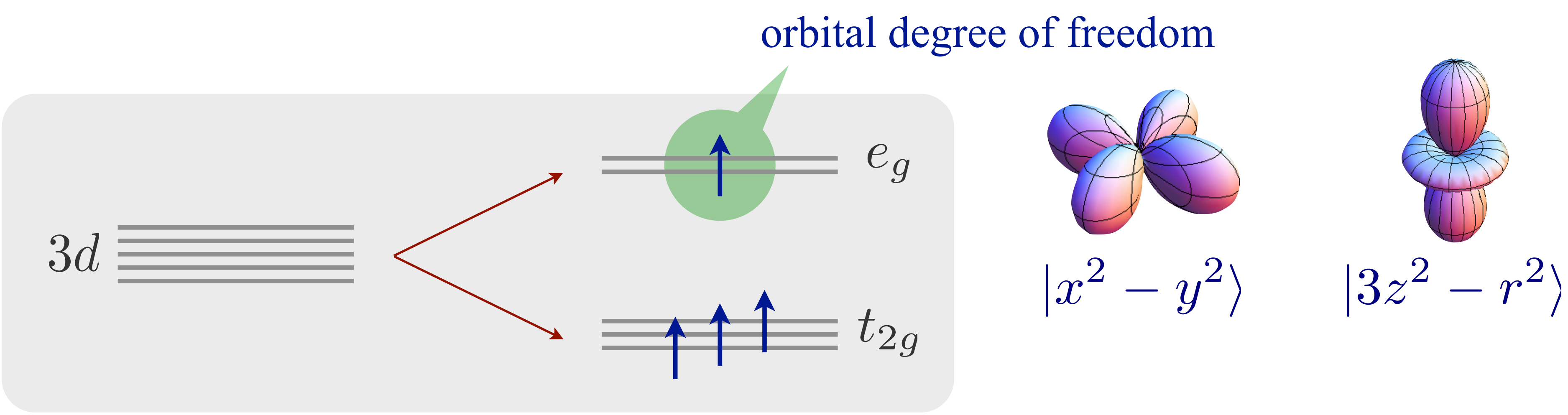
Mott insulators with partially filled *d*-shells

Mott insulating transition metal oxides with **partially filled 3*d*-shells** – such as the manganites – exhibit rich phase diagrams.

Non-trivial interplay of spin, charge, and orbital degrees of freedom.



crystal field splitting (perovskites)

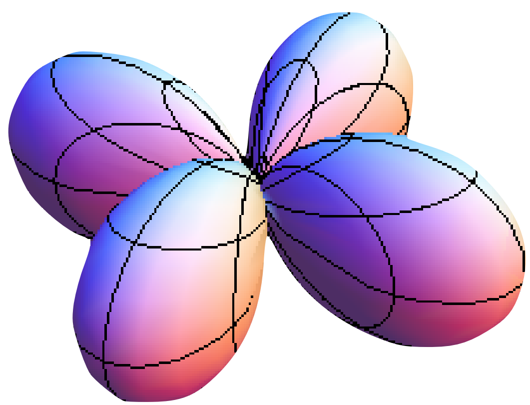
La**Mn**O_3
Rb_2**Cr**Cl_4 (d[4])
K**Cr**F_3

K**Cu**F_3
Li**Ni**O_2 (d[9])

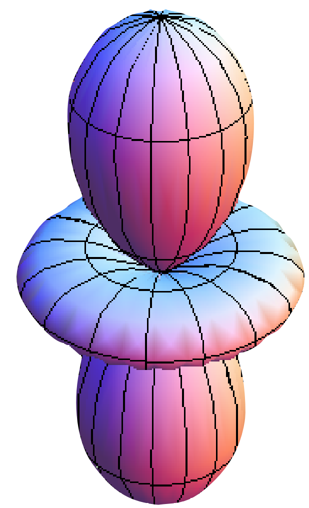
Orbital degrees of freedom

Orbitals are **spatially anisotropic** degrees of freedom.

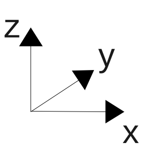
Point group symmetry of lattice is picked up by orbitals.



$$|x^2 - y^2\rangle$$



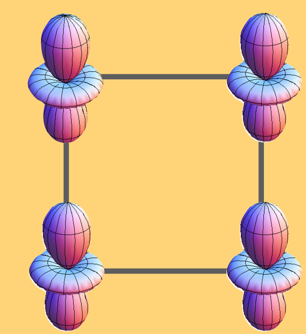
$$|3z^2 - r^2\rangle$$



Orbital degrees of freedom

Orbitals are **spatially anisotropic** degrees of freedom.
Point group symmetry of lattice is picked up by orbitals.

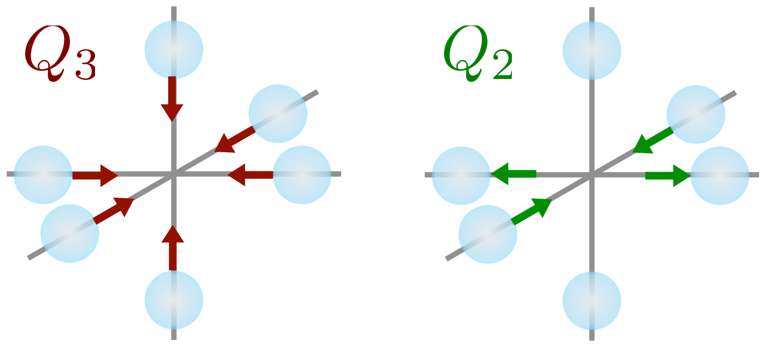
spins	feature	orbitals
weak	coupling to lattice	strong
high continuous	symmetry of Hamiltonian	[illegible]
often gapless	excitations	[illegible]
sometimes	frustration	almost always



Orbital exchange

Jahn-Teller interactions

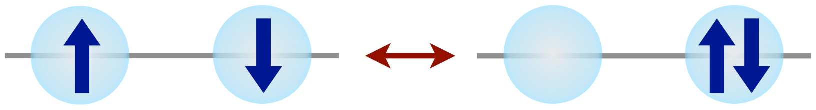
Jahn-Teller **lattice distortions**
mediate orbital-orbital exchange



classical orbital model

Kugel-Khomskii type interactions

induced by
magnetic superexchange



quantum orbital model

The 120 degree model

Both types of orbital exchanges give rise to the **same** Hamiltonian for the e_g orbital degrees of freedom

$$H_{120} = -\sum_{i,\gamma=x,y} \frac{1}{4}\Big[J_z T_i^z T_{i+\gamma}^z + 3J_x T_i^x T_{i+\gamma}^x \pm\sqrt{3}J_{\text{mix}}(T_i^z T_{i+\gamma}^x + T_i^x T_{i+\gamma}^z)\Big] - \sum_i J_z T_i^z T_{i+z}^z$$

Jahn-Teller distortions

pseudospins are classical O(2) spins

Kugel-Khomskii type superexchange

pseudospins are quantum SU(2) spins

The 120 degree model

Both type … miltonian

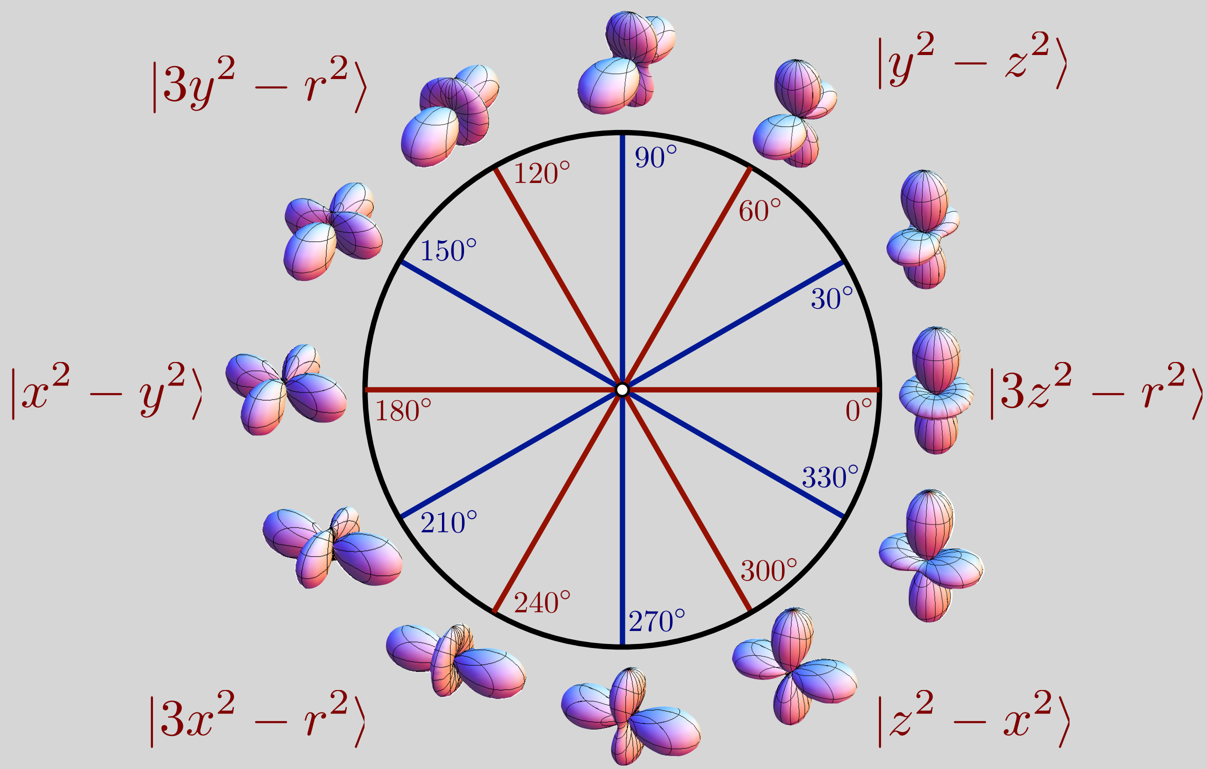
H_{120} … T^z_{i+z}

Jahn-Tell…

Kugel-Kh…

pseudospin representation

$$|\theta\rangle = \cos(\theta/2)|3z^2 - r^2\rangle + \sin(\theta/2)|x^2 - y^2\rangle$$
$$= (T^z, T^x)$$

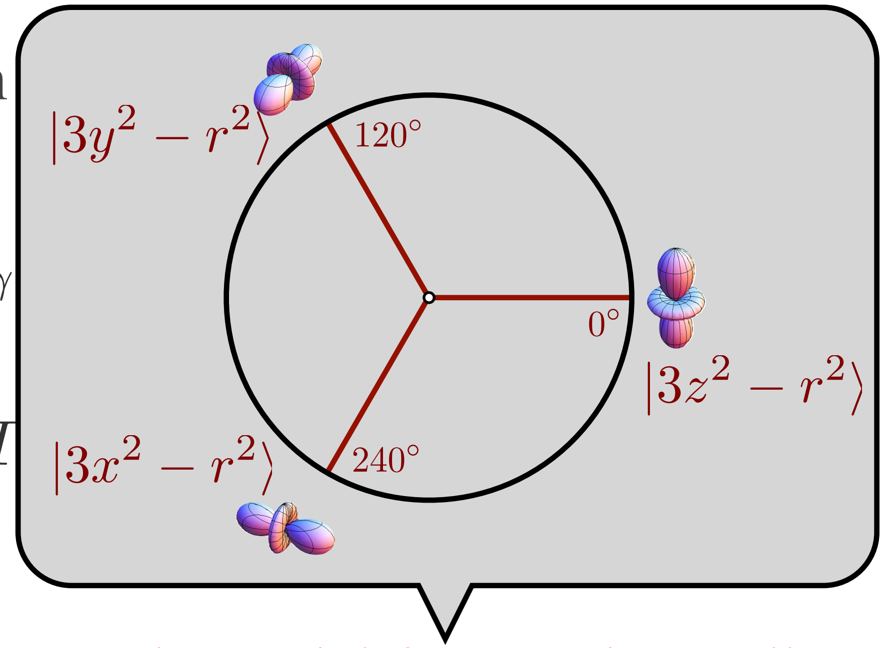


The 120 degree model

Our approach: explore 120º model in

$$H_{120} = -\sum_{i,\gamma=x,y} \frac{1}{4}\left[J_z T_i^z T_{i+\gamma}^z \right.$$

$$\pm\sqrt{3}J_{\text{mix}}(T_i^z T_{i+\gamma}^x + T$$

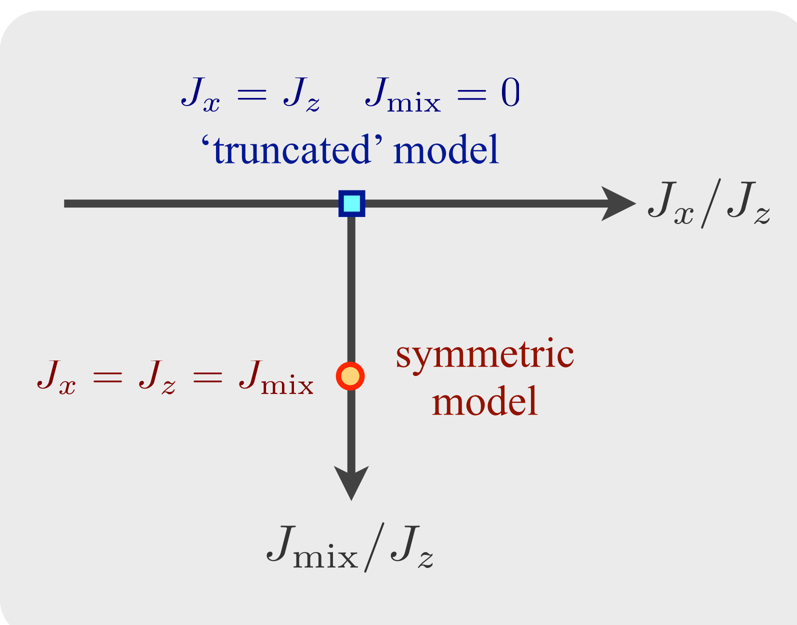


symmetric model for equal-coupling

$J_x = J_z = J_{\text{mix}}$

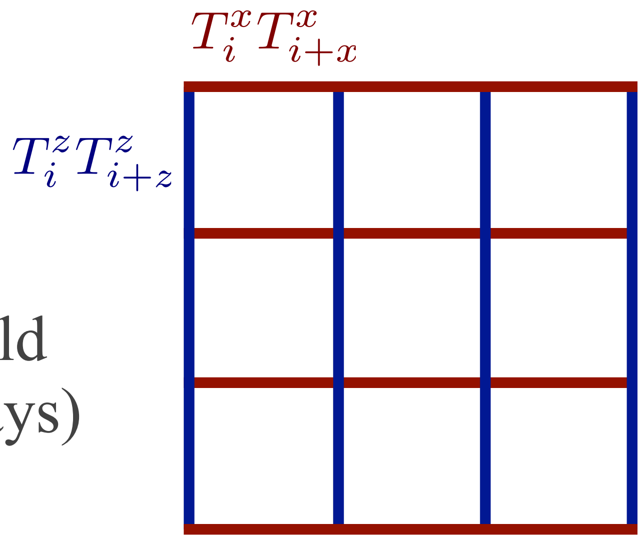
$$H_{120} = -J \sum_{i,\gamma=x,y,z} (\boldsymbol{\tau}_i \cdot \mathbf{e}^\gamma)(\boldsymbol{\tau}_{i+\gamma} \cdot \mathbf{e}^\gamma)$$

$$\boldsymbol{\tau}_i = \left([T_i^z + \sqrt{3}T_i^x]/2, [T_i^z - \sqrt{3}T_i^x]/2, T_i^z\right)$$



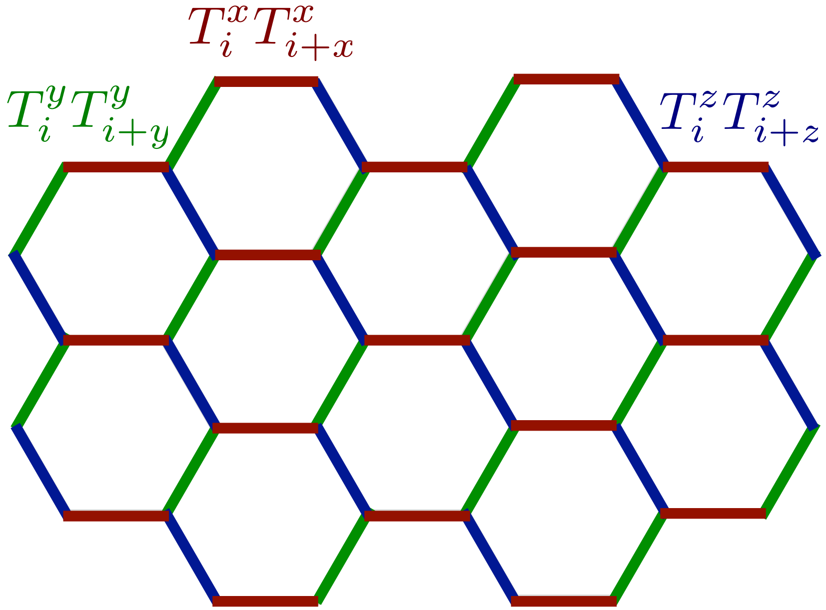
Orbital-only models

Planar compass model



topological order
dual to toric code in transverse mag. field
dual to Xu-Moore model (Josephson arrays)

Kitaev honeycomb model



topological order
gapless spin liquid

Ir oxides, polar molecules

The classical 120º model

pseudospins are classical O(2) spins

Zero temperature: degenerate ground states

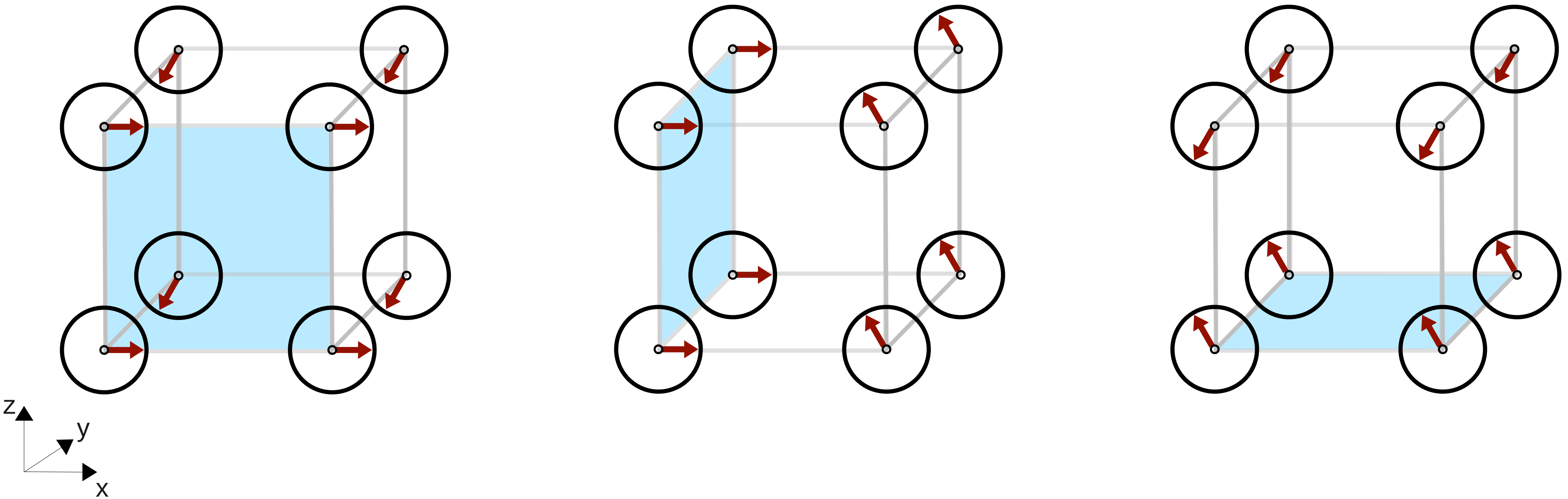
M. Biskup *et al.*, Comm. Math. Phys. **255**, 253 (2005).
Z. Nussinov *et al.*, Europhys. Lett. **67**, 990 (2004).

Emergent symmetries: U(1) and Z_2 symmetries

Ground-state manifold: infinite, but sub-extensive number of states

$$\mathcal{D} = 2^{3L}$$

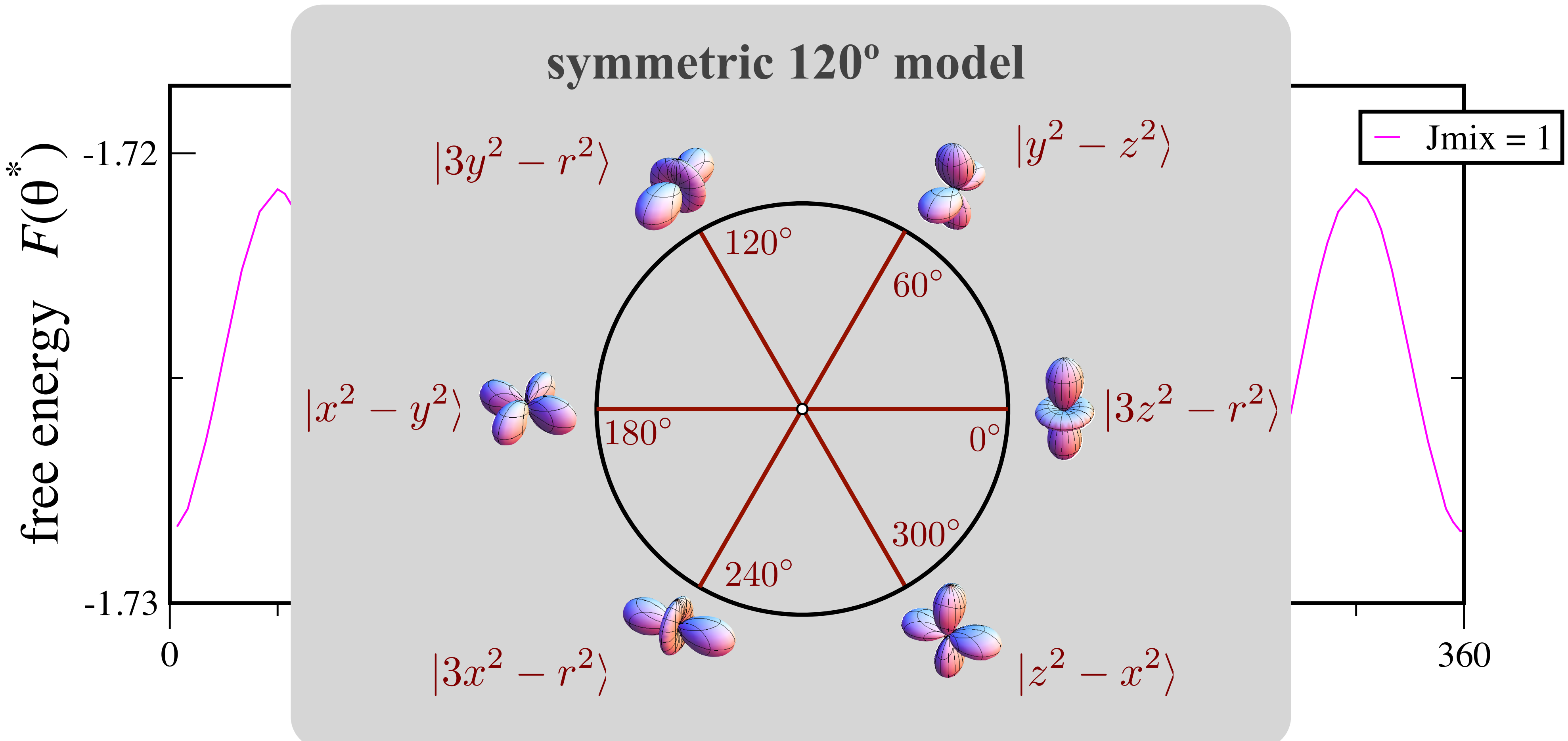
xz plane 120° | *yz* plane 240° | *xy* plane 0°



Low temperatures: Order by disorder

M. Biskup *et al.*, Comm. Math. Phys. **255**, 253 (2005).
Z. Nussinov *et al.*, Europhys. Lett. **67**, 990 (2004).

Spin-wave approximation: expansion in fluctuations $\delta\theta_i = \theta_i - \theta^*$
around ordered state with $\theta_i = \theta^*$ at each site.

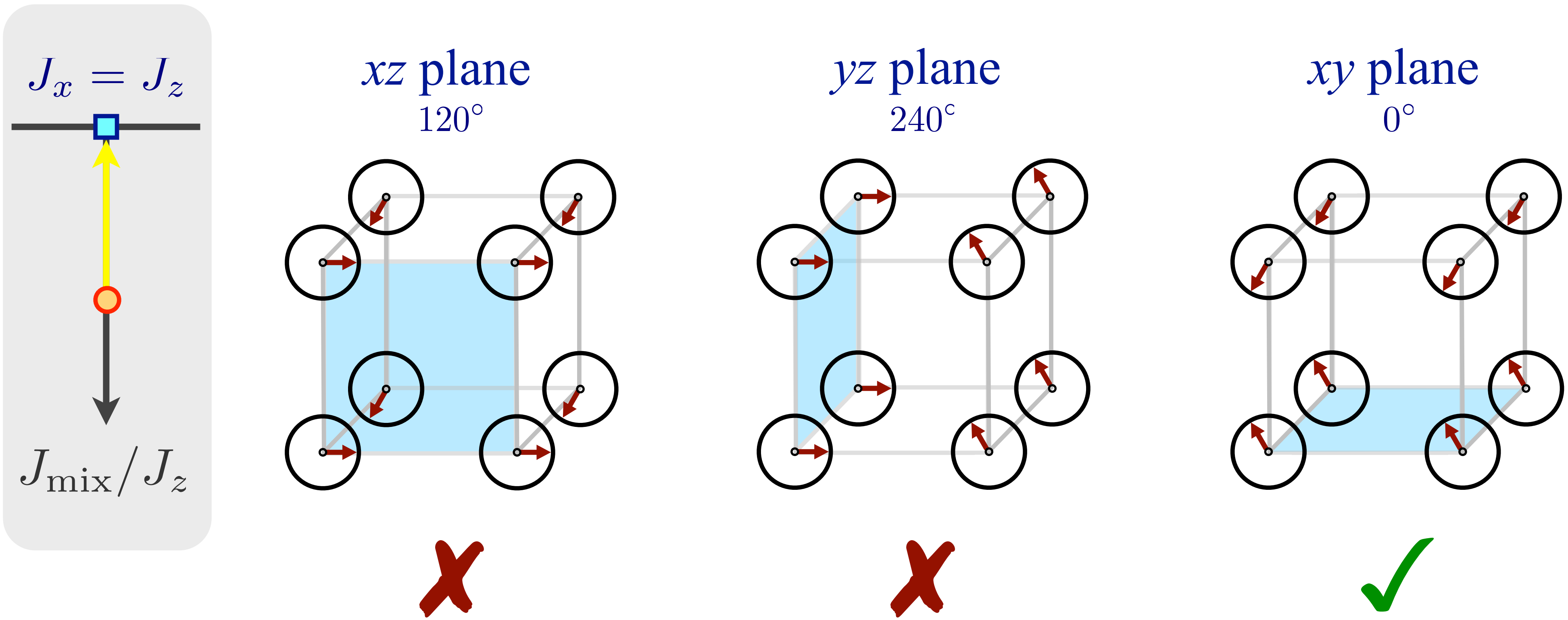


Moving away from symmetric point

Emergent symmetries: U(1) and Z_2 symmetries

Ground-state manifold: infinite, but sub-extensive number of states

$$\mathcal{D} = 2^{3L} \rightarrow \mathcal{D} = 2^{L}$$



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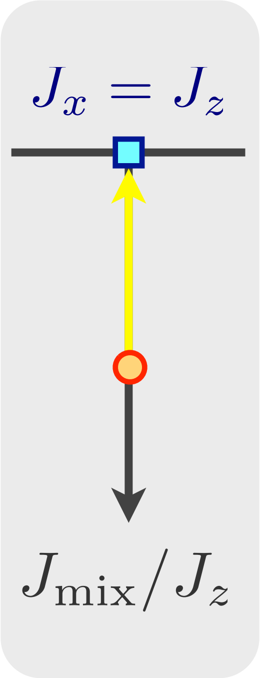

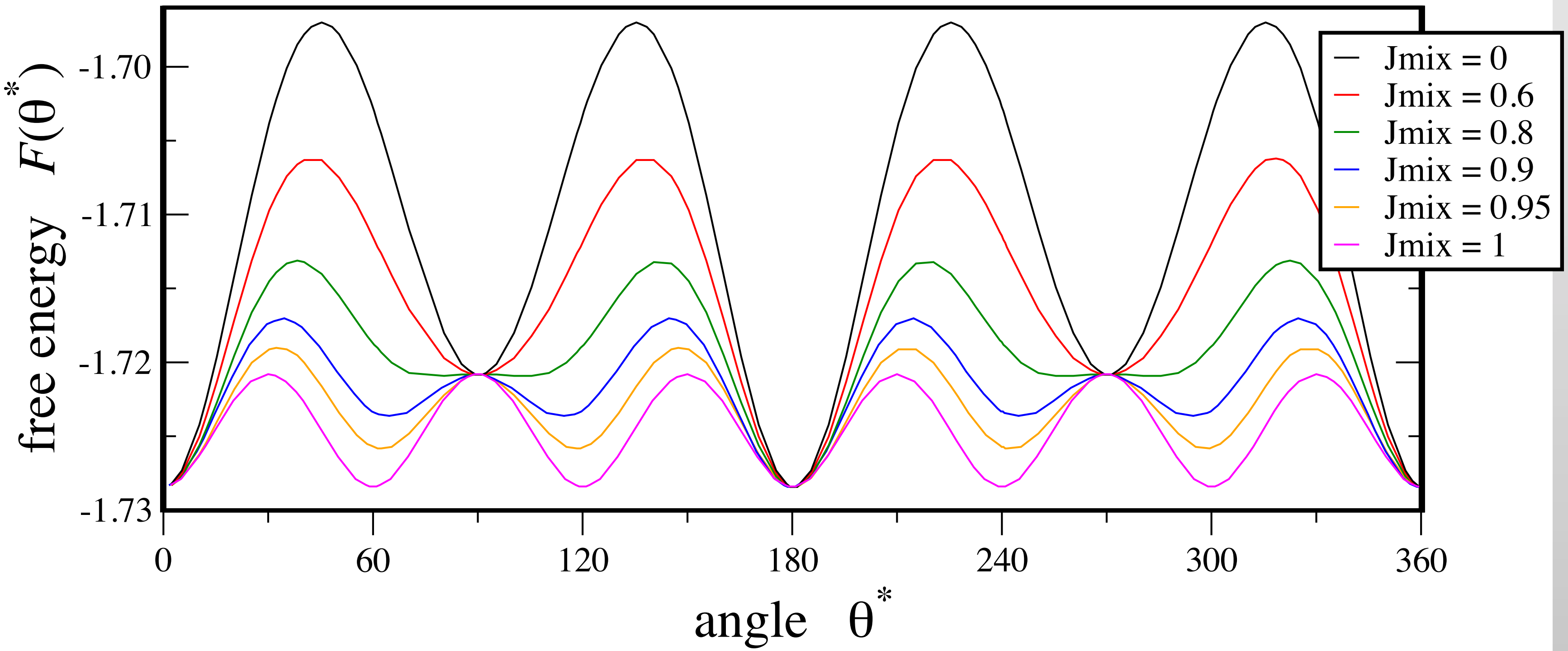

Low temperatures: Order by disorder

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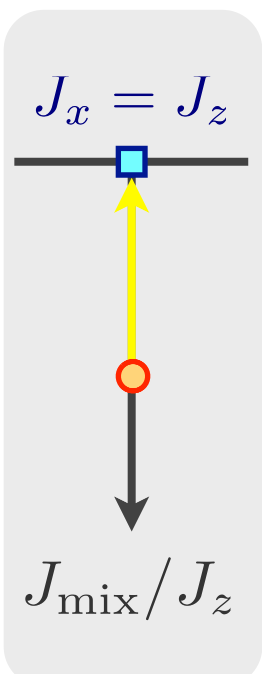
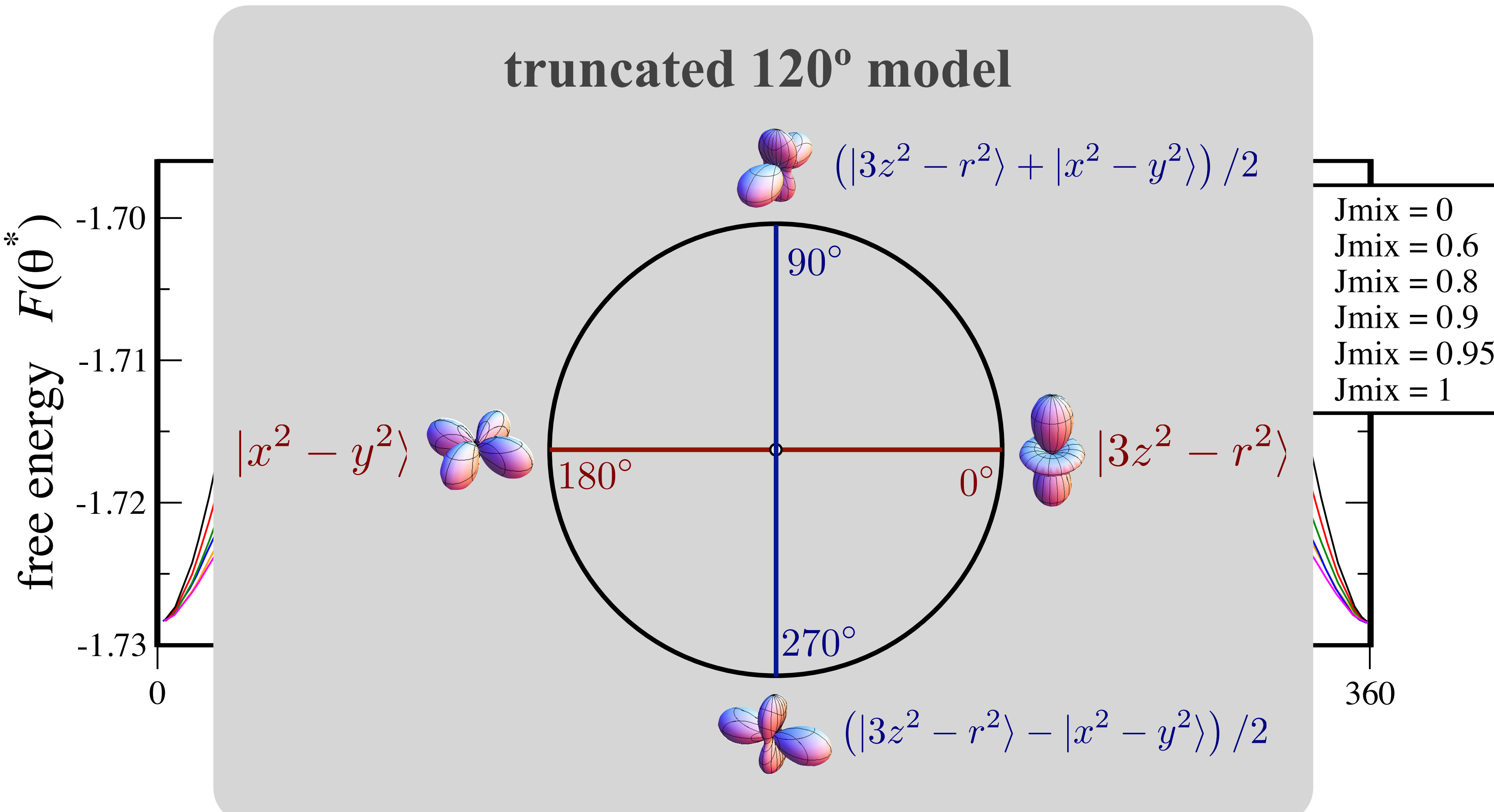
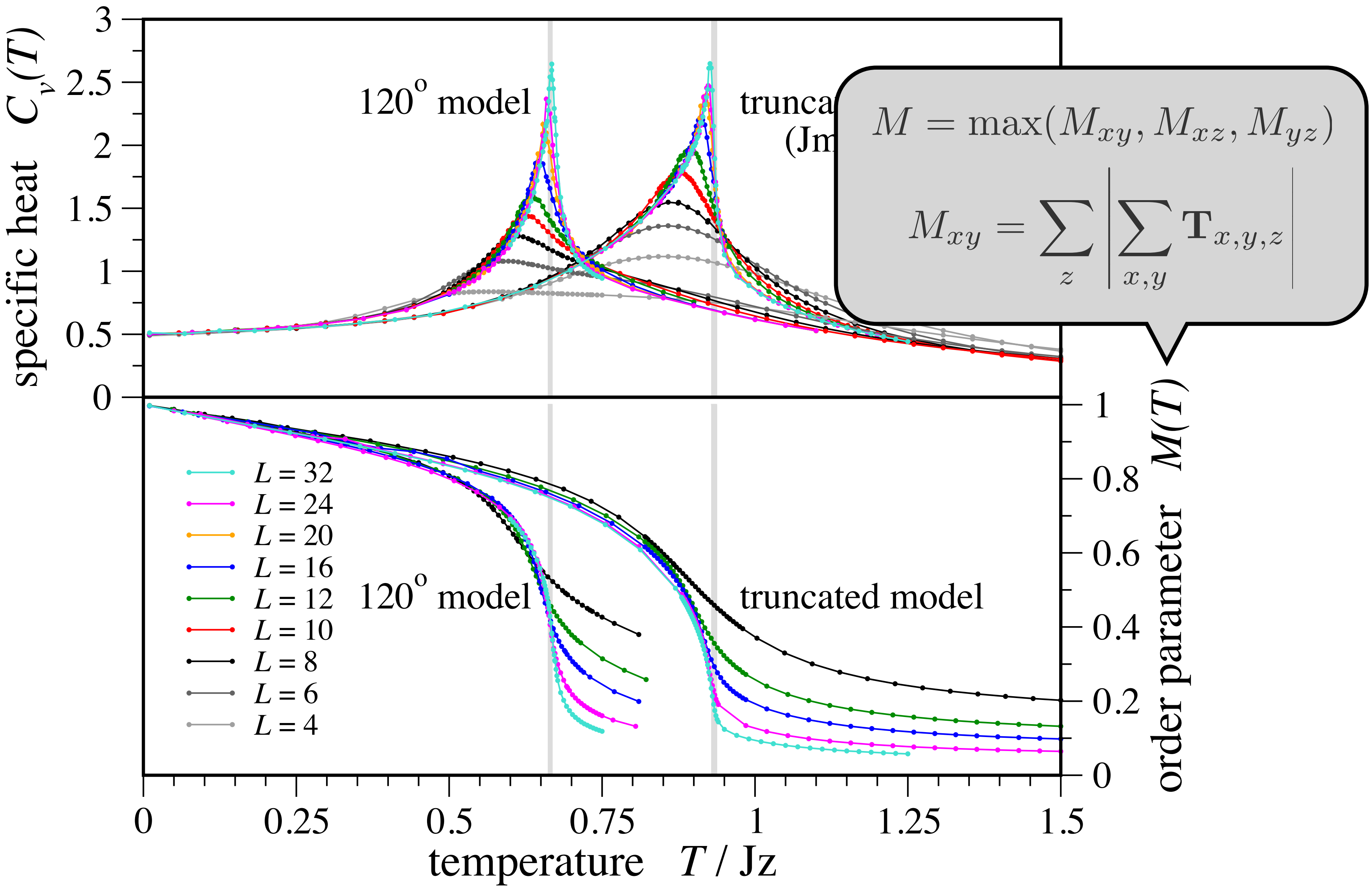


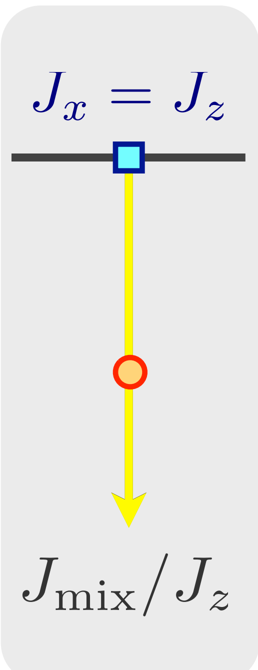


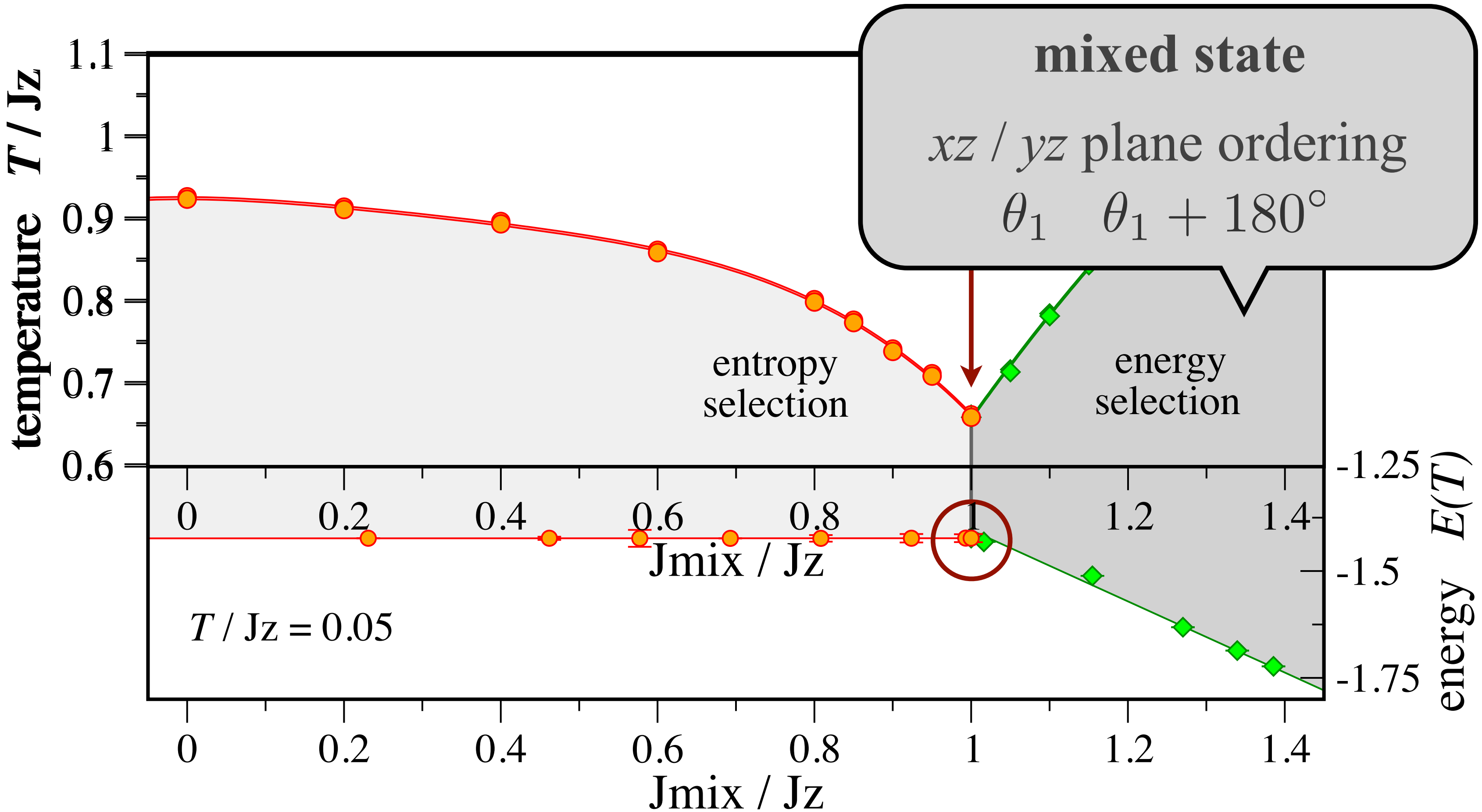
Thermal phase transitions



Moving back to the symmetric point

Finite temperature: A line of continuous thermal phase transitions.





Zero temperature: First-order transition to 'mixed state'.

Summary: classical 120º model

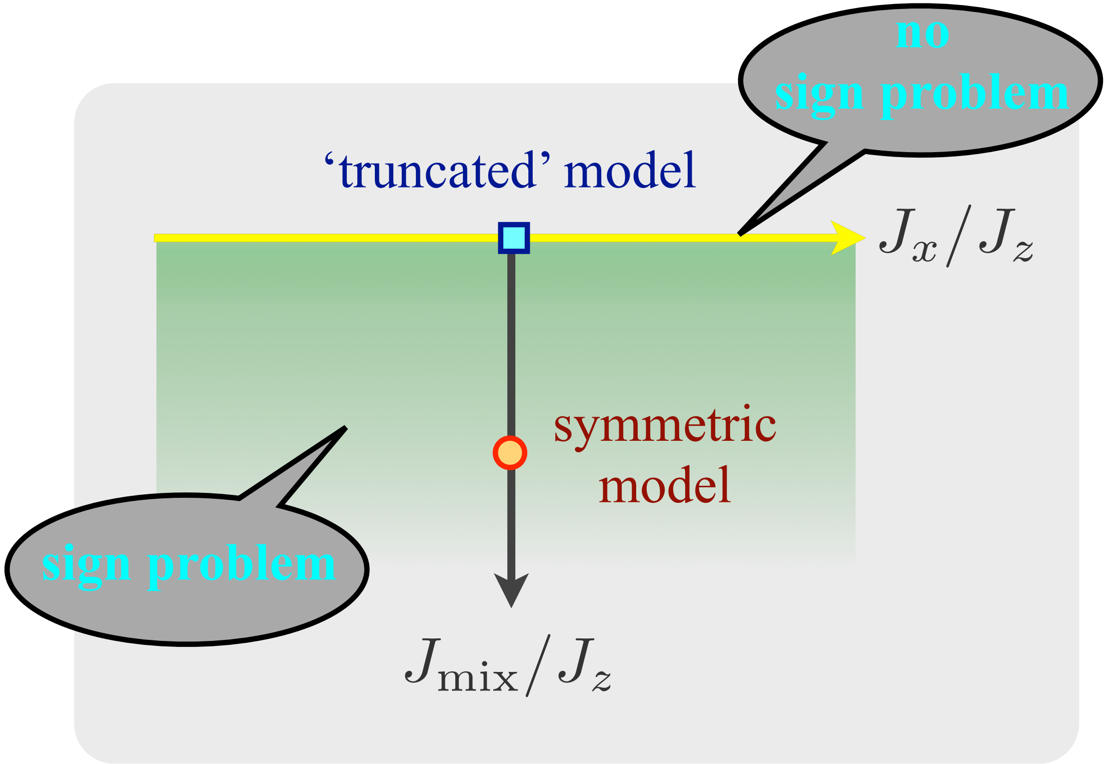
Considering the 120º model in an expanded parameter space, the symmetry of the original model manifests itself in various ways:

- **T=0:** first-order transition between family of models with subextensive ground-state manifold and a phase with unique ground state.
- **low T:** transition between *entropically* and *energetically* selected states.
- **finite T:** line of continuous thermal phase transitions with increasing Tc away from symmetric point.

The quantum 120º model

pseudospins are quantum SU(2) spins

Approaching the quantum 120º model

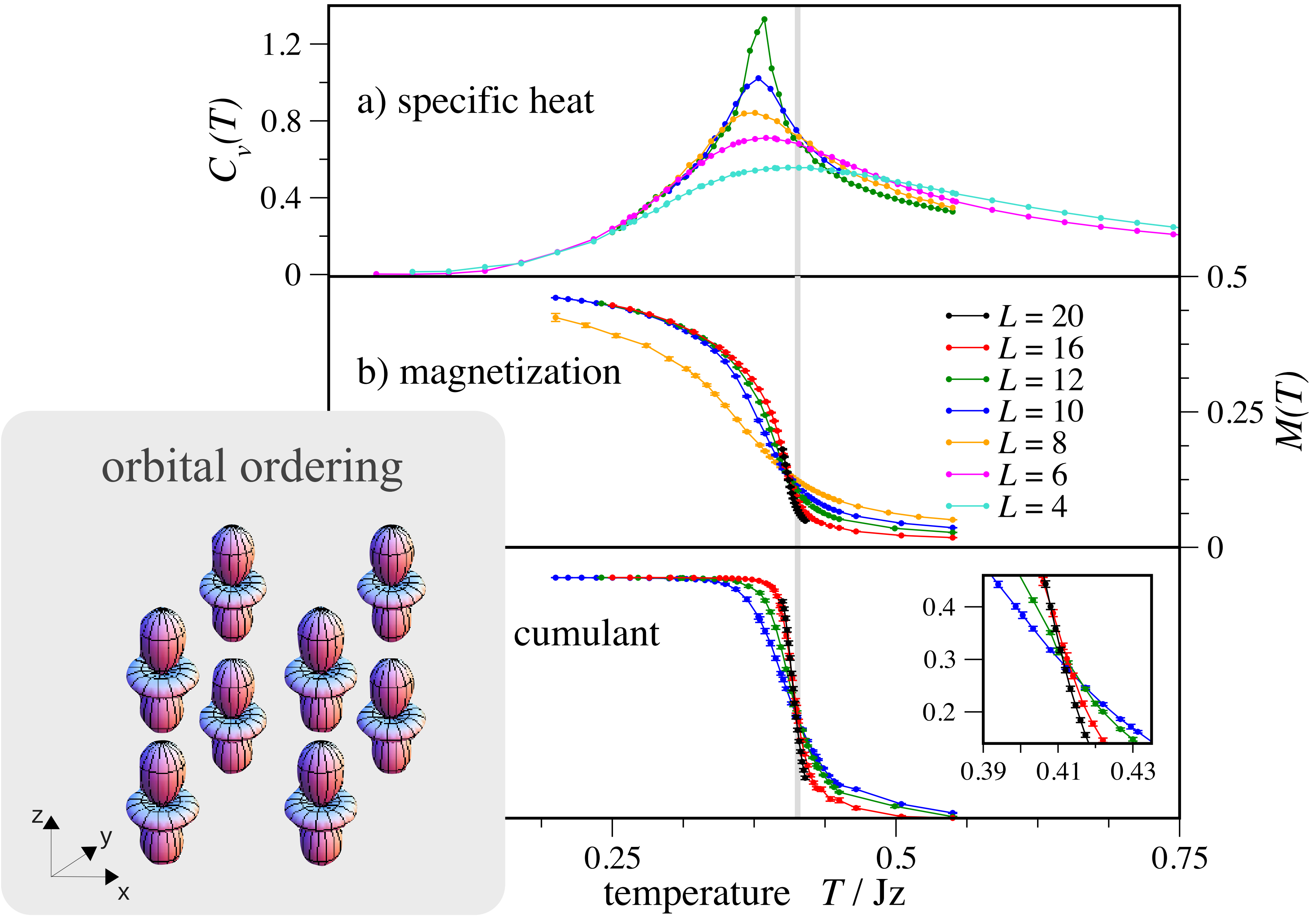


Truncated quantum model reminiscent of planar compass model

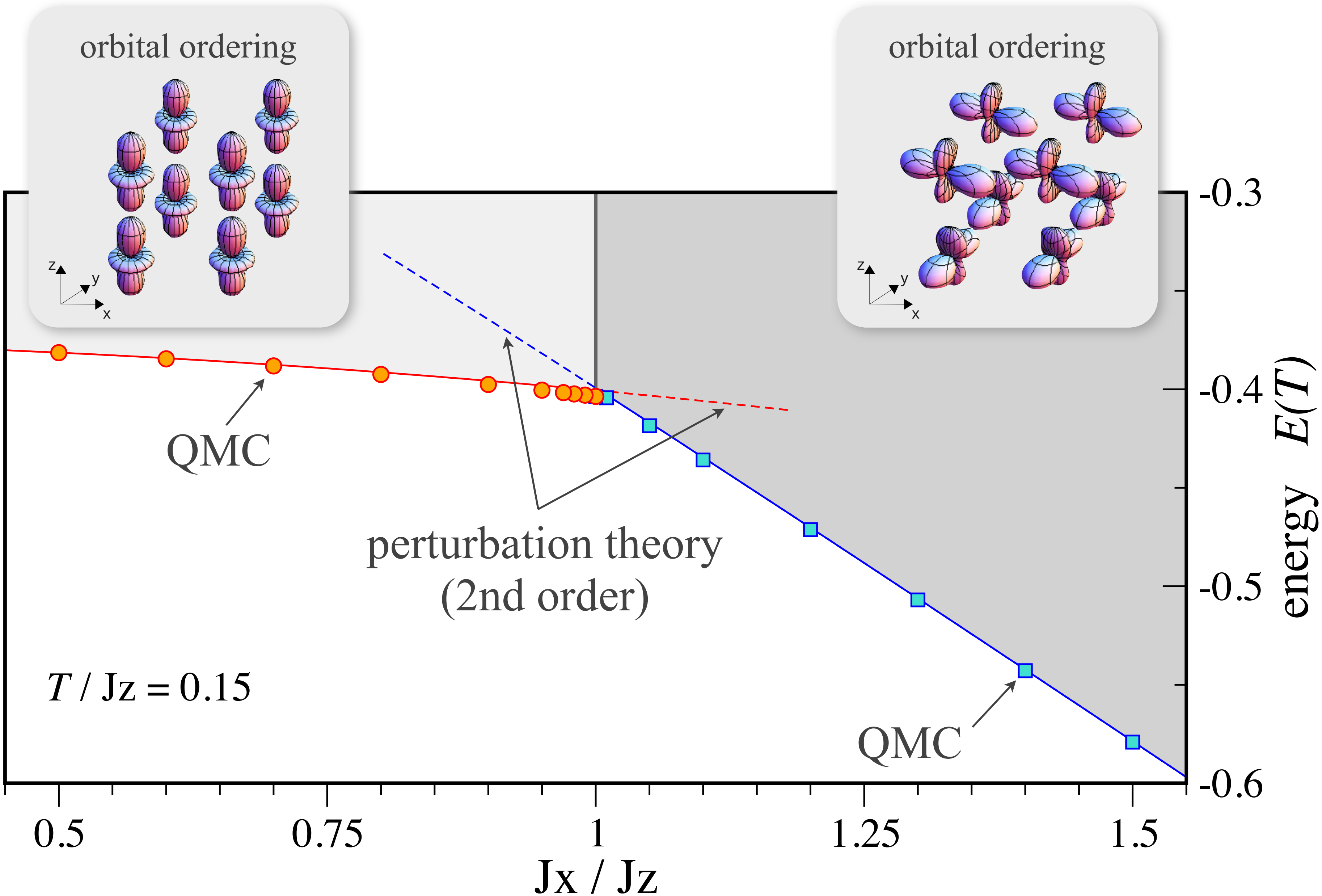
zero-temperature *first-order* phase transition

continuous thermal ordering transition
(but no directional ordering)

Thermal ordering transition (Jx=Jz)



Zero-temperature phase transition



1/S expansion

J. v.d. Brink *et al.*, Phys. Rev. B **59**, 6795 (1999).
K. Kubo, J. Phys. Soc. Jpn. **71**, 1308 (2002).

Can we understand the quantum ground states from a $1/S$ expansion?

Holstein-Primakoff

$$T_i^z = S - a_i^\dagger a_i$$

$$T_i^x = \sqrt{S/2}\left(a_i + a_i^\dagger\right)$$

$$T_i^z \to T_i^z \cos\theta + T_i^x \sin\theta$$

$$T_i^x \to T_i^x \cos\theta - T_i^z \sin\theta$$

Zero-point energy to linear order in S

$$E_0/N = -\frac{3}{2}S^2 + \Delta E_0(\theta) + O(S^{3/2}, S^{1/2})$$

does not explicitly include mixing terms

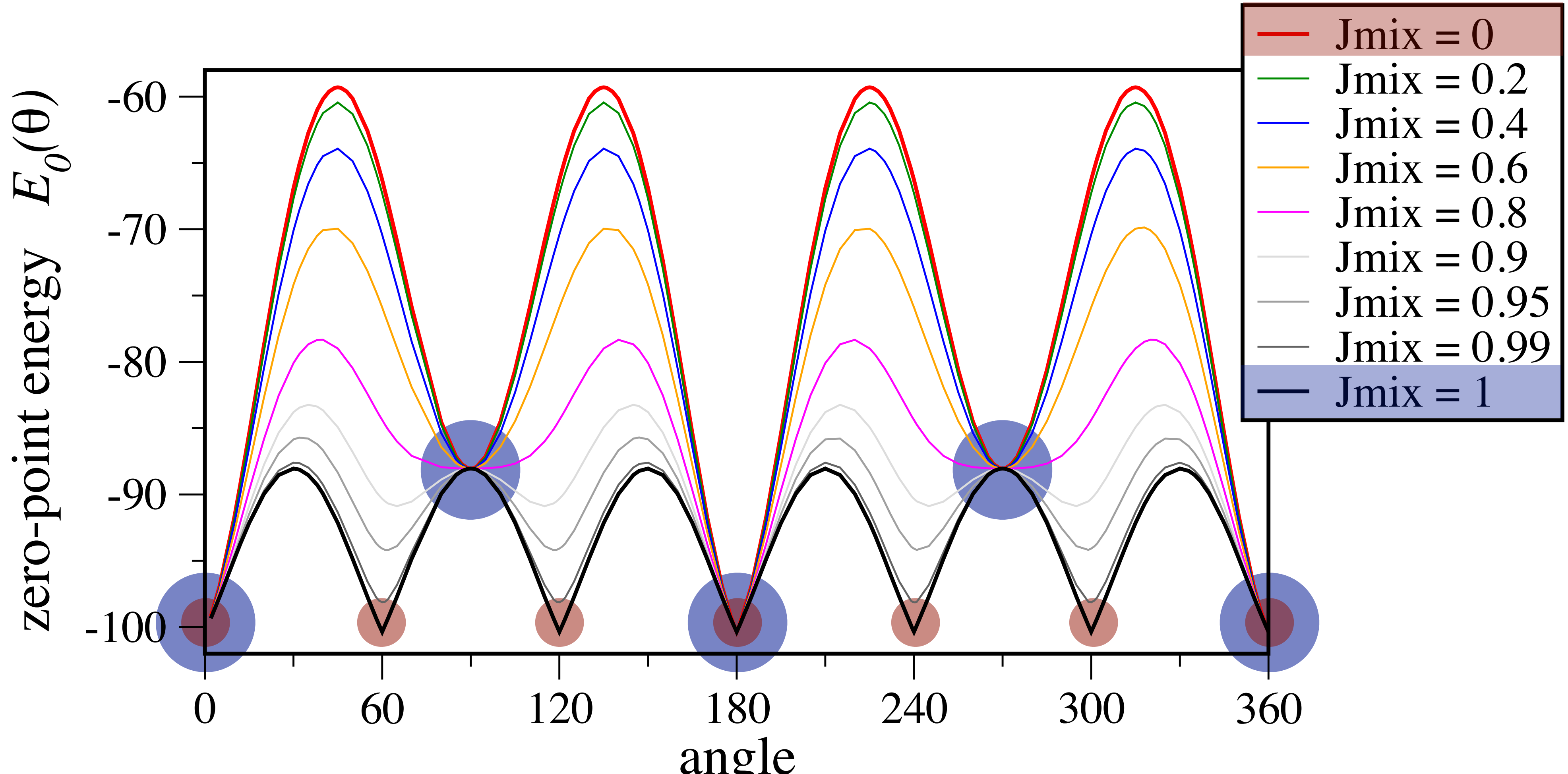
$$H_{120} = -\sum_{i,\gamma=x,y} \frac{1}{4}\left[J_z T_i^z T_{i+\gamma}^z + 3J_x T_i^x T_{i+\gamma}^x \pm\sqrt{3}J_{\mathrm{mix}}(T_i^z T_{i+\gamma}^x + T_i^x T_{i+\gamma}^z)\right] - \sum_i J_z T_i^z T_{i+z}^z$$

mixing terms

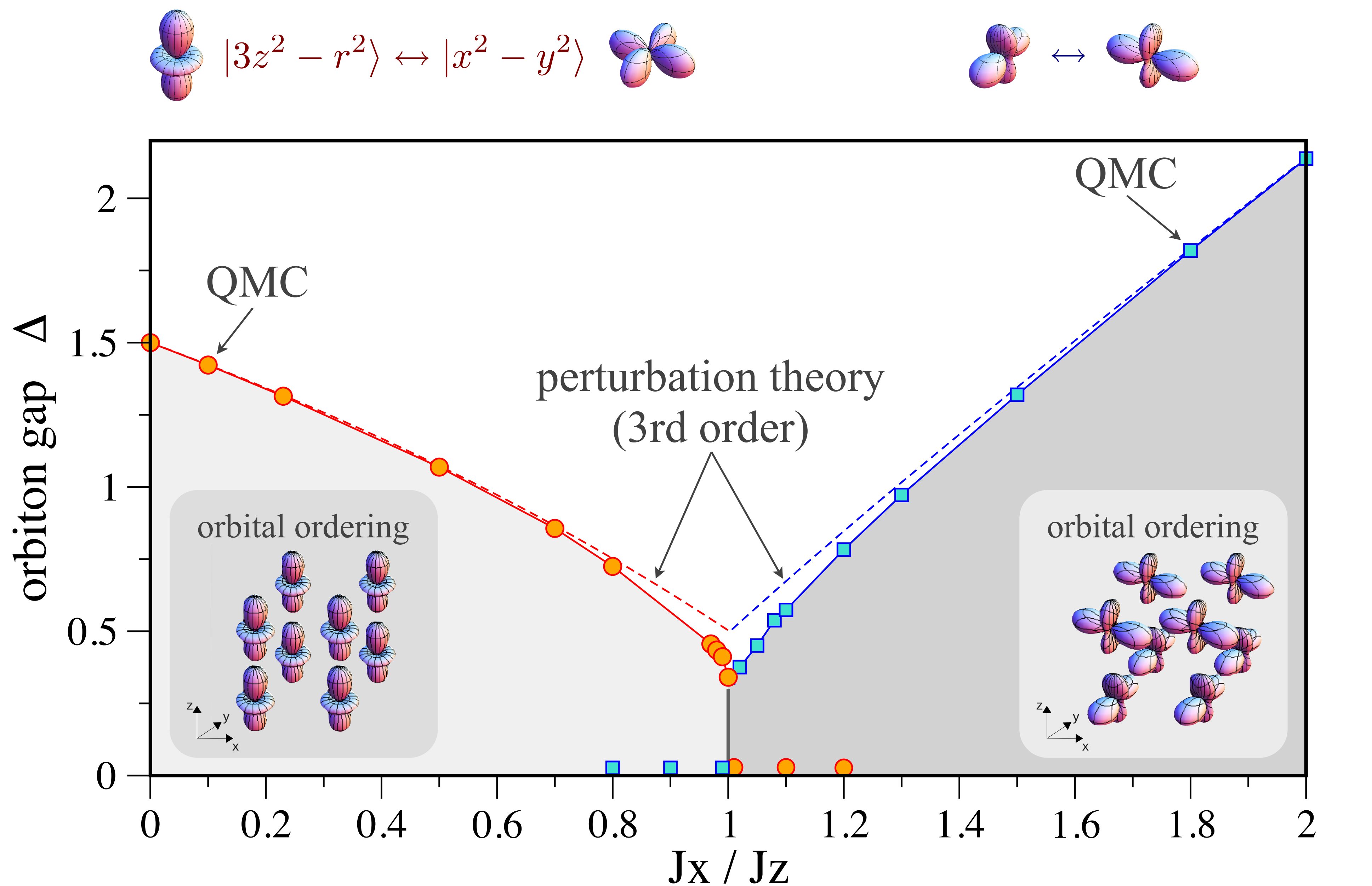
1/S expansion

Zero-point energy to linear order in S

$$E_0/N = -\frac{3}{2}S^2 + \Delta E_0(\theta) + O(S^{3/2}, S^{1/2})$$

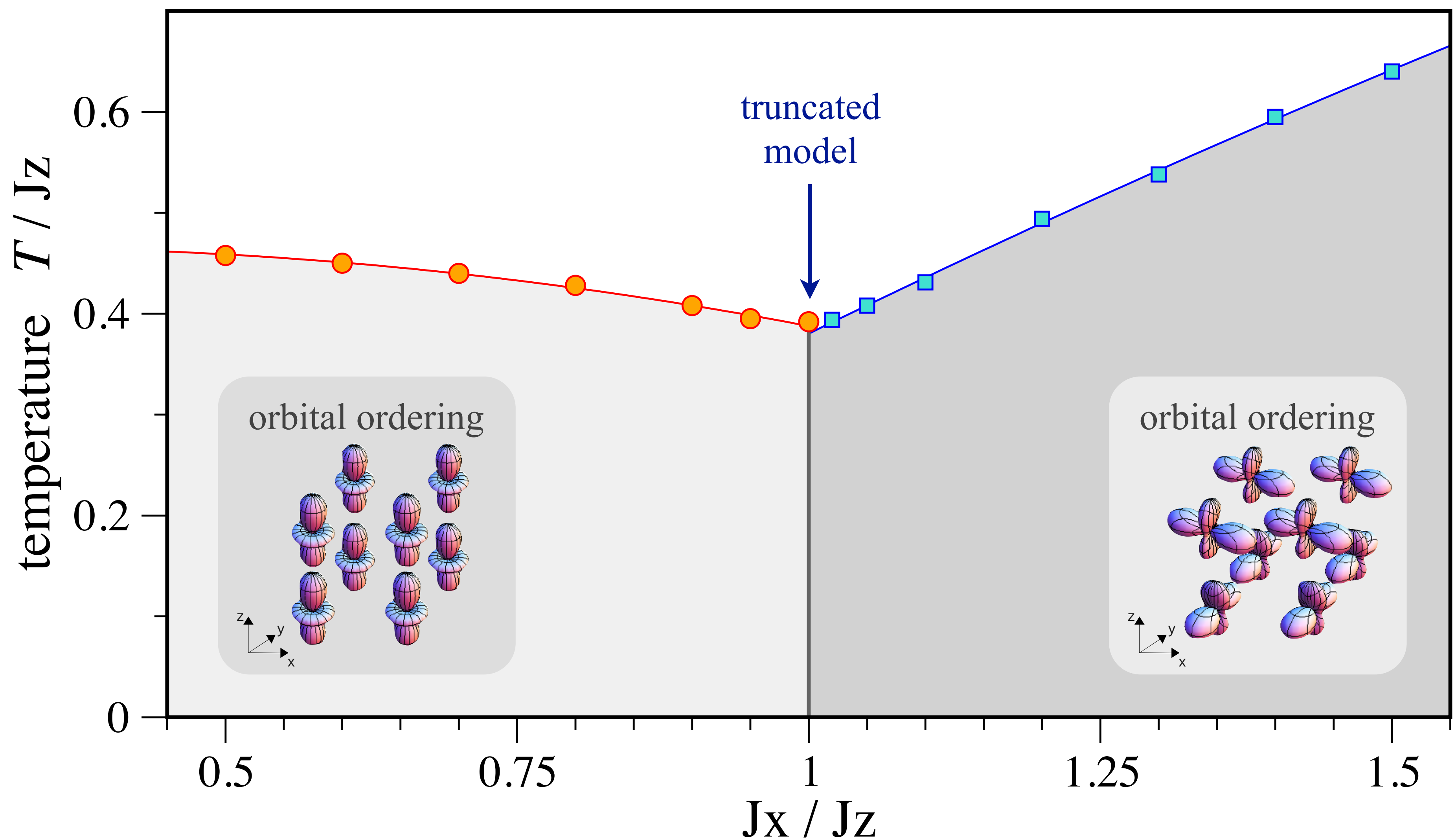


'Orbiton' excitations

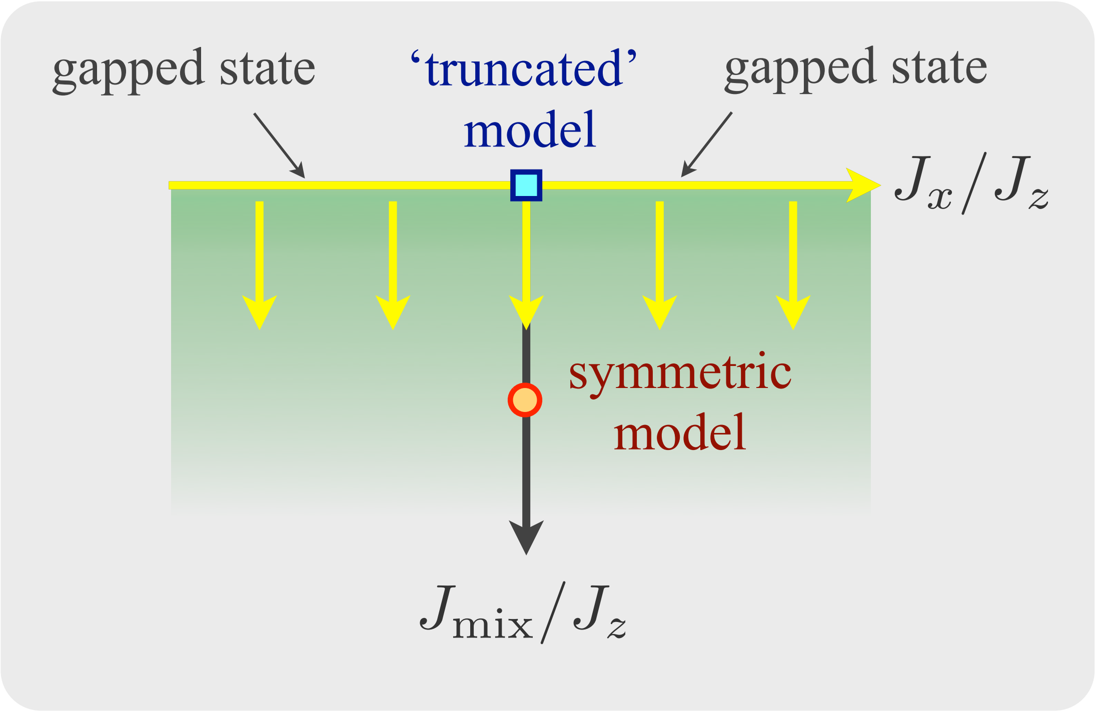


Thermal phase transitions

A line of continuous thermal phase transitions.



Approaching the quantum 120º model



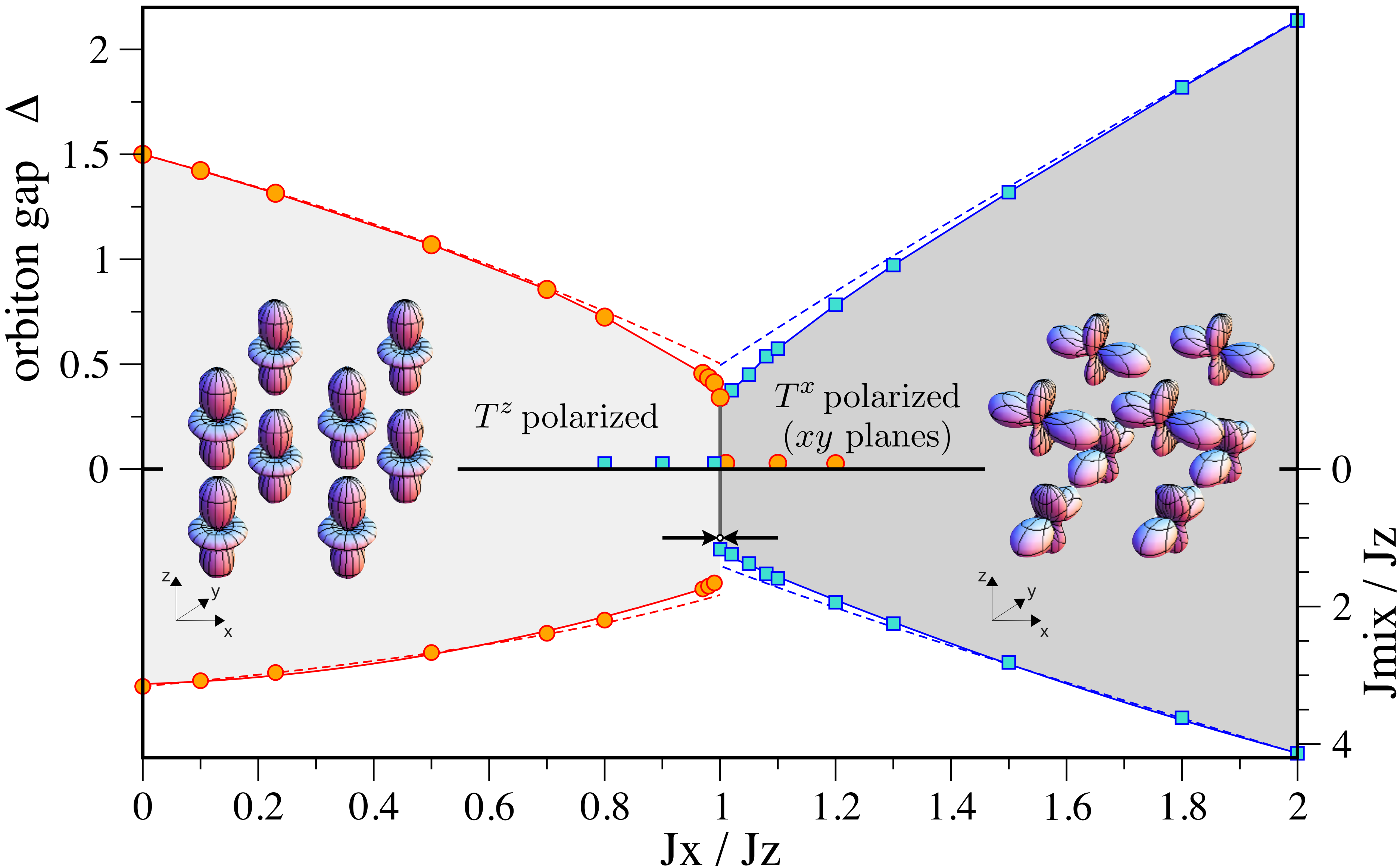
Going off into the Jmix > 0 plane

orbiton condensation

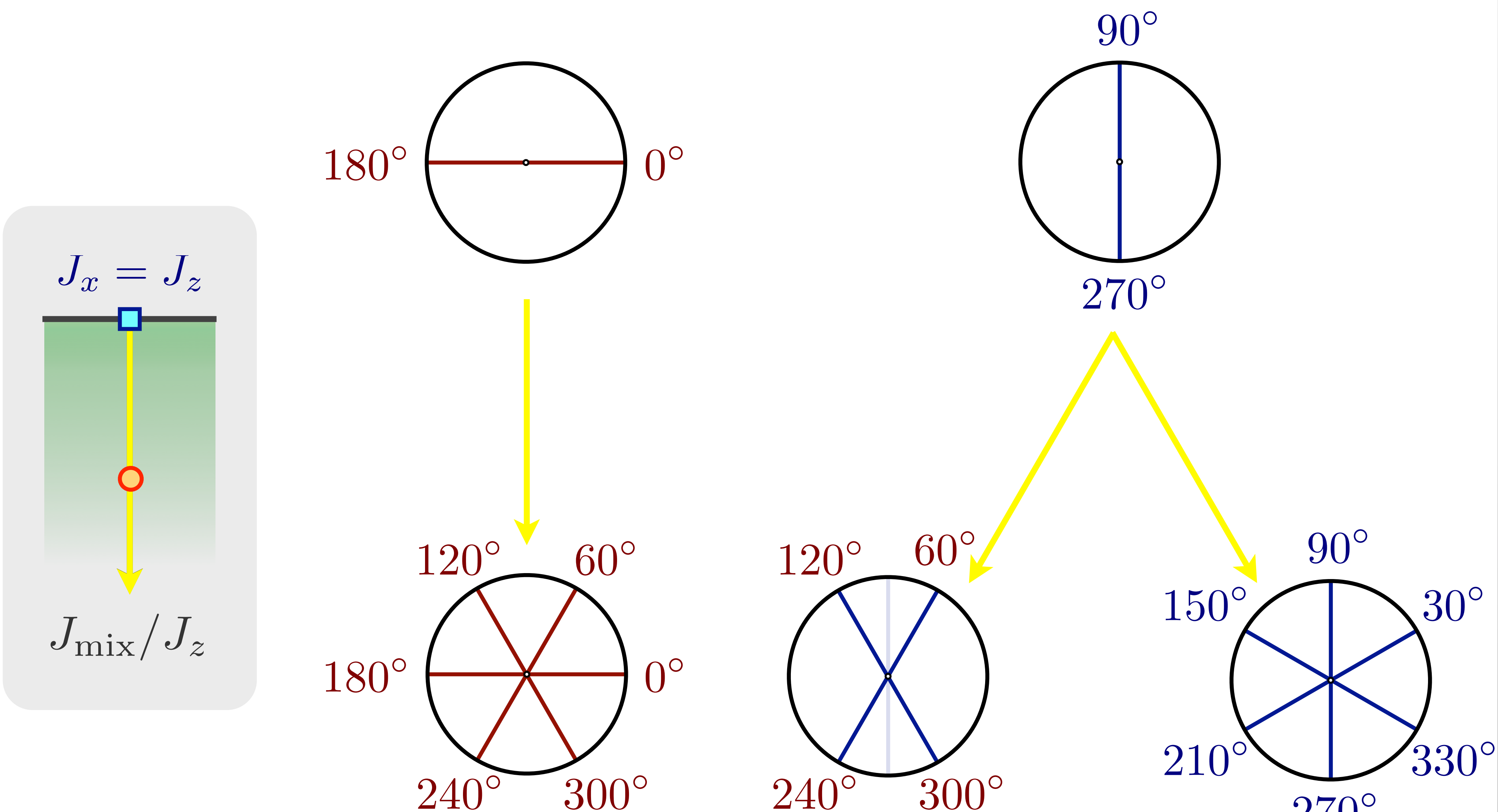
↓

phase boundaries of gapped, polarized states

Phase diagram from orbiton condensation



The symmetric 120° model

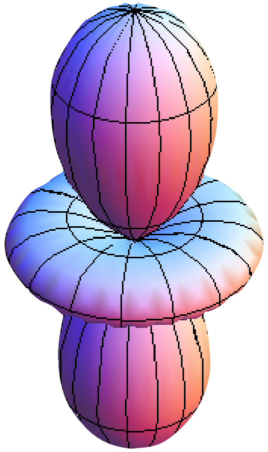


six ground states

twelve ground states

Summary

- Mott insulators with partially filled 3*d*-shells can give rise to orbital degrees of freedom.



- Orbital-only models can be interesting in their own right, because of their highly anisotropic and frustrated interactions.
- The 120º model for e_g orbitals
    - exhibits non-trivial quantum ground states
    - sits in the proximity of several T=0 phase transitions and various competing phases.