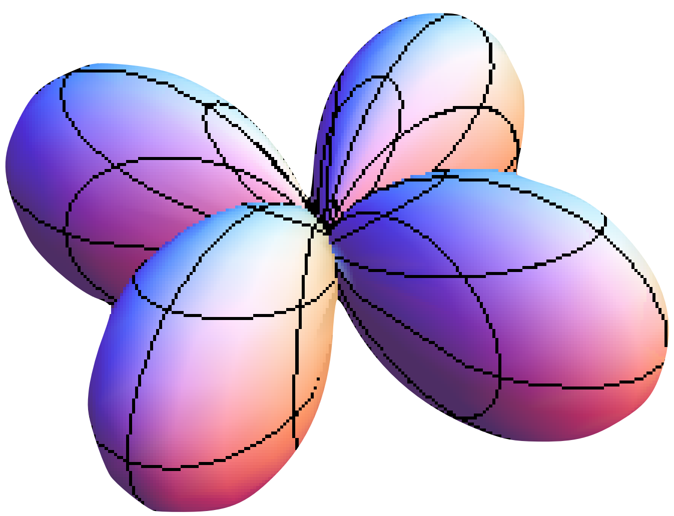
Orbital ordering in e_g orbital systems:

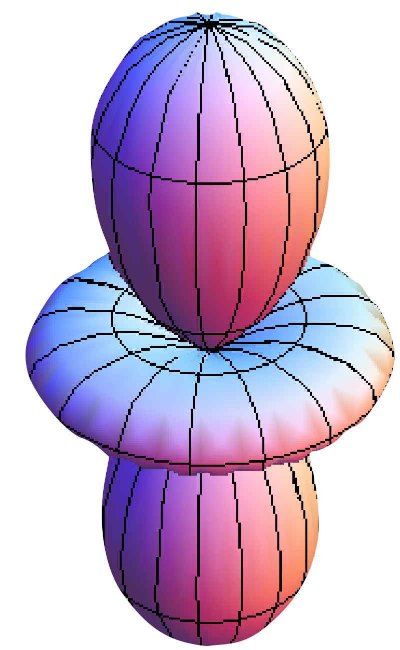
Critical properties of the classical 120º model

CompPhys'10, November 2010



Sandro Wenzel
EPF Lausanne

Andreas Laeuchli
MPI PKS, Dresden

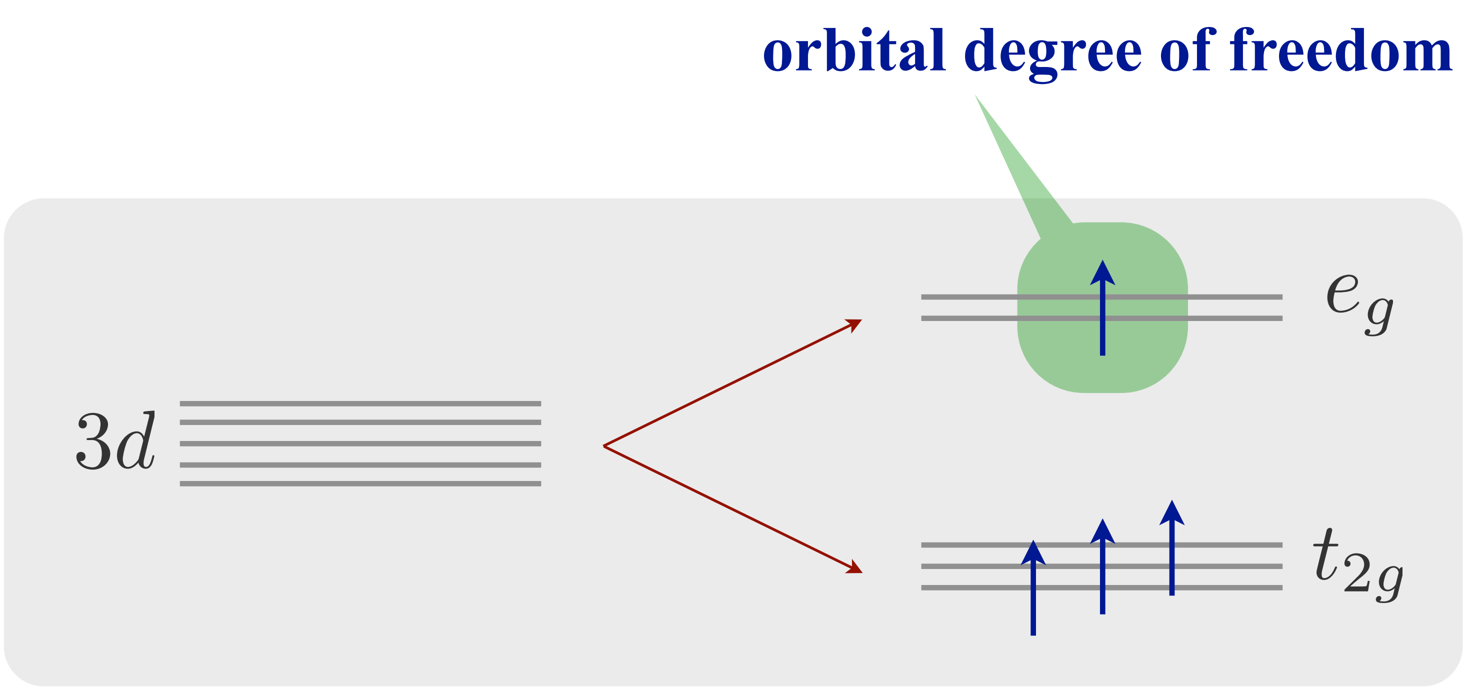


ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

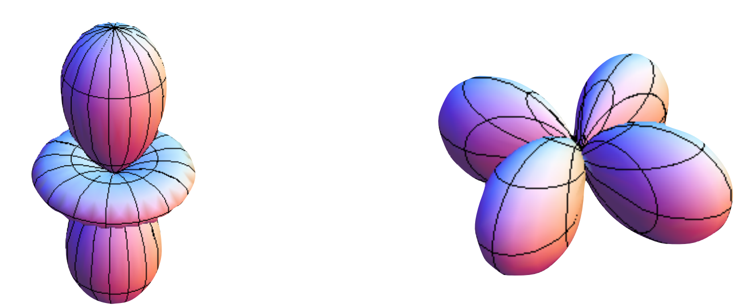
Mott insulators with partially filled *d*-shells

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)



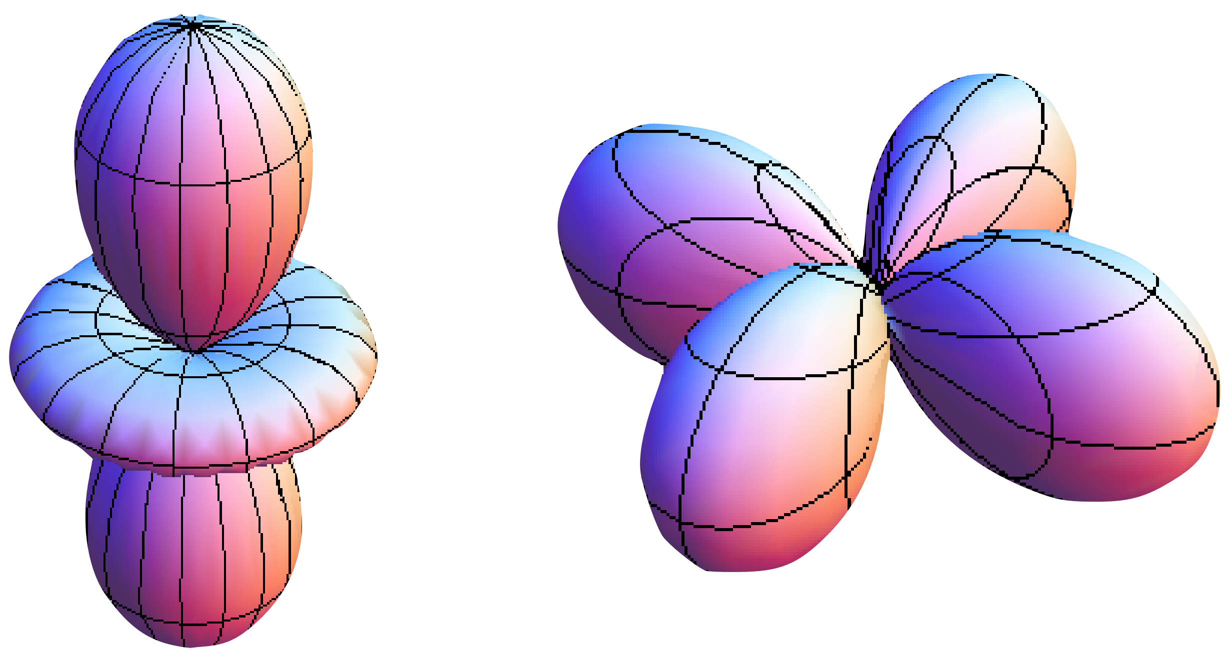
$|3z^2 - r^2\rangle$ $|x^2 - y^2\rangle$

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

K**Cu**F_3 (d^9)
Li**Ni**O_2

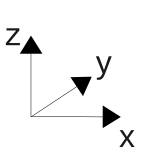
Description of orbital degree of freedom

General orbital state is superposition of e_g basis states



$|3z^2 - r^2\rangle$ $|1\rangle$ $\quad$ $|x^2 - y^2\rangle$ $|2\rangle$

$$|\psi\rangle = e^{i\phi}\cos(\theta/2)|1\rangle + e^{-i\phi}\sin(\theta/2)|2\rangle$$



J. van den Brink, New Journal of Physics **6**, 210 (2004).

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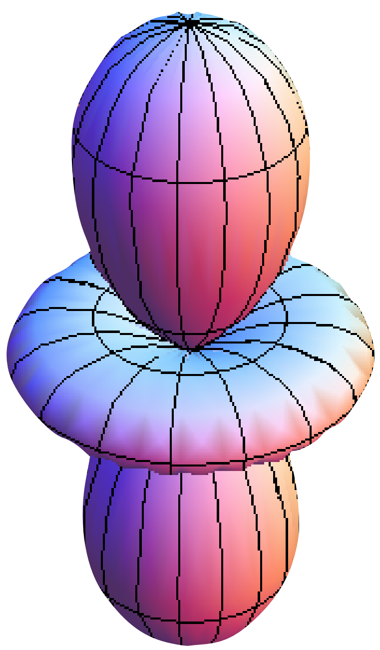

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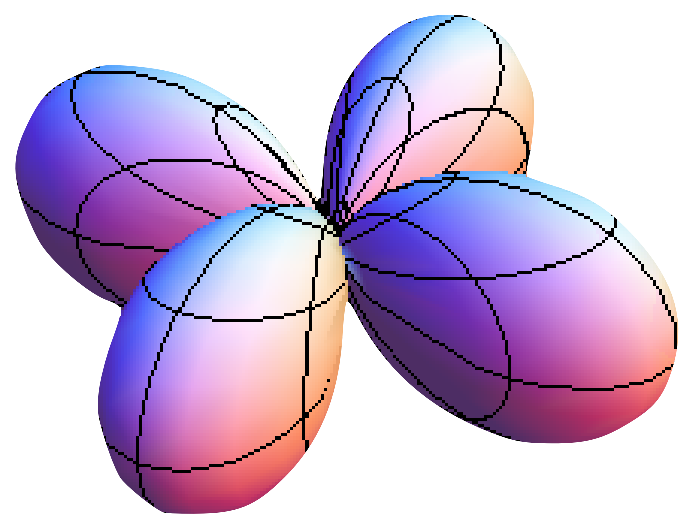

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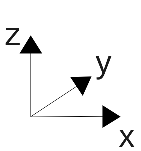

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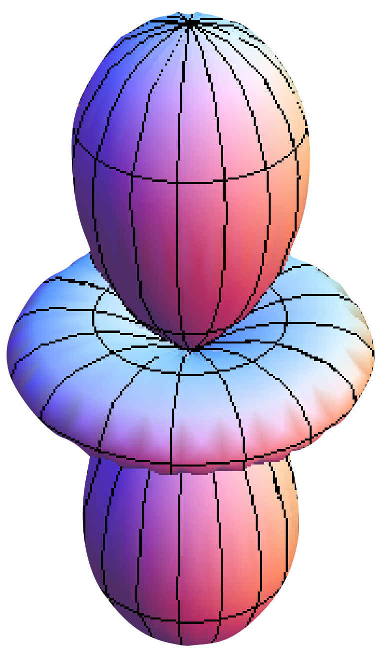

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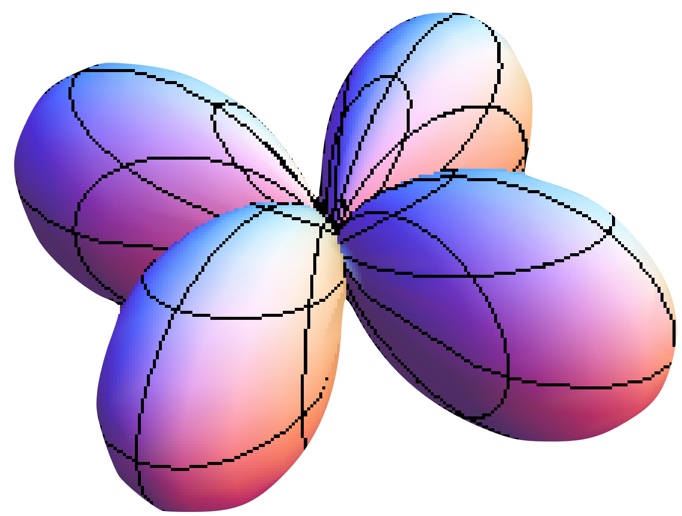

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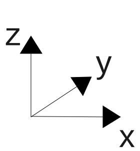

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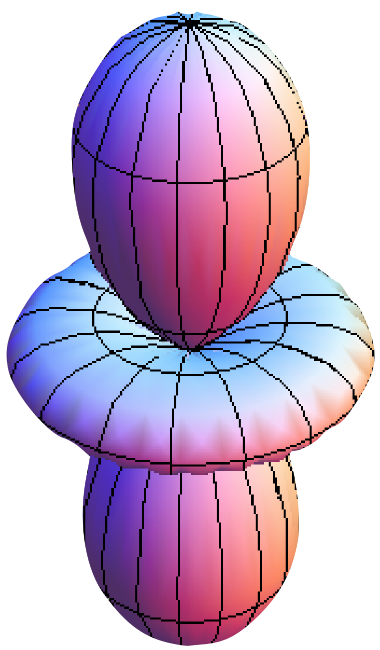

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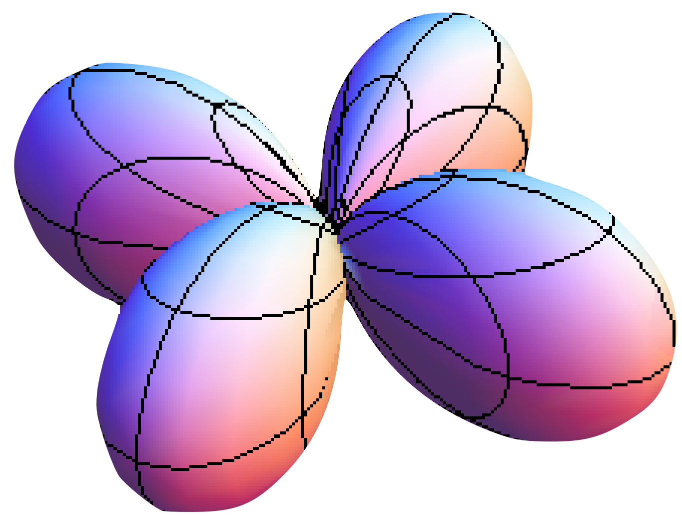

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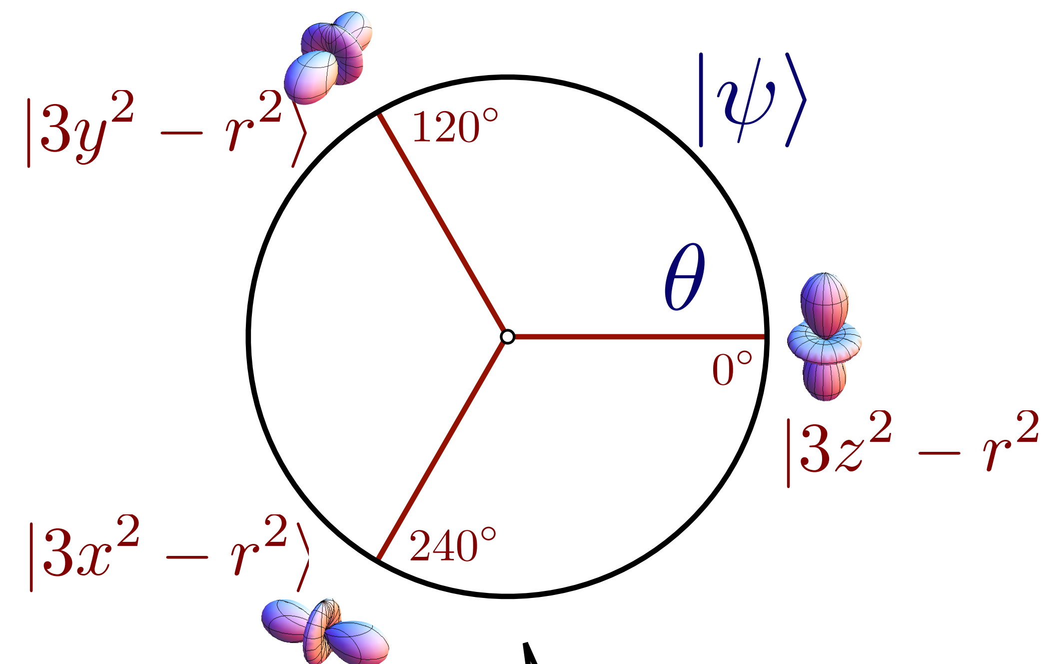
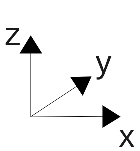


$$|\psi\rangle = \cos(\theta/2)|1\rangle + \sin(\theta/2)|2\rangle$$

defines a XY spin

$T = (T_z, T_x)$



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Orbital interactions: The 120° model

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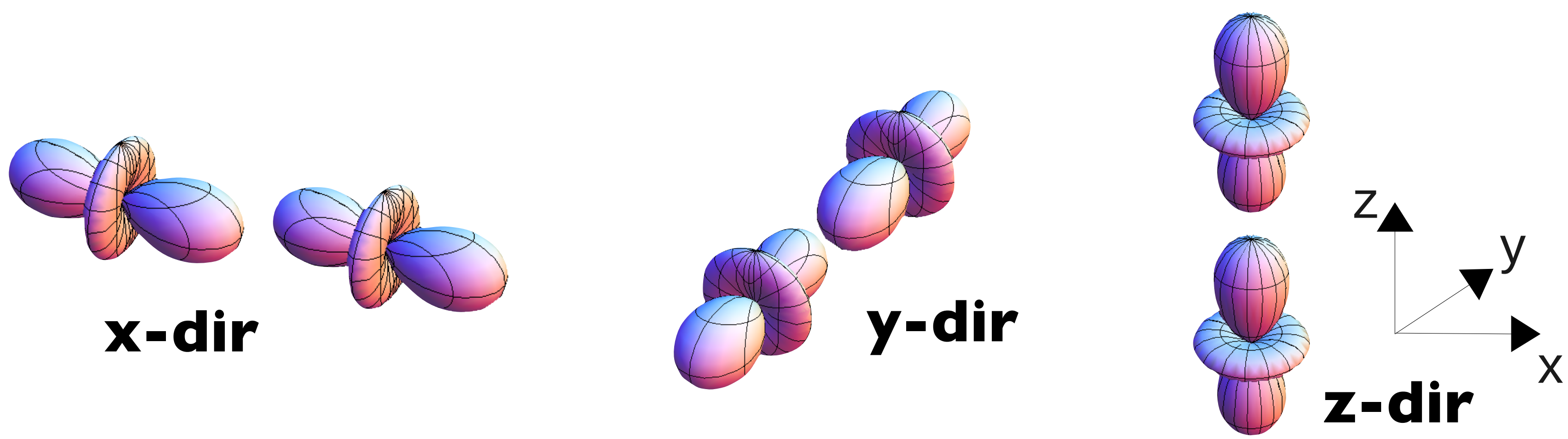
Jahn-Teller effect: orbital **interactions mediated by phonons**

favourable nearest neighbour configurations:



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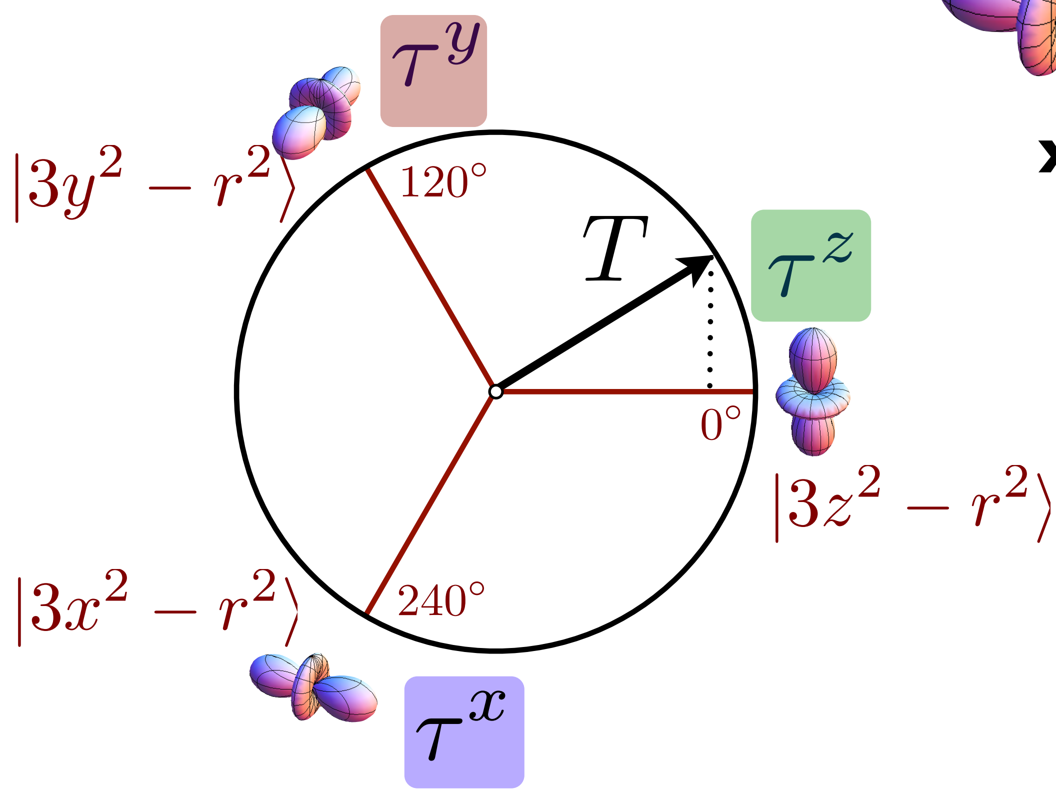

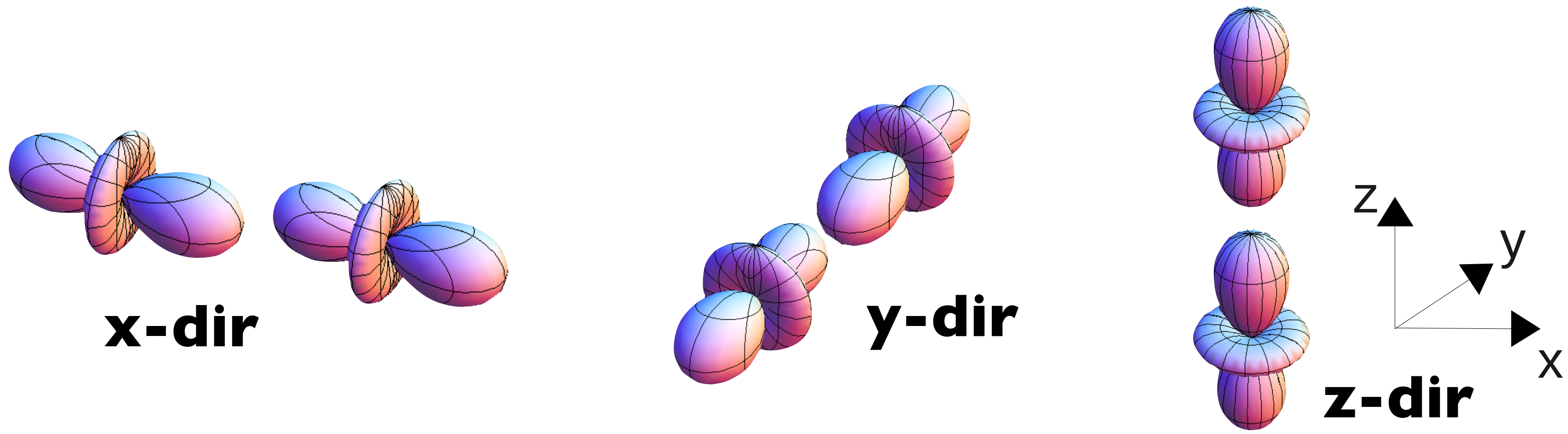

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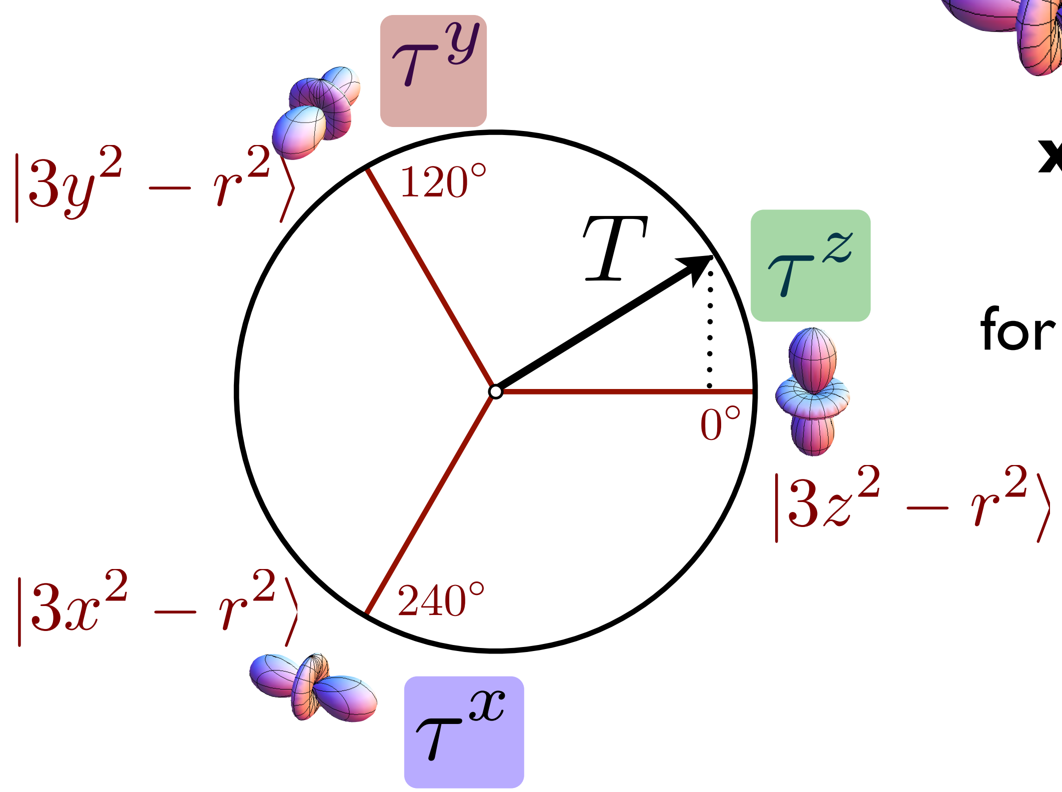
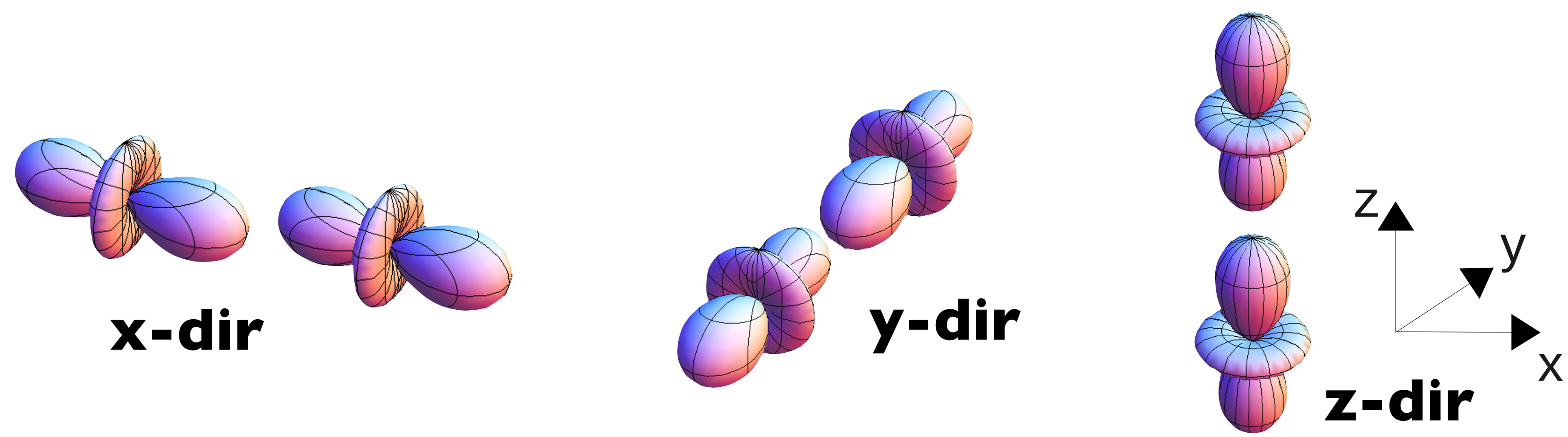




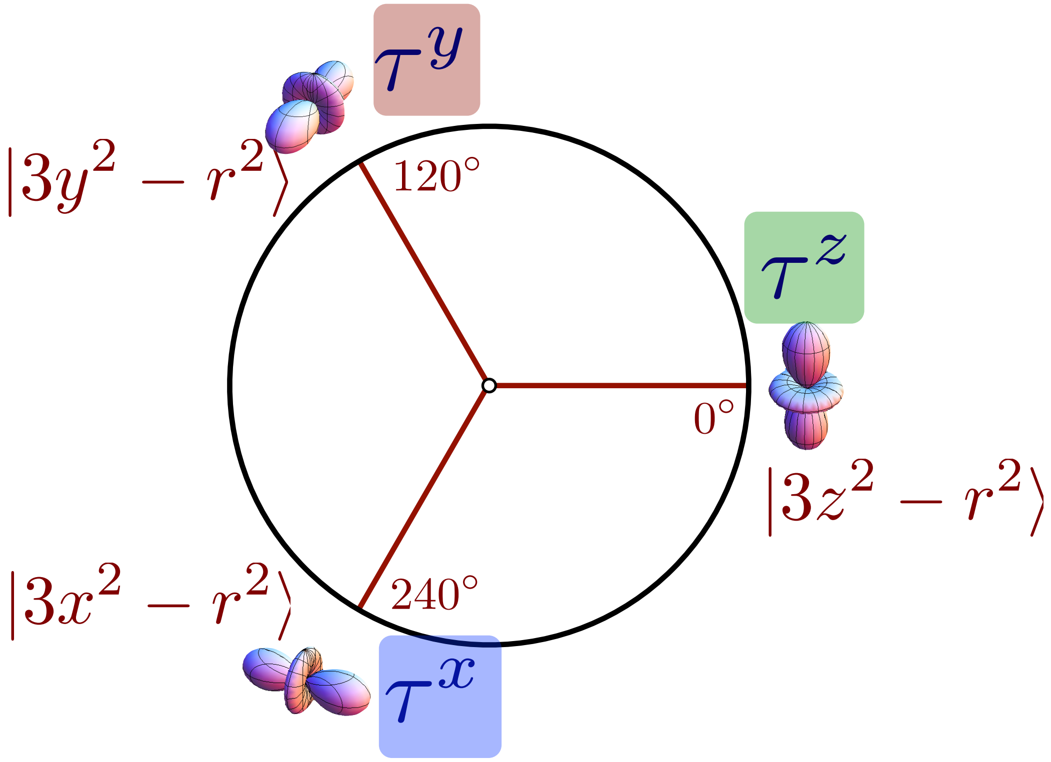
for arbitr. state T define **projection** onto favourable states

$$\boldsymbol{\tau}_i = \begin{pmatrix} \sqrt{3}/2 & 1/2 \\ -\sqrt{3}/2 & 1/2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} T_i^x \\ T_i^z \end{pmatrix}$$

$$H_{120} = -\sum_i \left[\tau_i^x \tau_{i+\mathbf{e_x}}^x + \tau_i^y \tau_{i+\mathbf{e_y}}^y + \tau_i^z \tau_{i+\mathbf{e_z}}^z \right]$$

Critical properties of the classical 120º model

pseudospins are classical O(2) spins



1. Is there collective ordering at finite T?
2. What are the critical properties (universality)?

our approach: extensive Monte Carlo simulations!

$$H_{120} = \sum_i \left[\tau_i^x \tau_{i+\mathbf{e_x}}^x + \tau_i^y \tau_{i+\mathbf{e_y}}^y + \tau_i^z \tau_{i+\mathbf{e_z}}^z \right]$$

Zero temperature: degenerate ground states

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

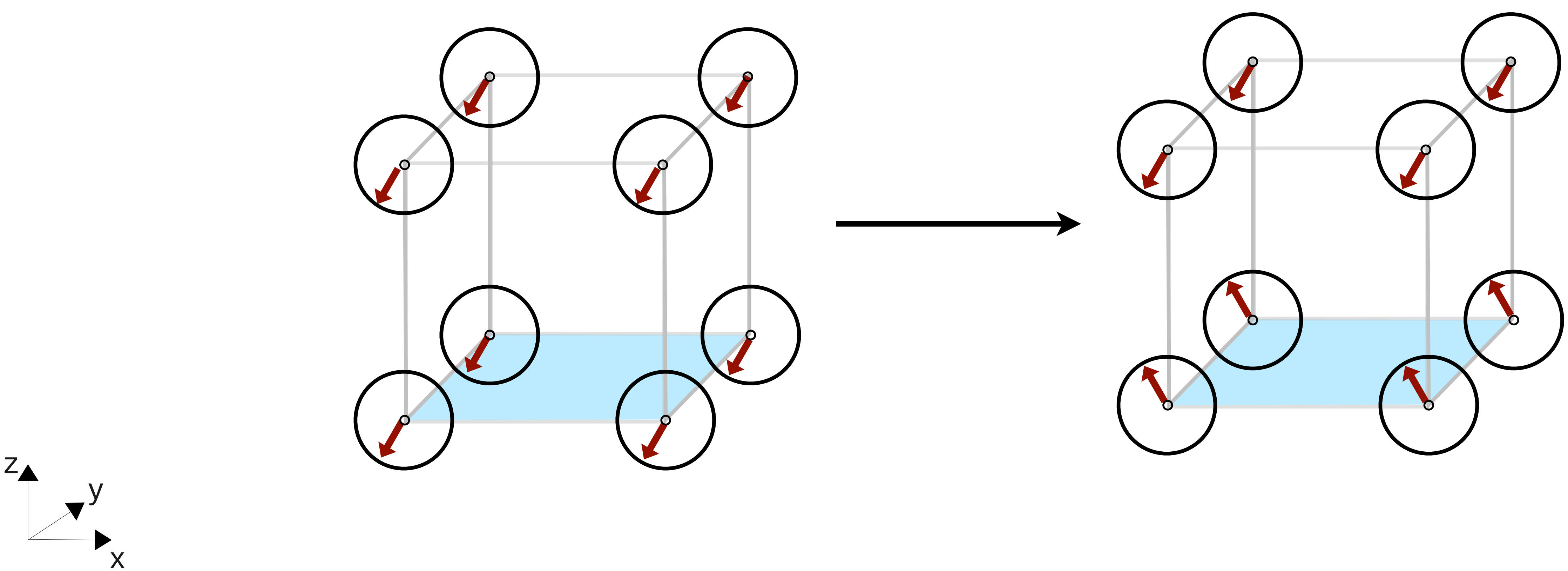
Emergent symmetries: U(1) and Z_2 symmetries

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

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

example of Z2 symmetry:

reflect all spins in *xy* plane at 0°



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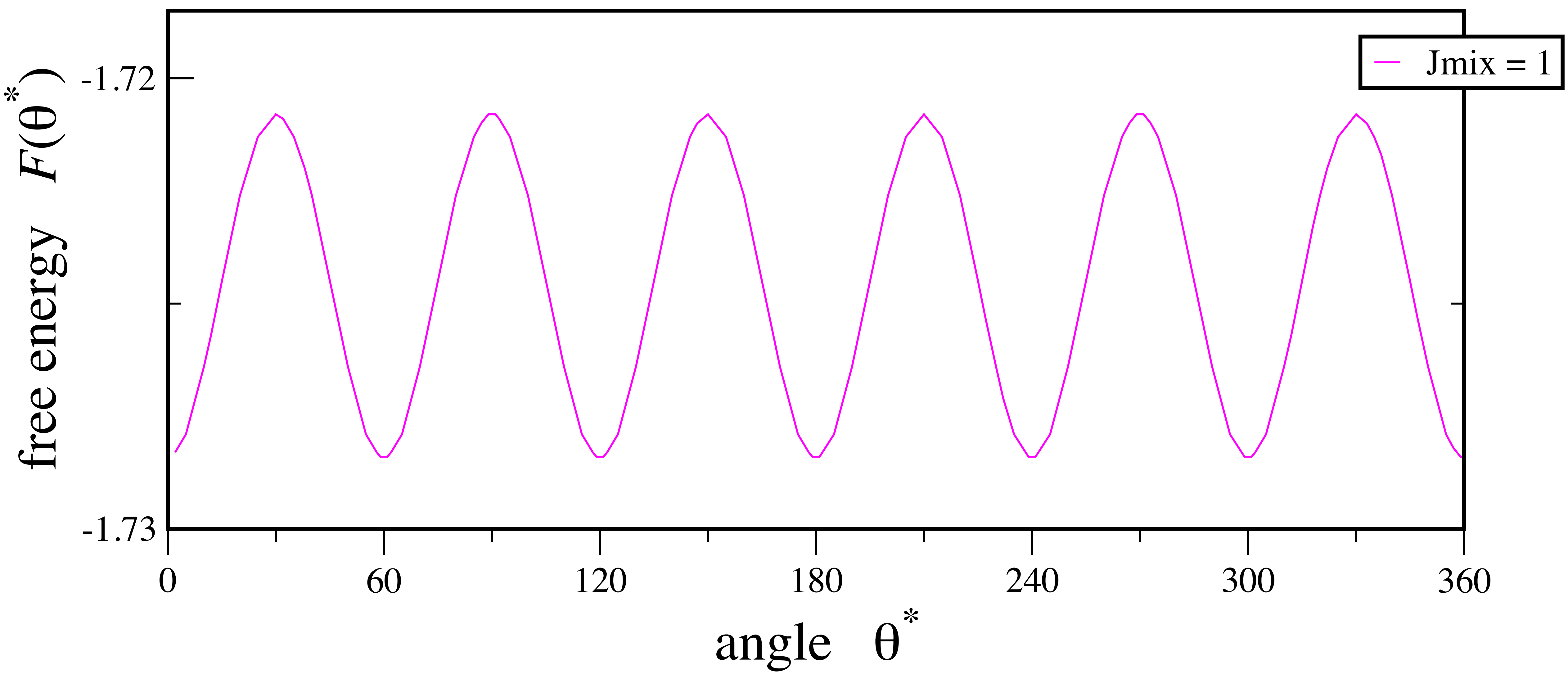
Spin-wave approximation: expansion in fluctuations $\delta\theta_i = \theta_i - \theta^*$ around ordered state with $\theta_i = \theta^*$ at each site.



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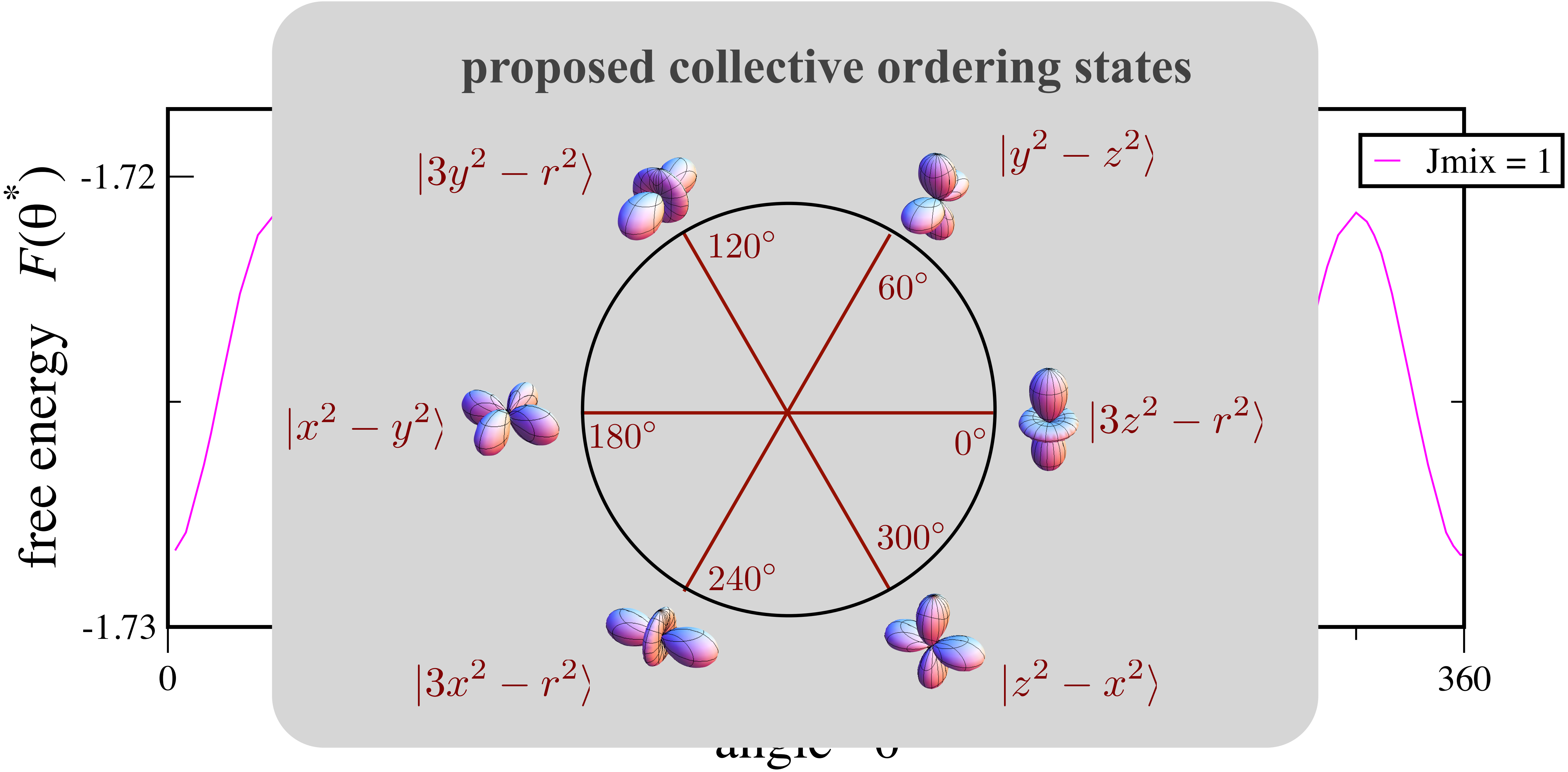
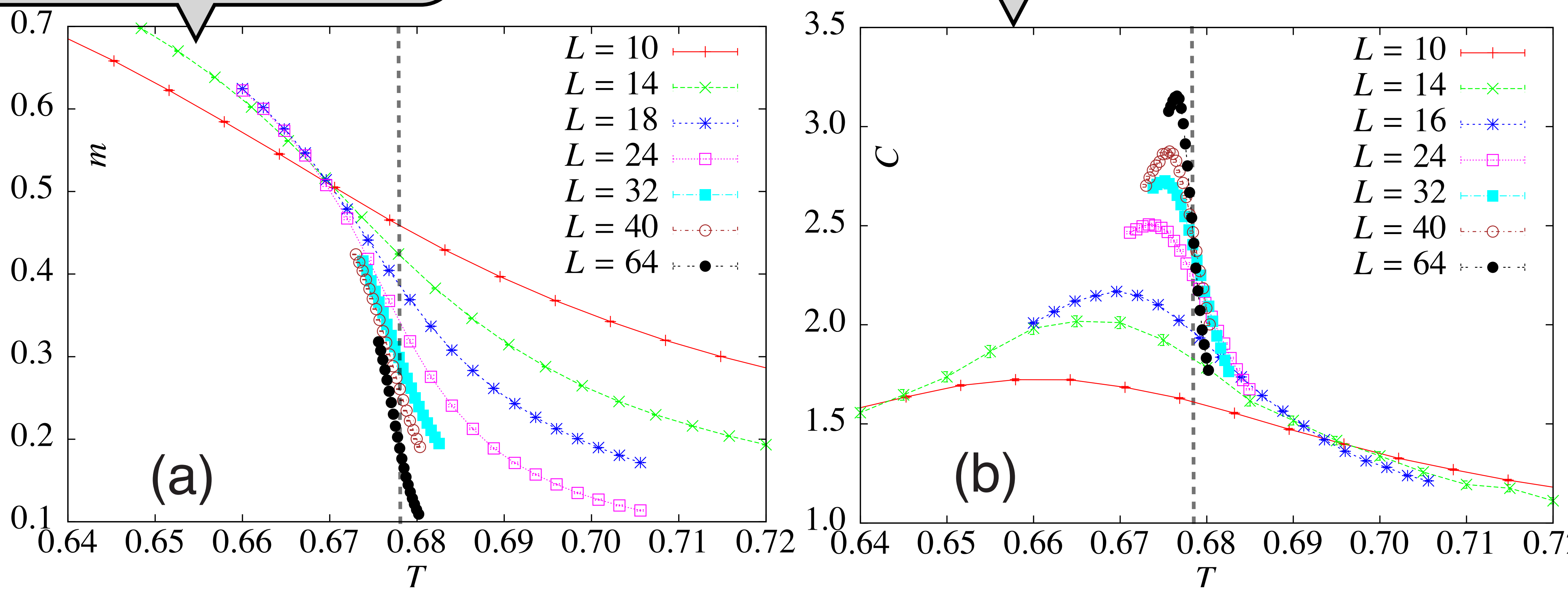


Orbital-ordering phase transition

$$m = \frac{1}{N}\sqrt{\left(\sum_i T_i^x\right)^2 + \left(\sum_i T_i^z\right)^2}$$

heat capacity

$T_c = 0.6775(1)$



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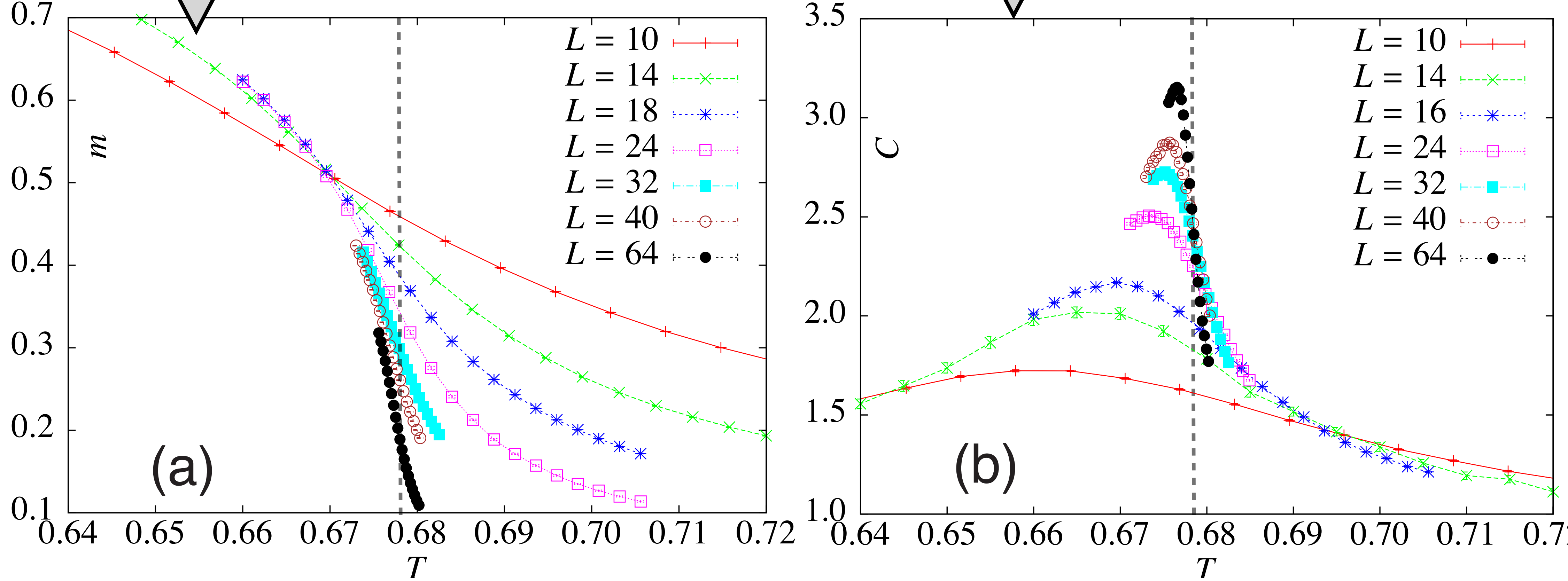

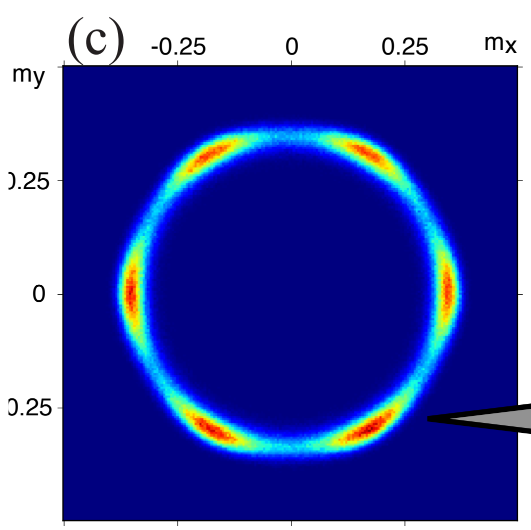

distribution of order parameter

below Tc:
6 fold symmetry

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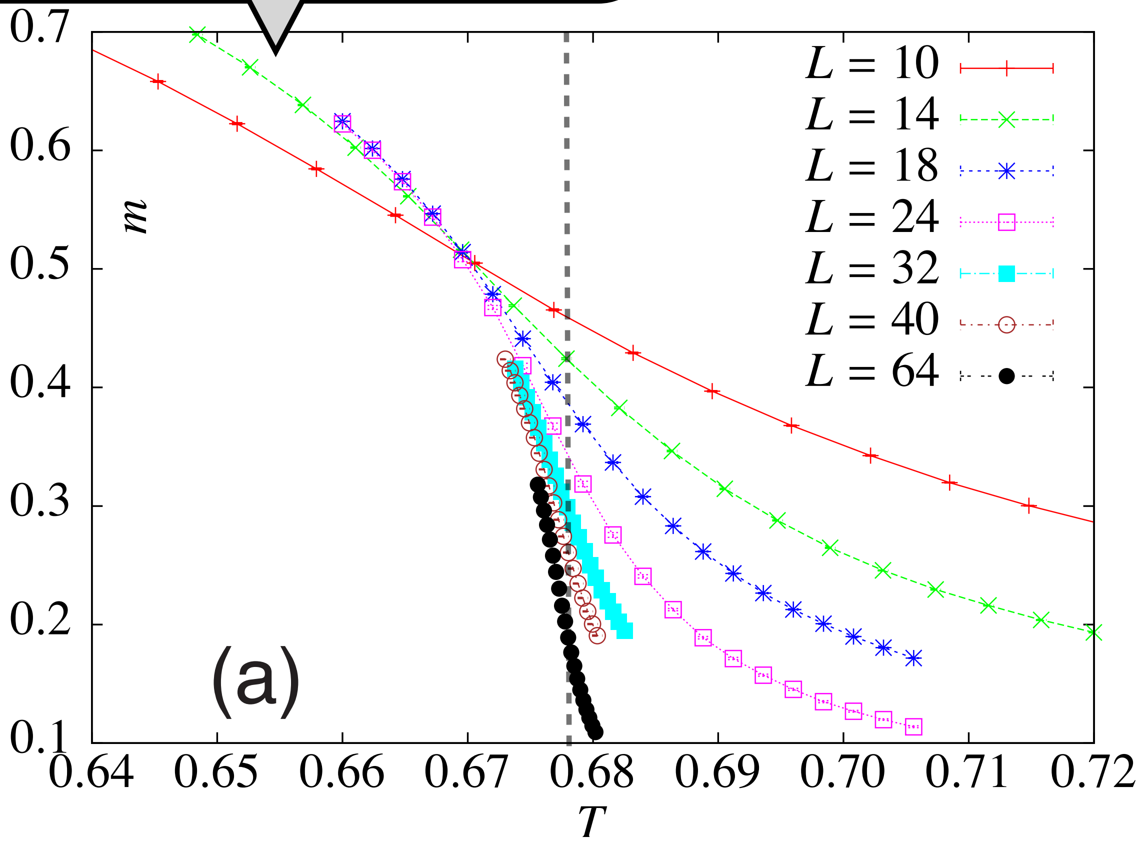

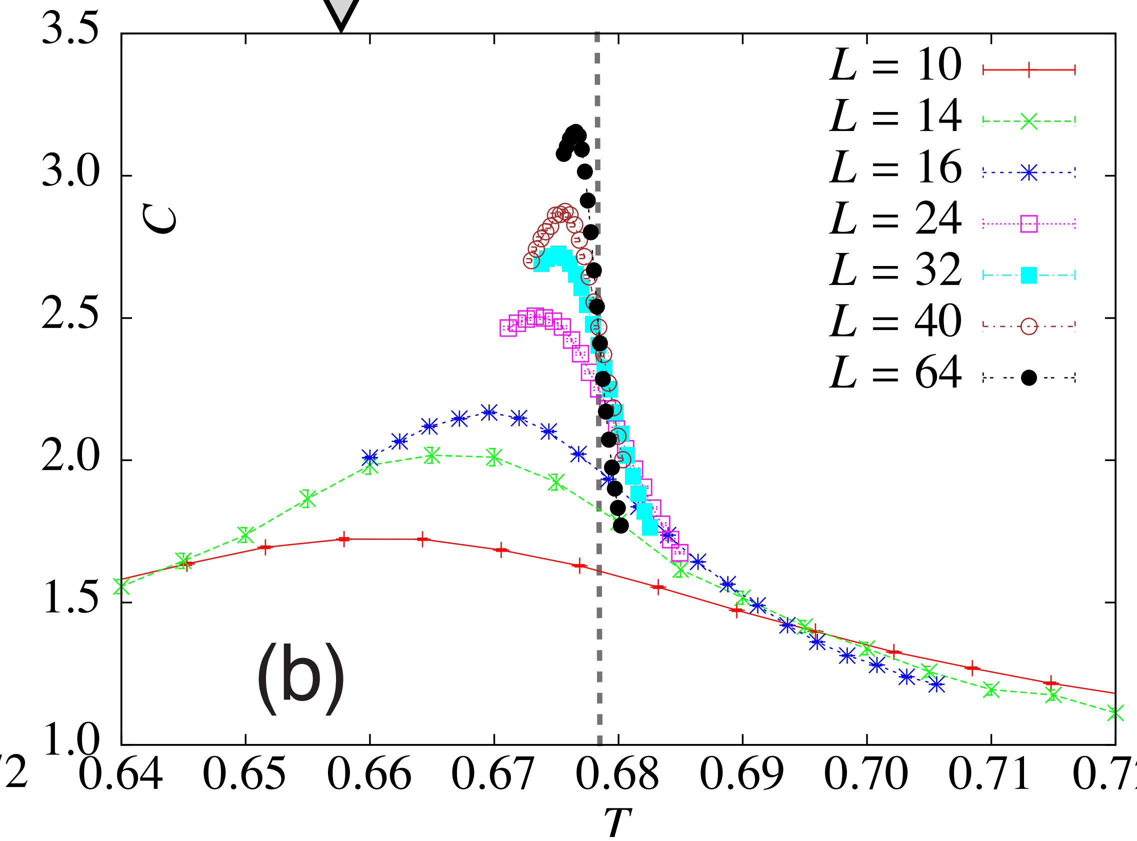

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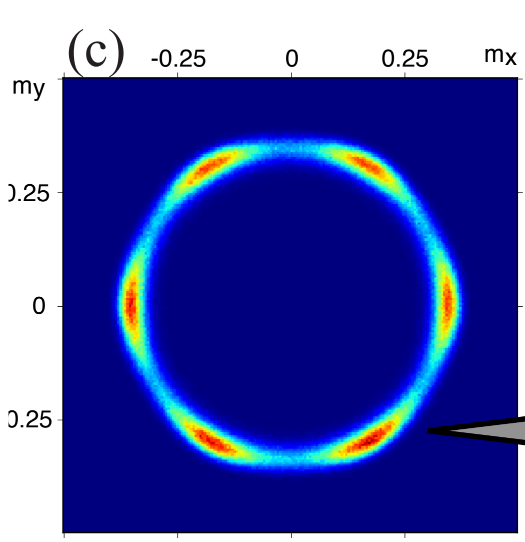

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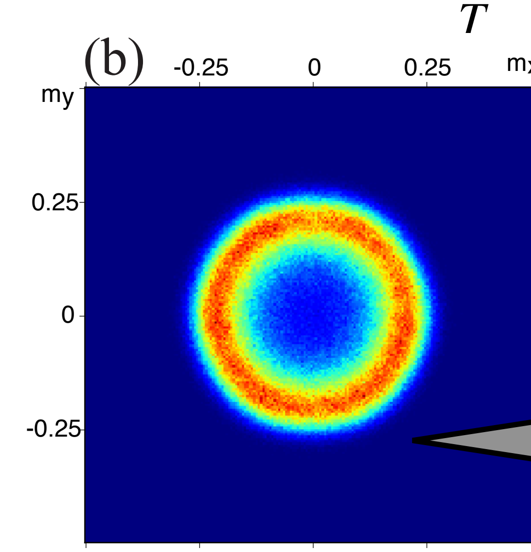

at Tc: emergent U(1) symmetry

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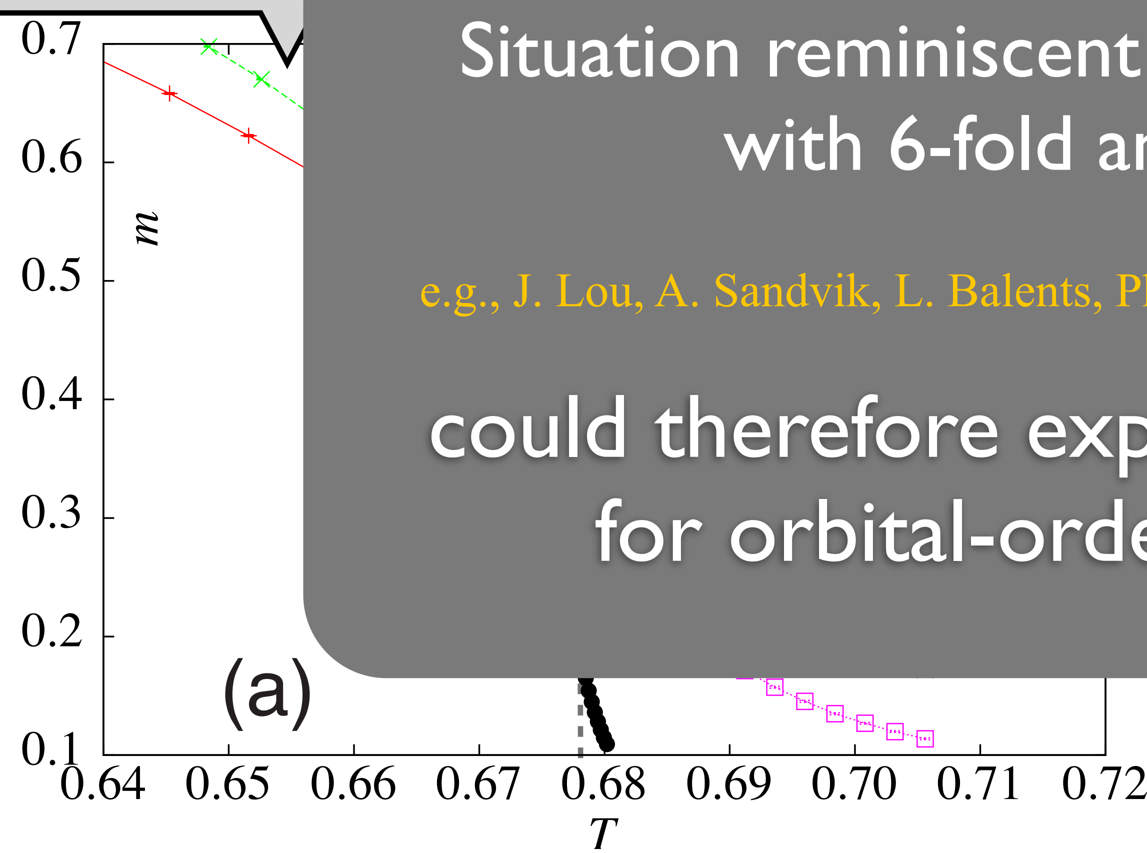
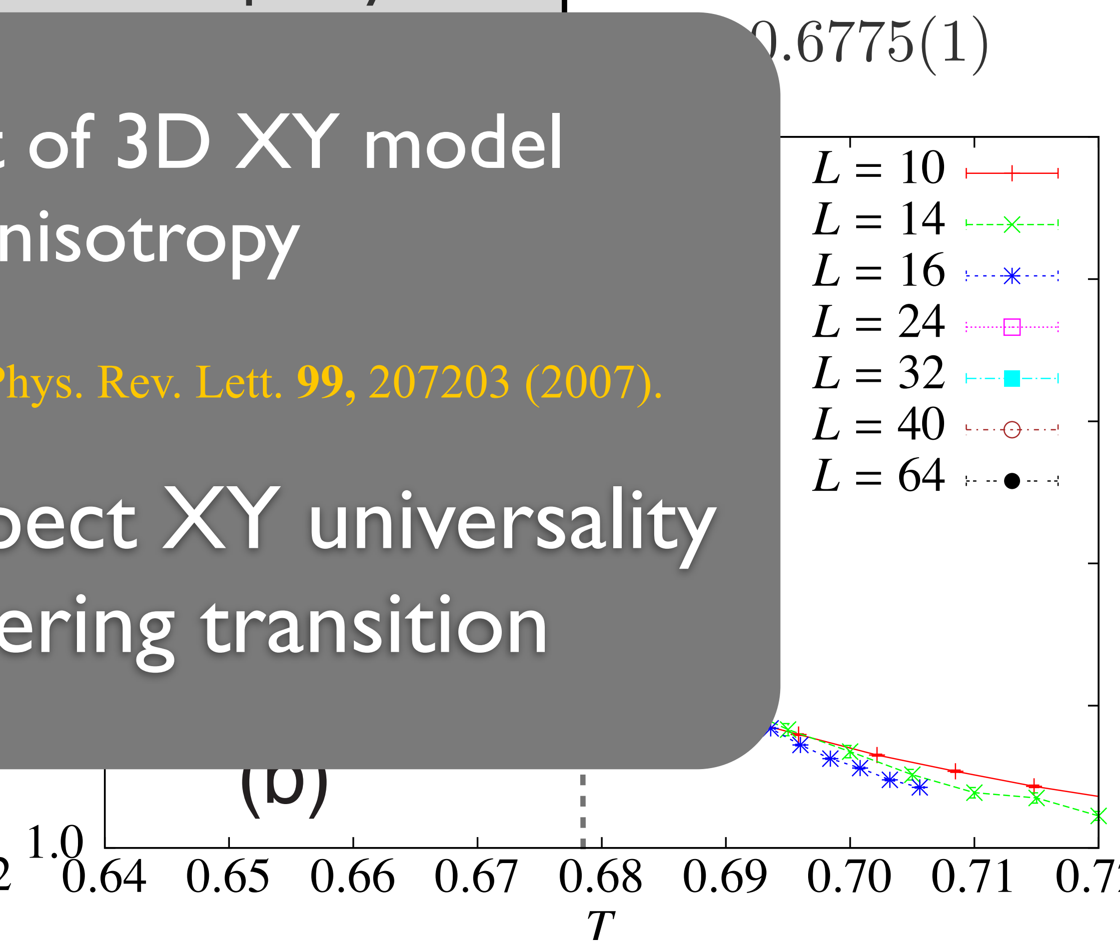
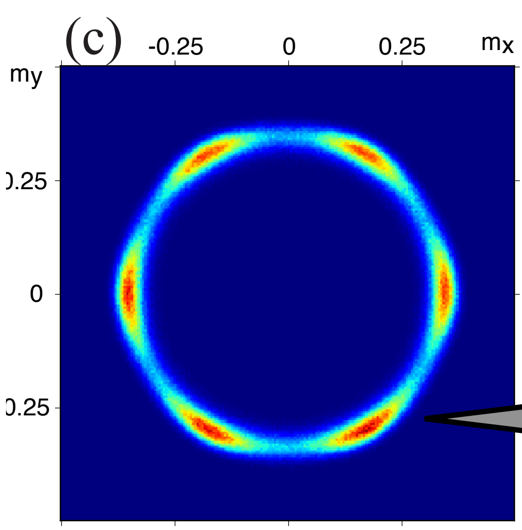




Situation reminiscent of 3D XY model with 6-fold anisotropy

e.g., J. Lou, A. Sandvik, L. Balents, Phys. Rev. Lett. **99,** 207203 (2007).

could therefore expect XY universality for orbital-ordering transition



distribution of order parameter

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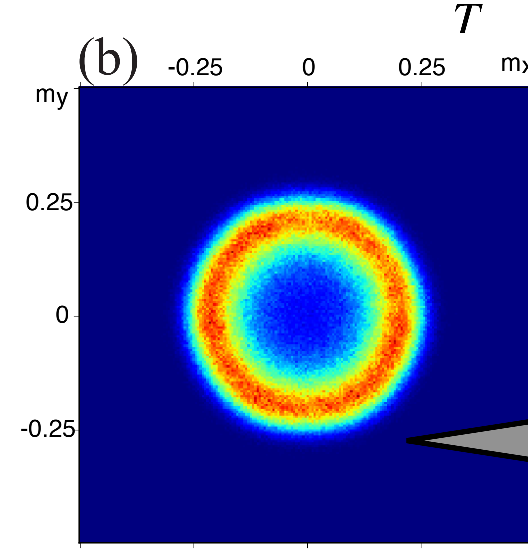
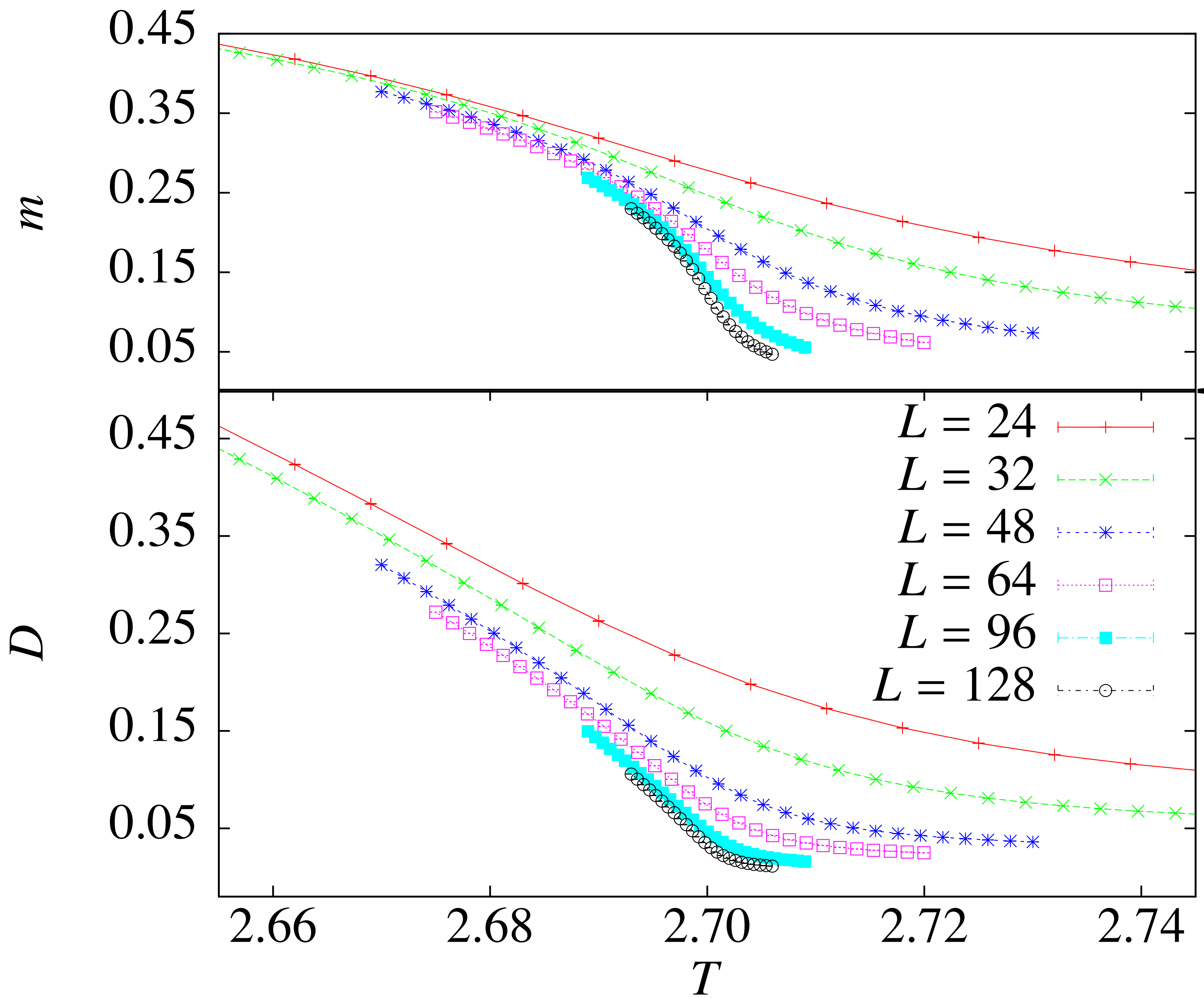


at Tc: emergent U(1) symmetry

Additional directional ordering

a key feature not present in an ordinary XY spin model:

$$D = (1/N)\left([E_x - E_y]^2 + [E_y - E_z]^2 + [E_z - E_x]^2\right)$$



simultaneous onset of orbital and directional order

anisotropic fluctuations in ordered state

Critical exponents of the120° model

$$\xi \sim |t|^{-\nu}$$

orbital-orbital
correlation length

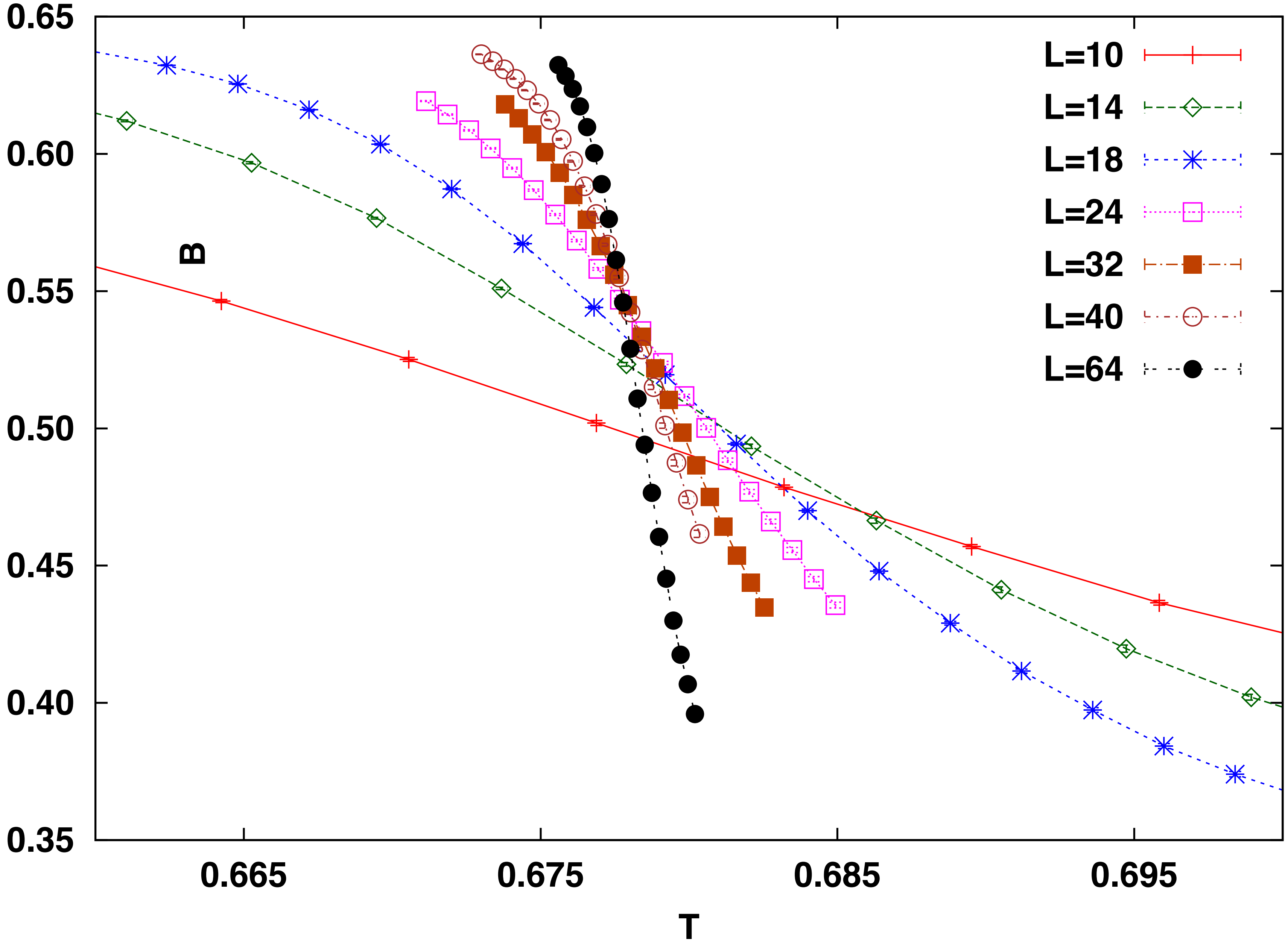
$$G(r) = r^{-2+d-\eta}$$

decay of orbital-orbital correlations
at critical temperatur

Critical exponents of the 120° model

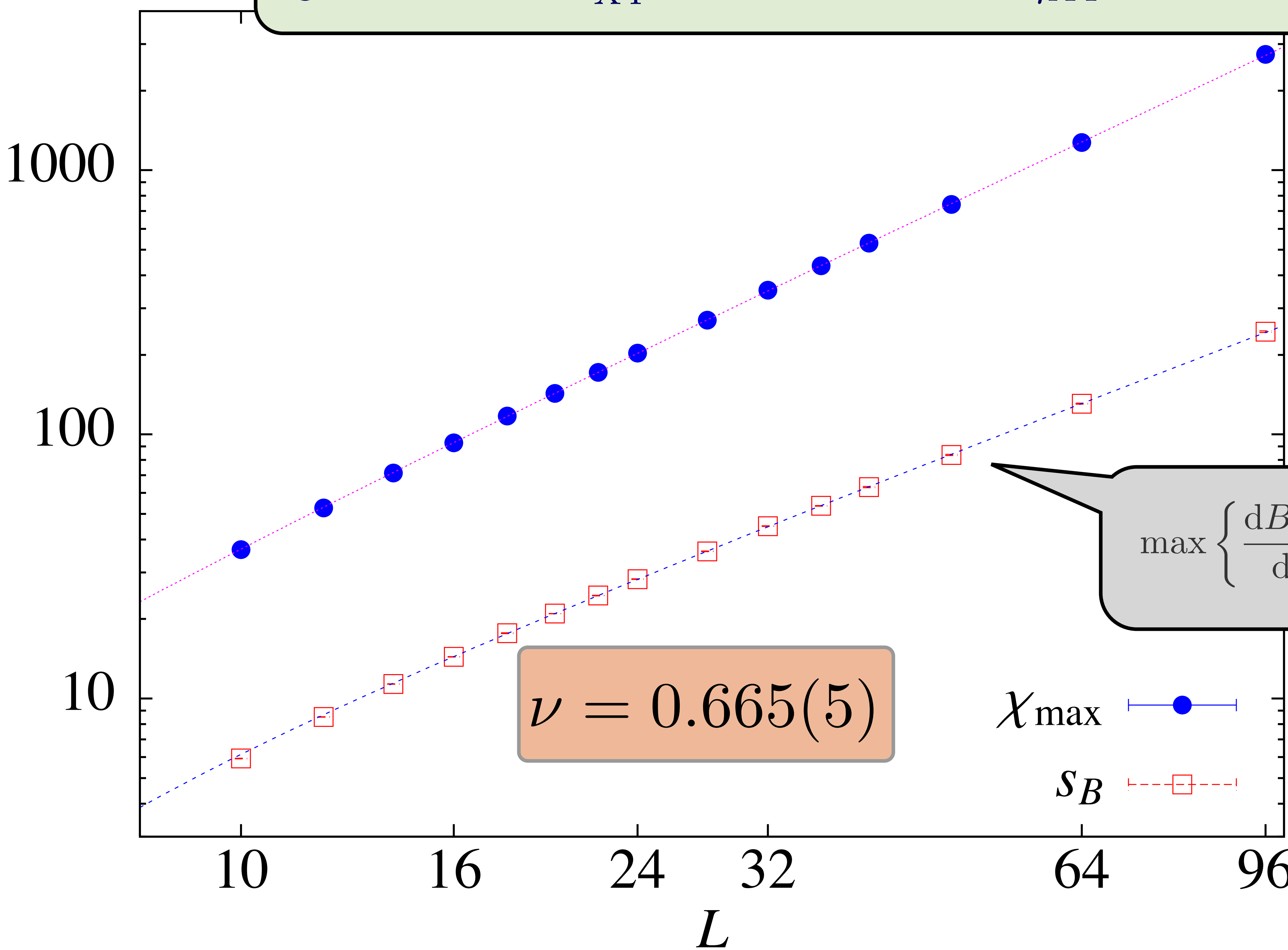
$$\xi \sim |t|^{-\nu}$$

$$B = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \qquad \max\left\{\frac{\mathrm{d}B(L)}{\mathrm{d}T}\right\} = aL^{1/\nu}(1 + cL^{-\omega})$$



Critical exponents of the120° model

3DXY $\quad \nu_{\mathrm{XY}} = 0.671 \quad \eta_{\mathrm{XY}} = 0.0385$



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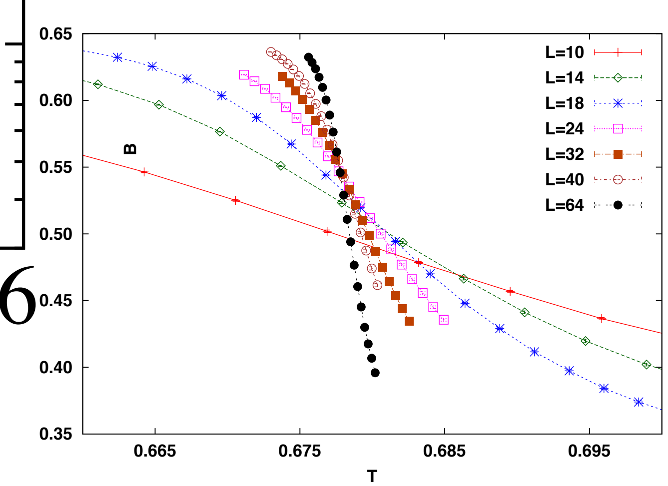
$\nu = 0.665(5)$



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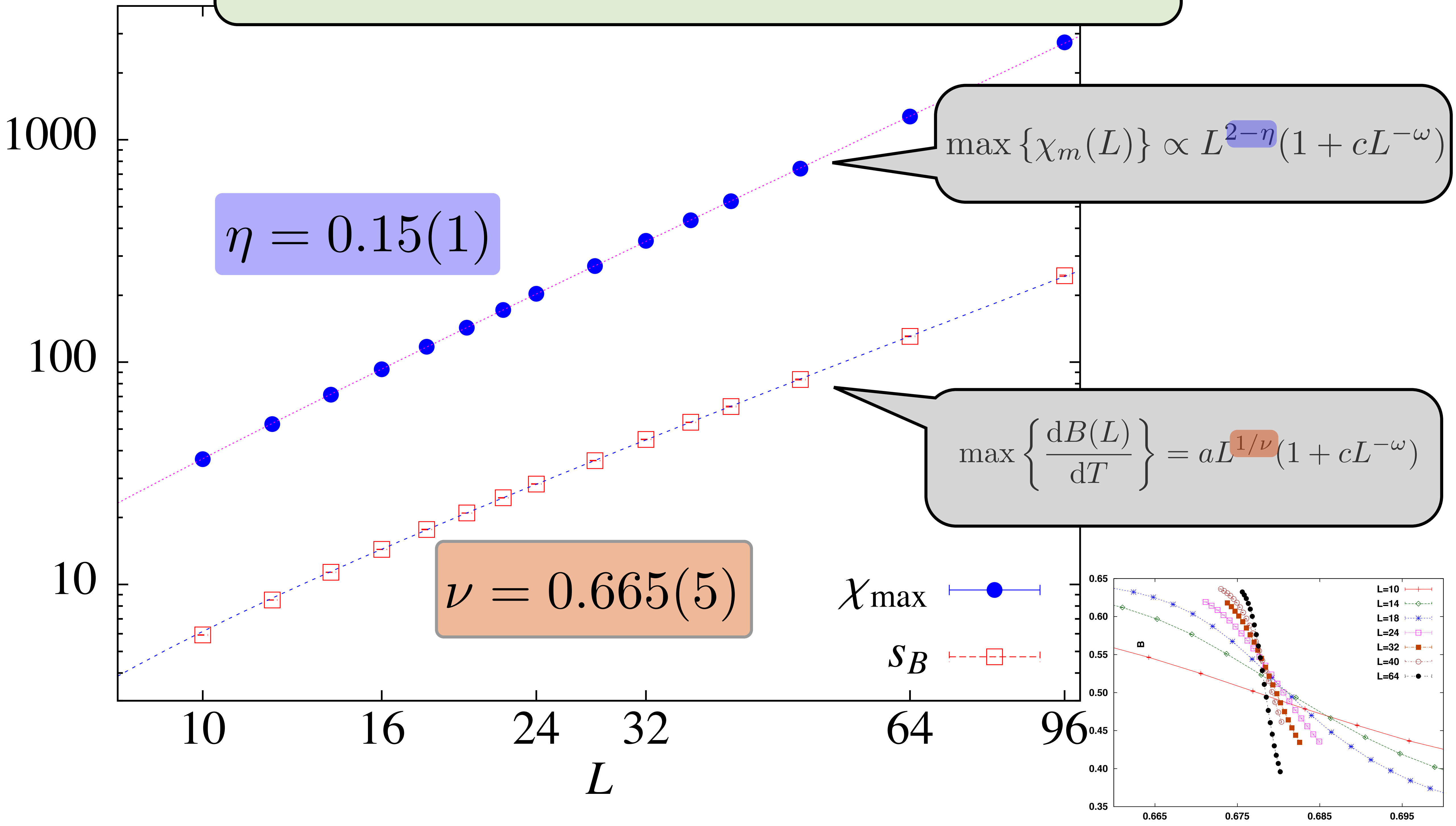
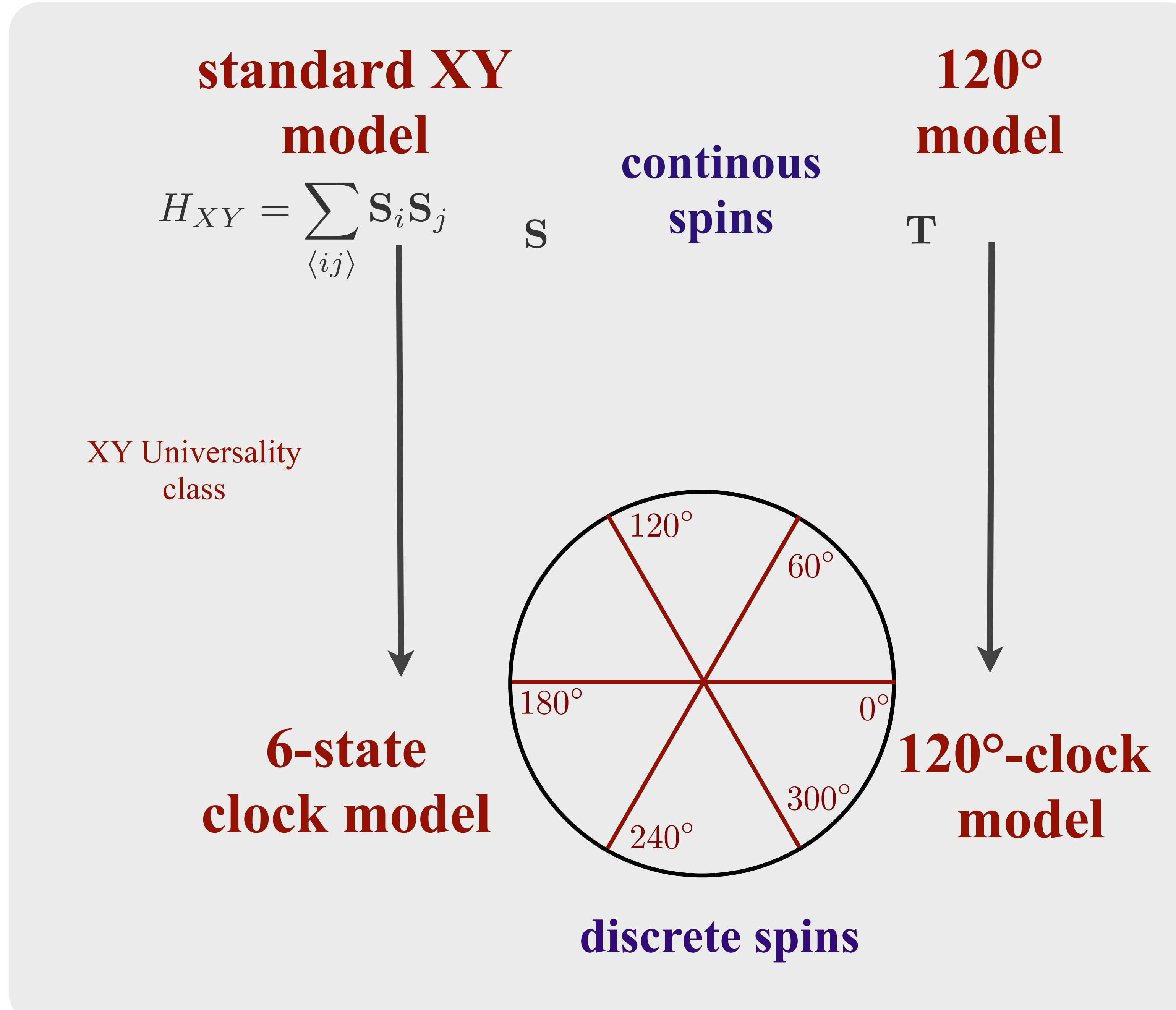


The discrete 120° (clock) model

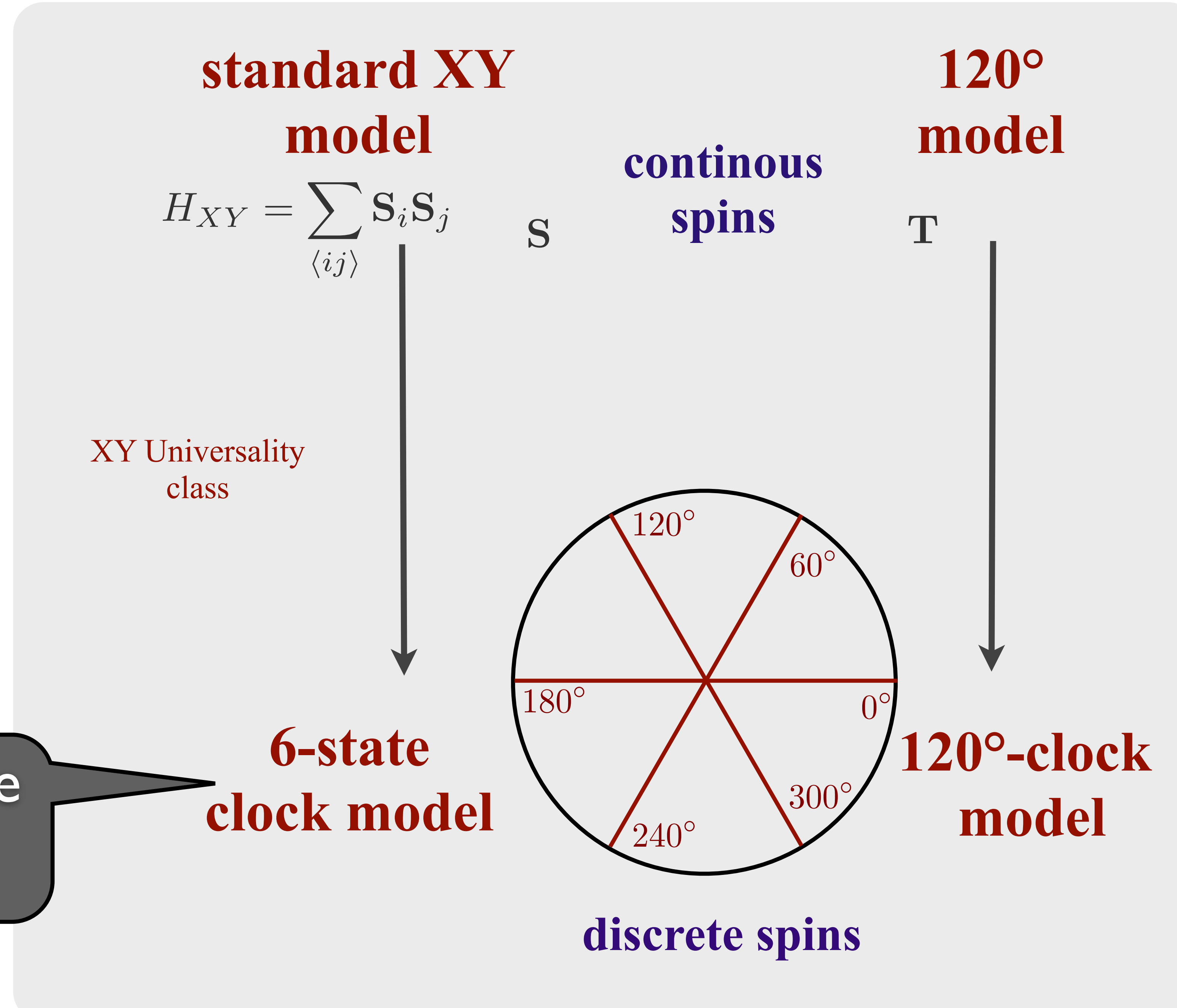
Want a simplified model ...



The discrete 120° (clock) model

Want a simplified model ...

discrete models have the same ordered state on spin level!



The discrete 120° (clock) model

Want a simplified model ...

standard XY model

$$H_{XY} = \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j$$

S

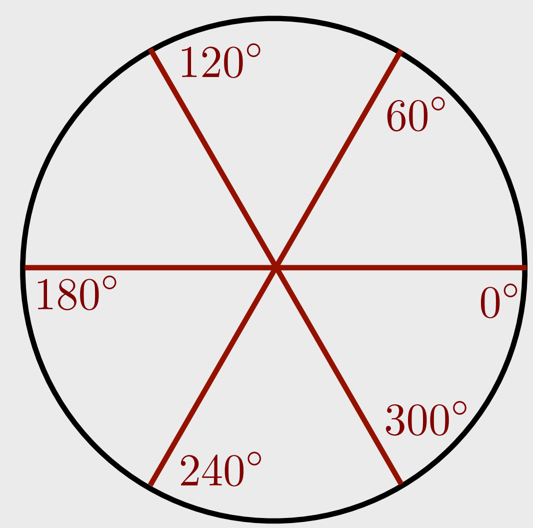
continous spins

T

120° model

XY Universality class

6-state clock model



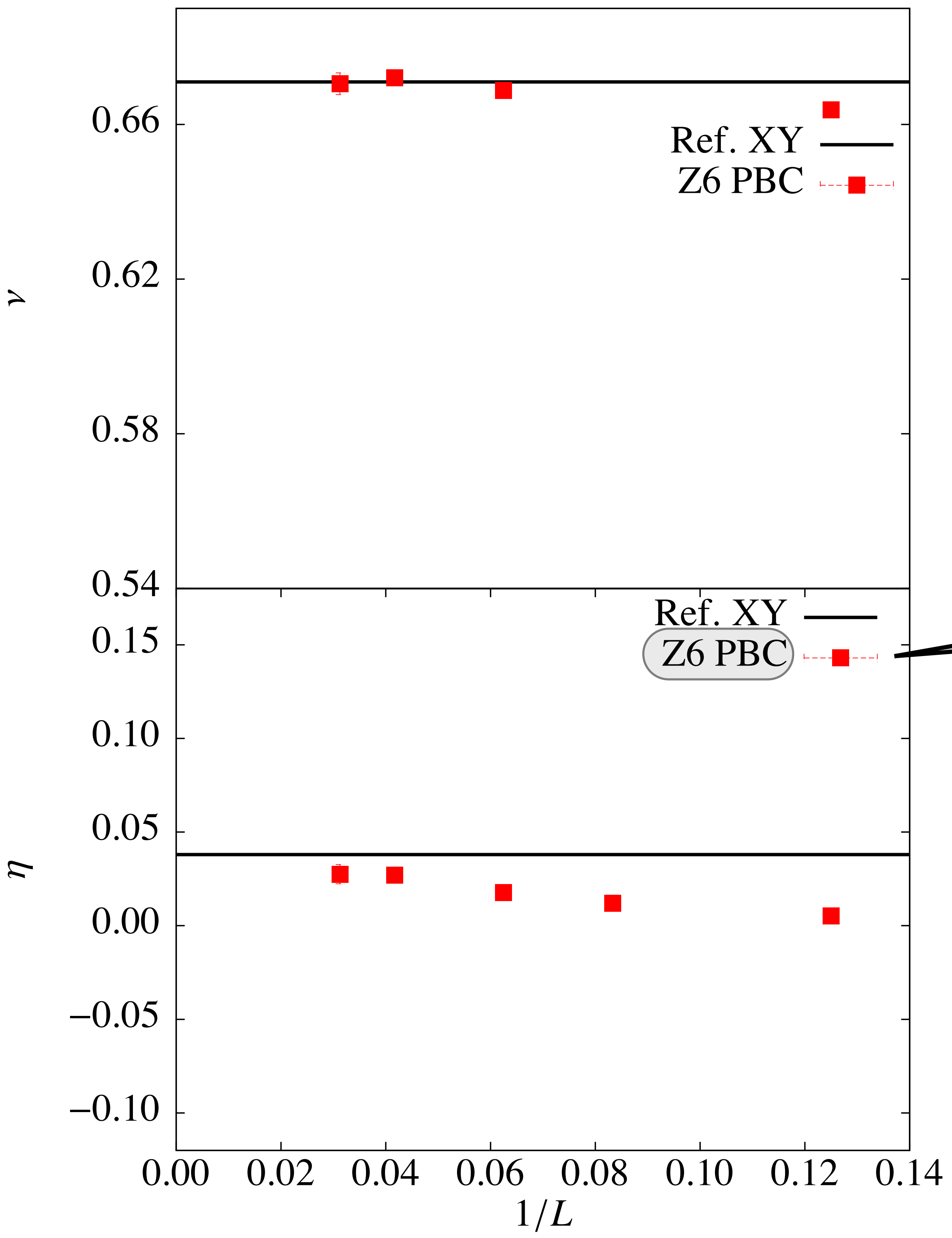
120°-clock model

discrete spins

discrete models have the same ordered state on spin level!

discrete structure allows for VERY efficient MC simulations: can reach N=128^3 sites (2.09 million spins !)

Detailed comparison of FSS



systematic comparison of critical scaling:
scaling of **effective** critical exponents

$$\chi(L) \propto L^{2-\eta}(1+\cdots)$$

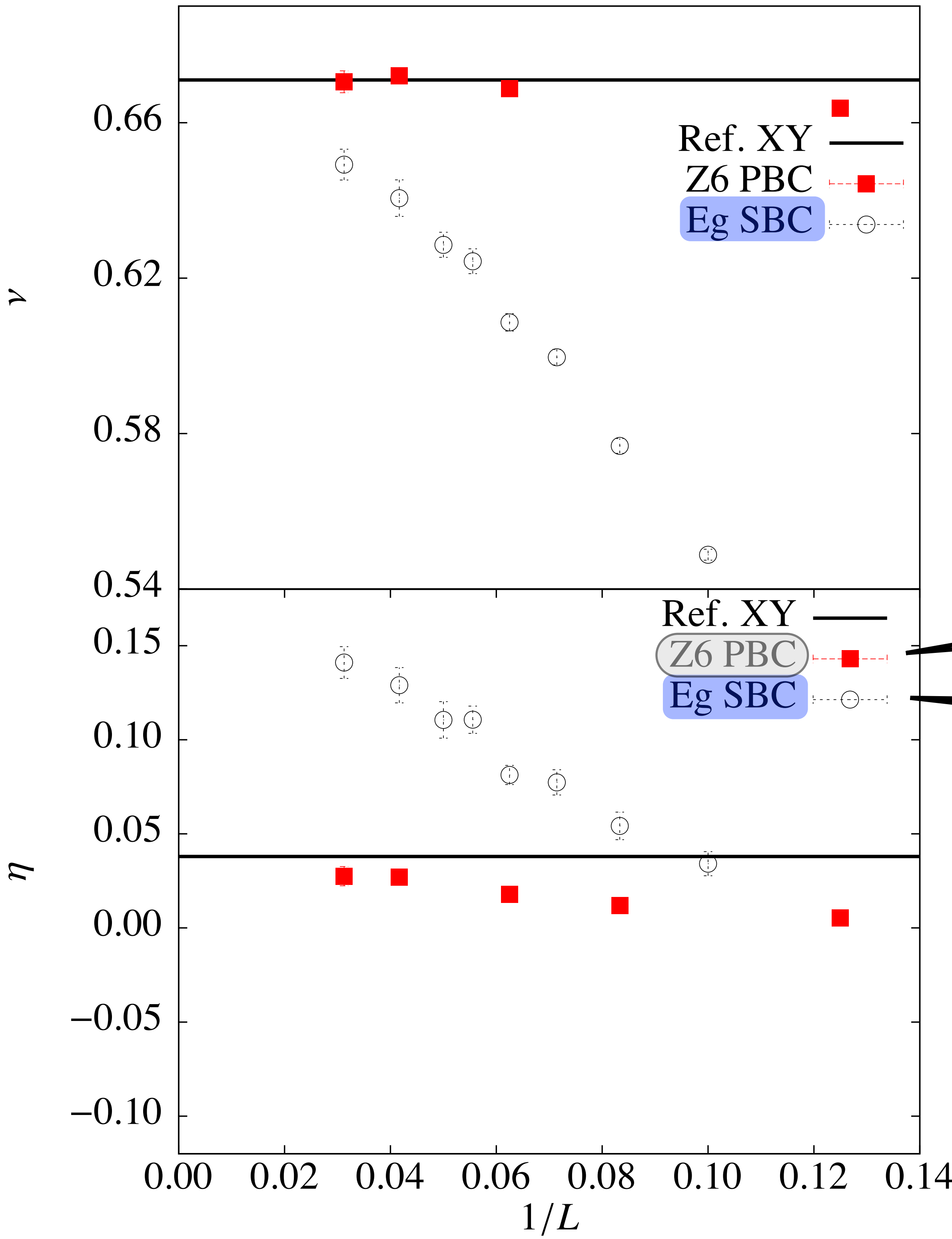
$$\downarrow$$

$$\eta = 2 - \ln\left(\chi(2L)/\chi(L)\right) / \ln(2)$$

6 state clock model

XY? ✓

Detailed comparison of FSS



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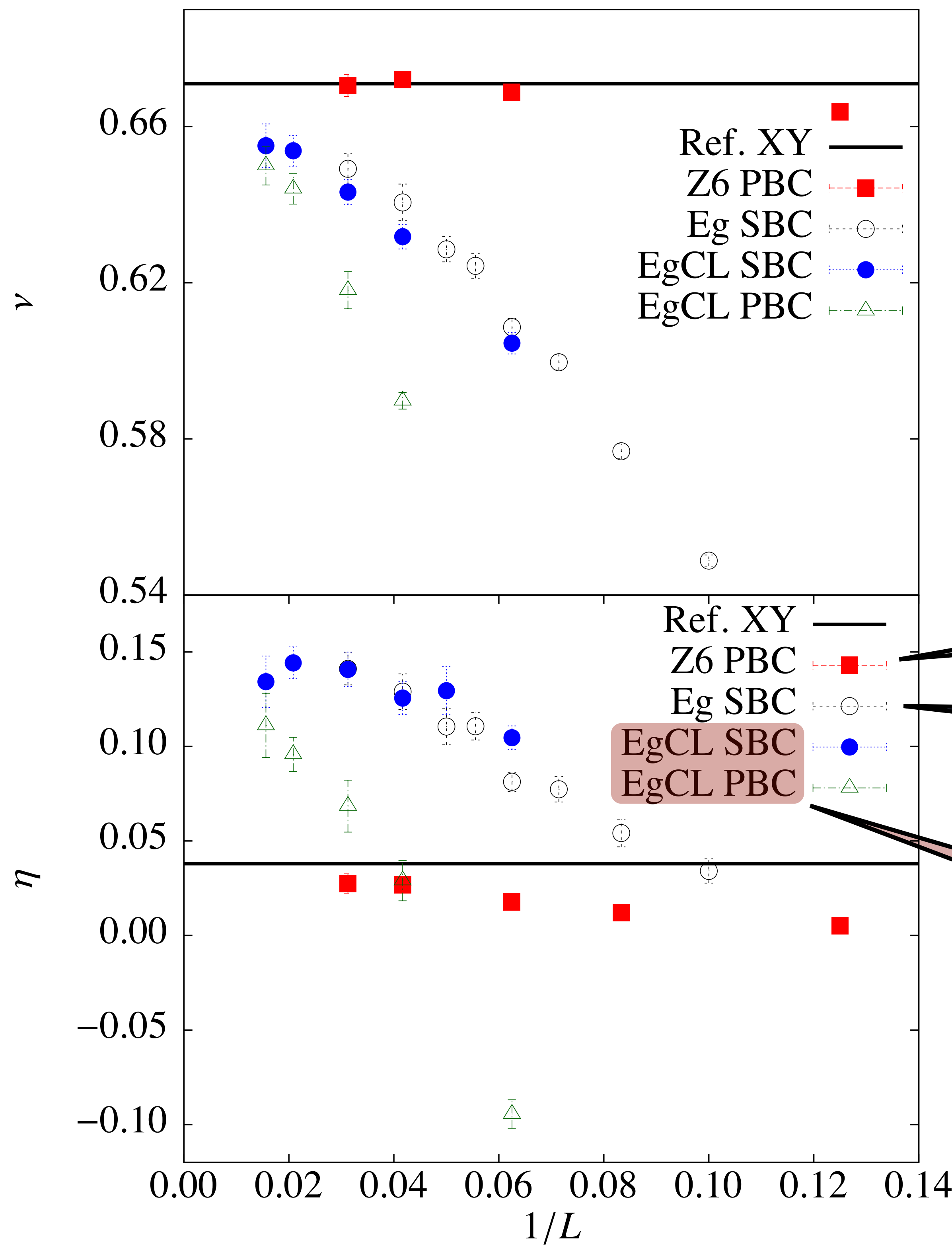
6 state clock model ✓

120° model ✗

Detailed comparison of FSS



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XY?

6 state clock model ✓

120° model ✗

120°-clock model (for multiple bc) ✗

Summary

first large scale Monte Carlo study of the prototypical classical 120^{o} model for orbital ordering

- **ordering nature: verified orbital ordering with 6-fold degeneracy**
- **criticality: obtained critical exponents which differ from standard magnetic universality classes (XY)**
- **consequence:** expect to see **novel physics** different from ordinary spin models of magnetisms (e.g. disorder, ...)

T. Tanaka, M. Matsumoto, and S. Ishihara, Phys. Rev. Lett. **95**, 267204 (2005)

- **outlook**: write down a Ginzburg-Landau theory..., simulations on GPUs, ...

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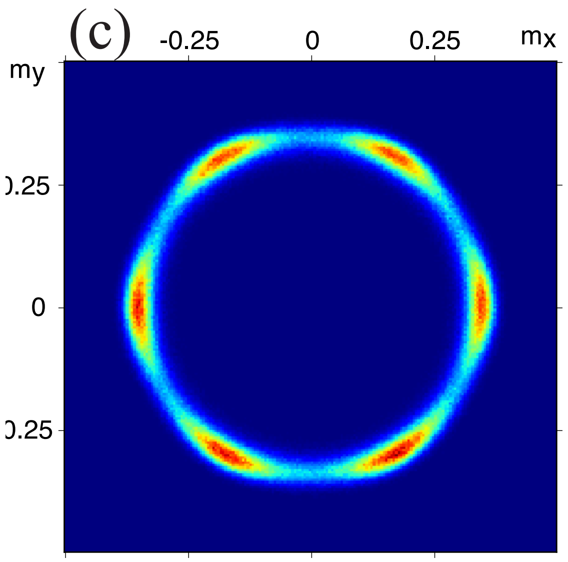
!! THANKS !!

- ... for your attention
- ... to Simon Trebst for providing some slides/figures

Influence of U(1) length-scale for T<Tc

J. Lou, A. Sandvik, L. Balents, Phys. Rev. Lett. **99,** 207203 (2007).



consider order distribution function for T < Tc:

- T= Tc: U(1) symmetry
- T<Tc:
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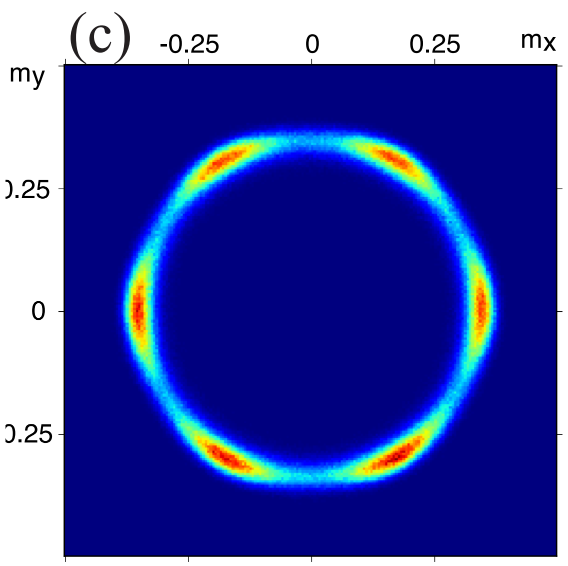

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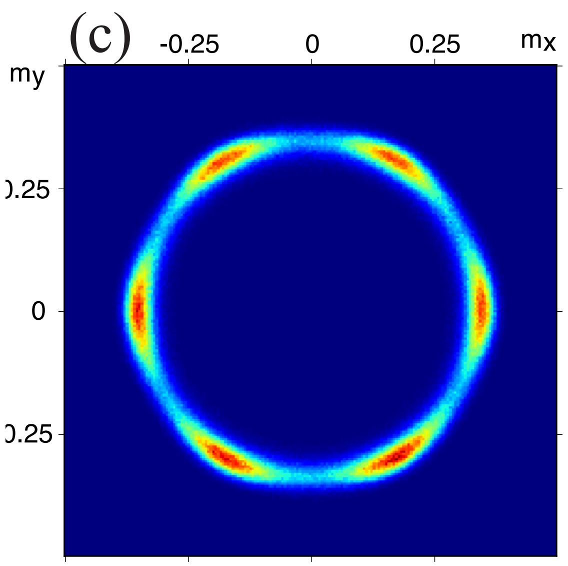

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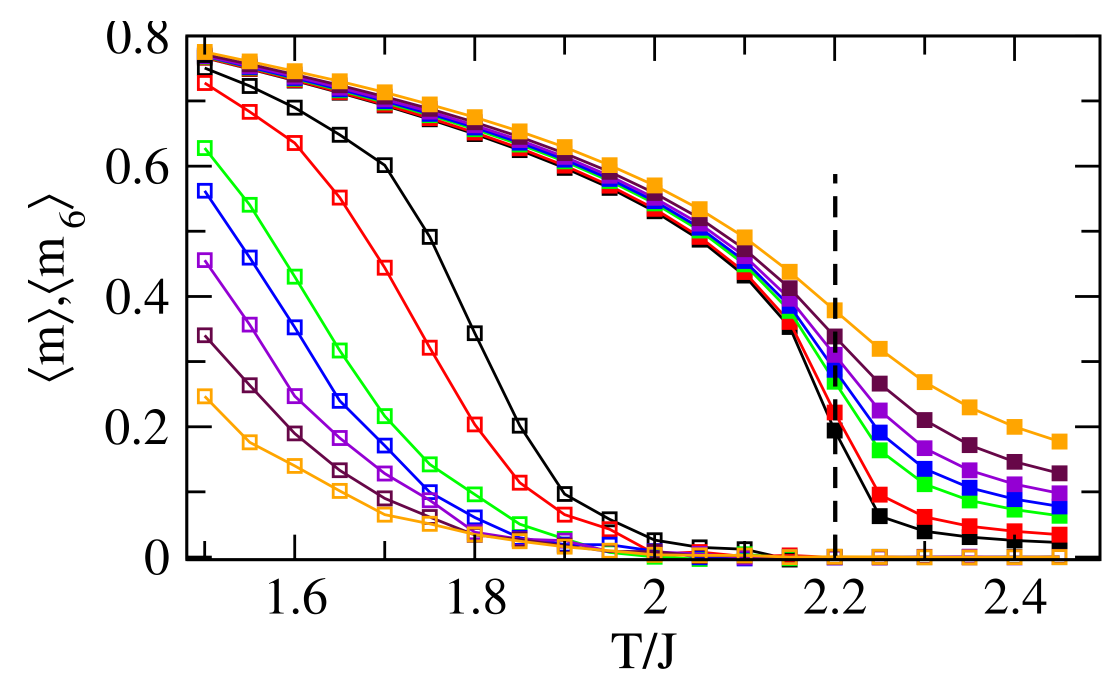

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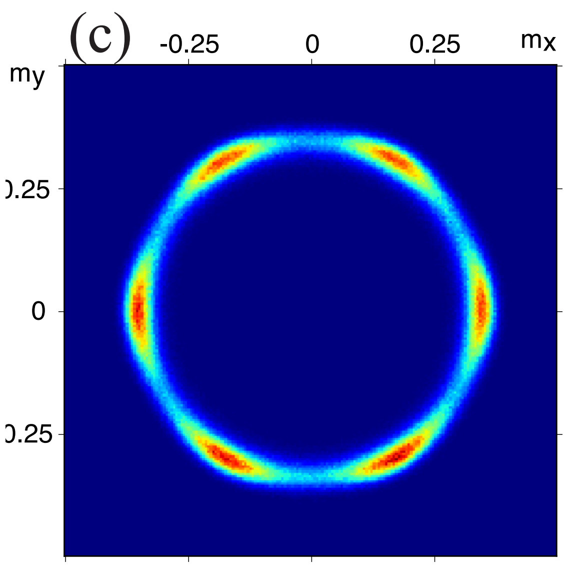

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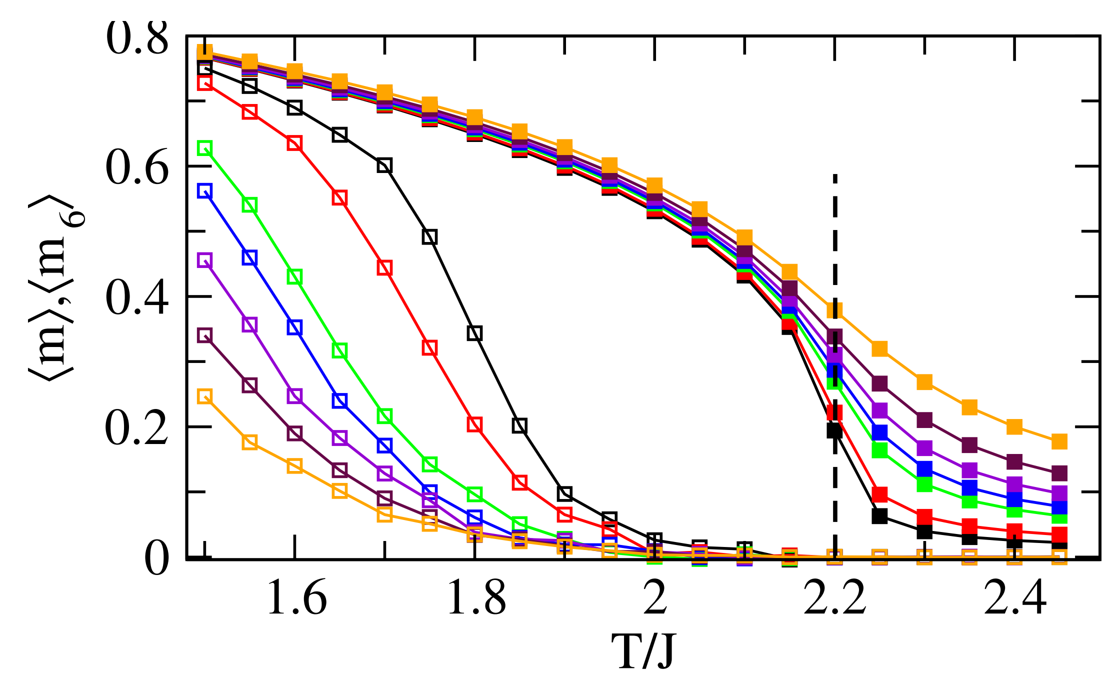

$$a_{q=6;\mathrm{XY}} = 2.2(1)$$

$$a_{120^\circ} = 1.2(1)$$