

# Orbital orders glasses

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Batista, LANL [arXiv:cond-mat/04](#)

Biskup, L. Chayes, UCLA; J. van den Br  
[arXiv:cond-mat/0309691](#) (Comm M  
0309692 (EPL)

Fradkin, UIUC [arXiv:cond-mat/0410](#)

tiz, E. Cobanera, Indiana [arXiv:cond-r](#)

# Conclusions (new results)

Orbital systems can order by **thermal disorder" fluctuations** even in their class (no  $(1/S)$  zero point quantum fluctuation necessary).

Similar to charge and spin driven quantum behavior, it is theoretically possible to have **order driven quantum critical** behavior (Prediction.)

**Orbital glasses appear in exactly solvable models**

Orbital systems can exhibit topological **dimensional reductions** due to their unique

What are orbital orders?

Models for orbital order

*“Order by disorder” in orbital systems*

Orbital order driven quantum criticality and  
*exact solutions as a theoretical proof of concept*

Symmetries and topological order

*Dimensional gauge like symmetries and dimerizations: experimentally testable selection rules*



... are orbital orders. (old)

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Models for orbital order (old)

*“Order by disorder” in orbital system.  
(situations) (new)*

Orbital order driven quantum criticality  
*Exact solutions as a theoretical proof of*

Symmetries and topological order  
*n dimensional gauge like symmetries an*

els in  $3d$  shell split by crystal field.

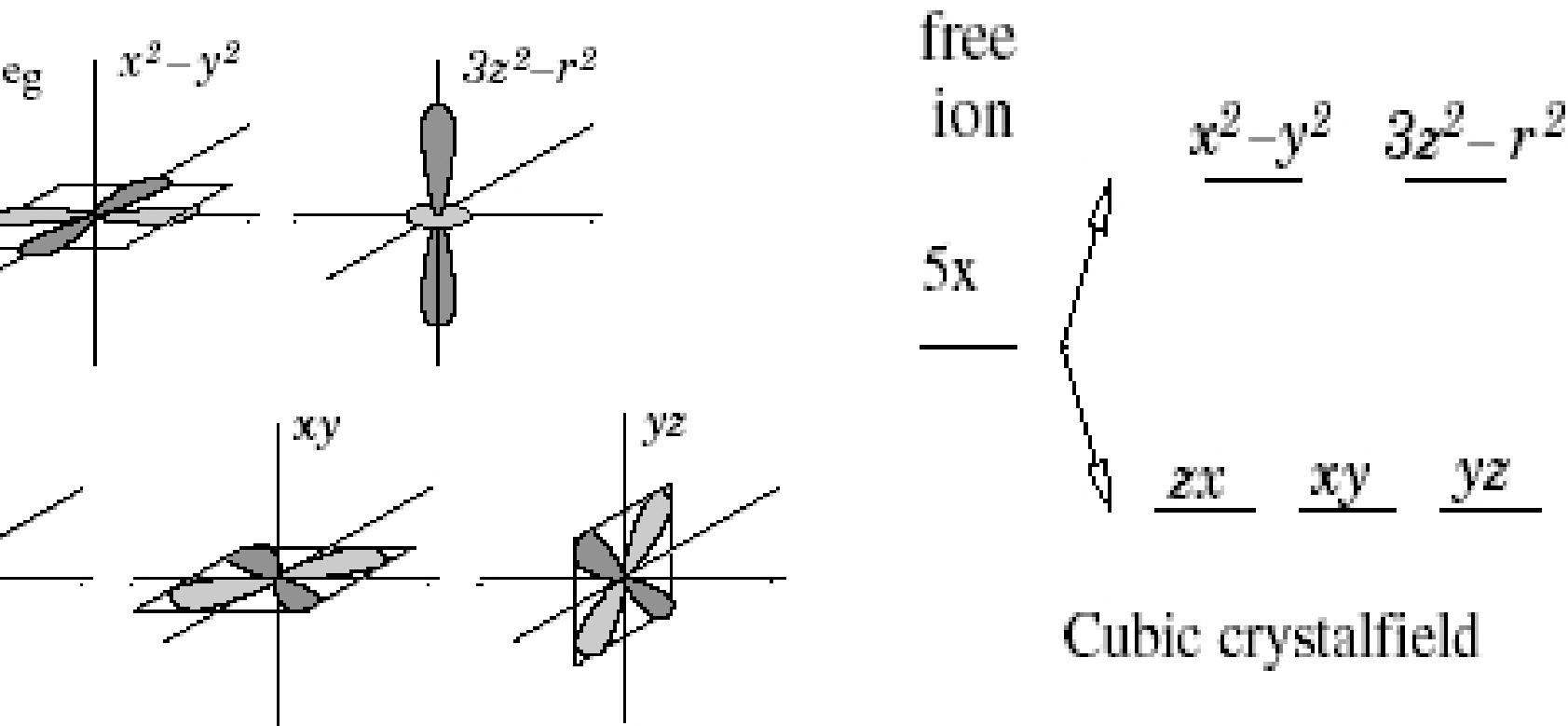
$e_g$

gle itinerant electron @ each site  
multiple *orbital* degrees of freedom.

$t_{2g}$



# The 3d orbitals



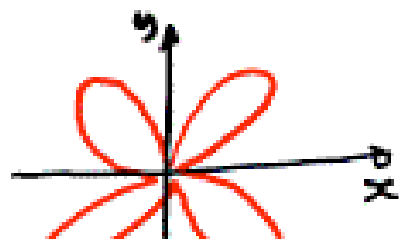
The five 3d orbital states share the  
 Function Their angular dependen

$d'$

$Ti^{3+}$

$= e_g$

$= t_{2g}$

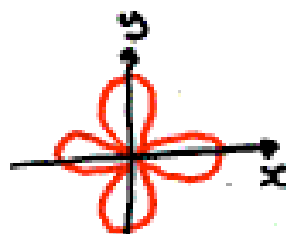


$d^3$

$Mn^{4+}$

$= e_g$

$= t_{2g}$

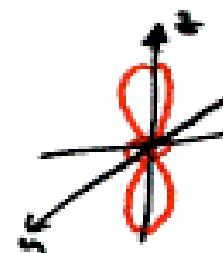


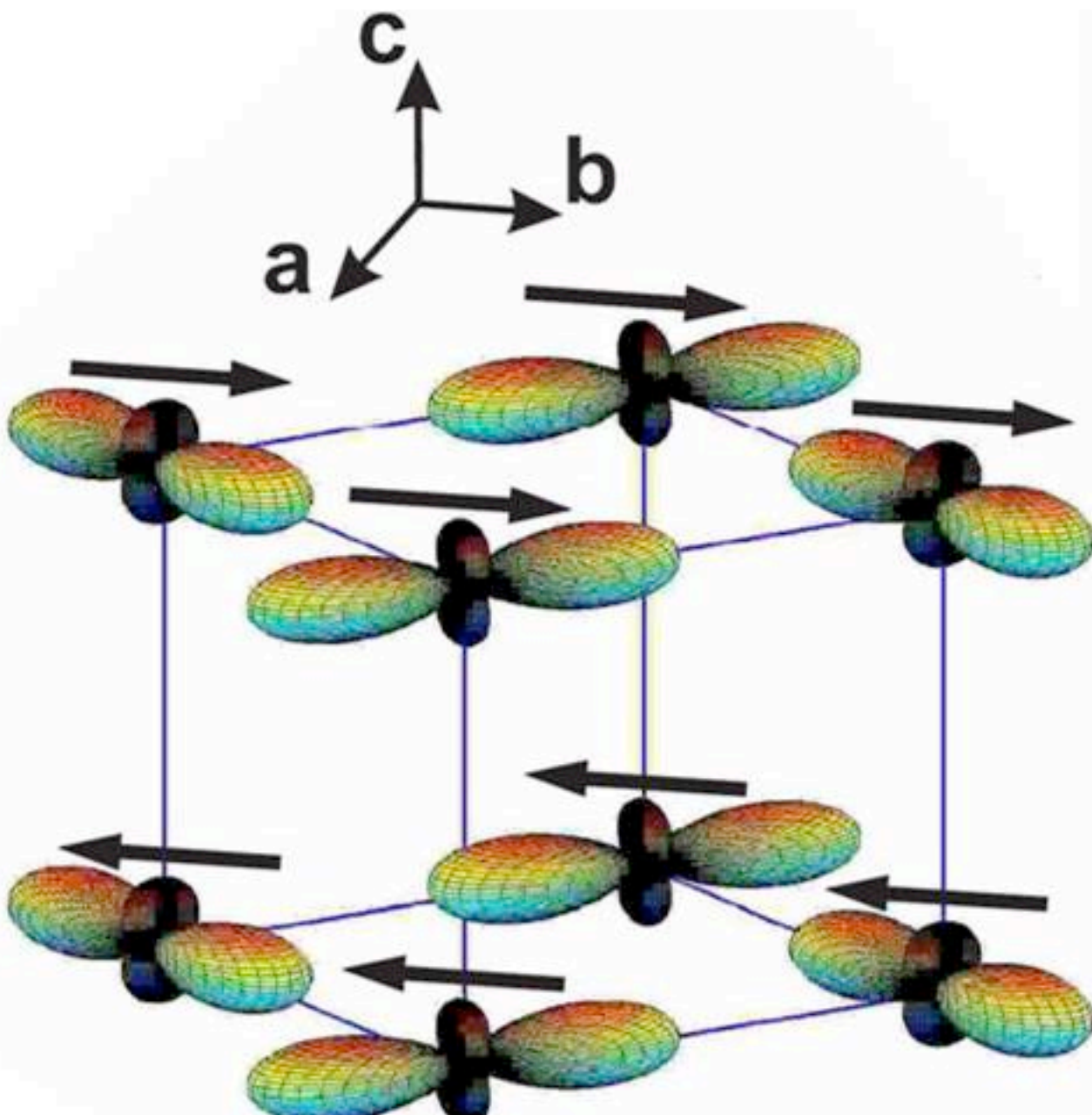
$d^4$

$Mn^{3+}$

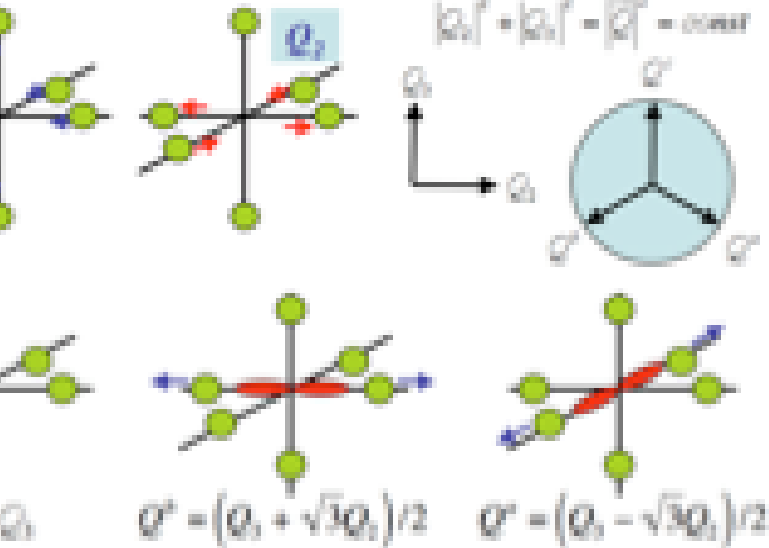
$= e_g$

$= t_{2g}$





# Jahn-Teller distortions



$$|x^2 - y^2\rangle = |S = -m = 1/2\rangle \equiv$$

$$|xy\rangle = |S = 1, m = 0\rangle; |yz\rangle = 2$$

$$|zx\rangle = -i2^{-1/2}(|11\rangle - |1-1\rangle)$$

The Hilbert space of the  $e_g$  orbitals is spanned by two states. The associated Jahn-Teller distortions can be expressed on a two dimensional unit disk (linear combinations of independent distortions  $Q_{2,3}$ ). An effective pseudo-spin  $S=1/2$  representation. There is an angle of *120 degrees* between the

Models for orbital order (old)

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*“Order by disorder” in orbital system  
(situations) (new)*

Orbital order driven quantum criticality

*Exact solutions as a theoretical proof of*

Symmetries and topological order

*n-dimensional gauge like symmetries and*

*Unlike spins, orbitals live in real space.  
The orbital interactions  
are not isotropic. Reduced symmetry  
and frustration.*



levels in  $3d$  shell split by crystal field.

$e_g$

single itinerant electron @ each site  
multiple *orbital* degrees of freedom.

$t_{2g}$

exchange approximation (and neglect of strain-field induced interactions)

$$\sum_{\langle r, r' \rangle} H_{\text{orb}}^{r, r'} (\mathbf{s}_r \cdot \mathbf{s}_{r'} + \frac{1}{4})$$

$$H_{\text{orb}}^{r, r'} = J[4\hat{\pi}_r^\alpha \hat{\pi}_{r'}^\alpha - 2\hat{\pi}_r^\alpha$$

[Hubbard–Kohn–Hohenberg–Kohn Hamiltonian]

$120^\circ$ -model ( $e_g$ -compounds)

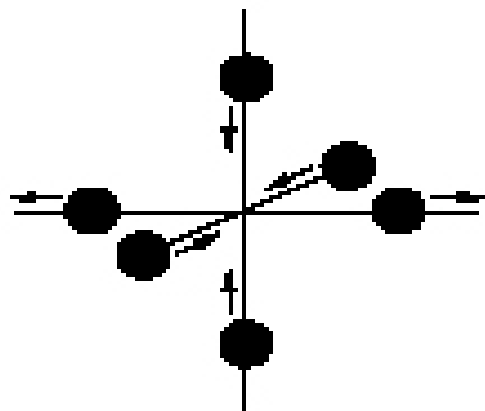
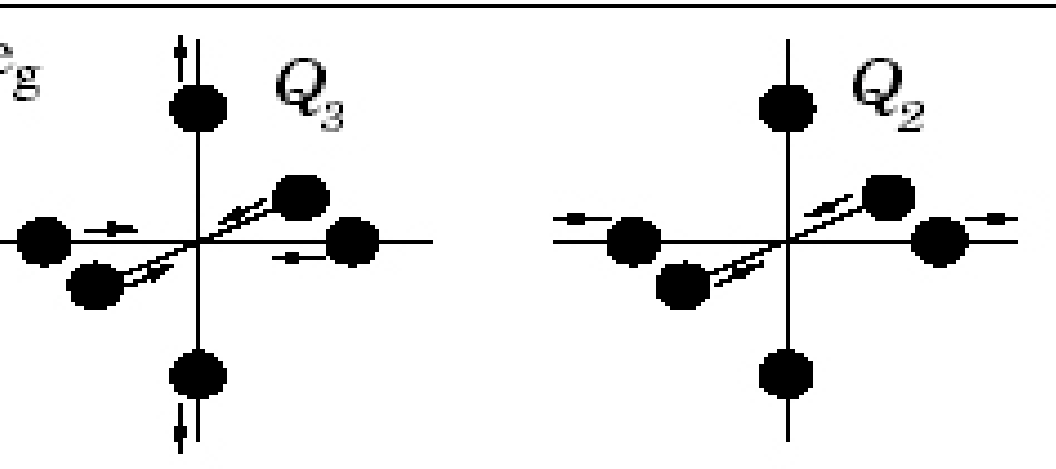
$\text{V}_2\text{O}_3$ ,  $\text{LiVO}_3$ ,  $\text{LaVO}_3$ ,  $\text{LaMnO}_3$ , ...

$$\hat{\pi}_r^x = \frac{1}{4}(-\sigma_r^z + \sqrt{3}\sigma_r^x)$$

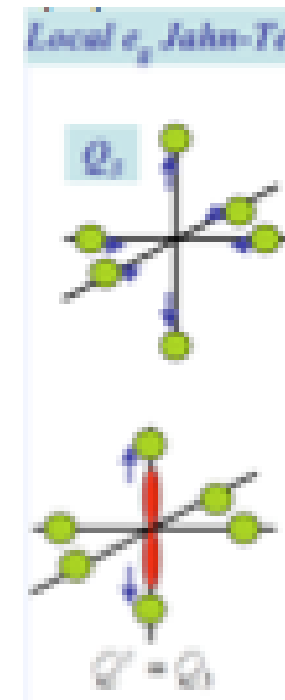
$$\hat{\pi}_r^z =$$

# Jahn-Teller distortion

distortions preferred by different c



$$Q_3 \cos \phi + Q_2 \sin \phi$$



# *The orbital only interact*

The orbital component of the orbital dependent exchange as well as the direct Jahn-Teller interactions have a similar form:

$$H_{orb} = J \sum_{\alpha} \sum_r \pi_r^{\alpha} \pi_{r+e_{\alpha}}^{\alpha}$$

al only approximation: Neglect spin degree

120° Hamiltonian:

$$= J \sum_r (S_r^{[a]} S_{r+e_x}^{[a]} + S_r^{[b]} S_{r+e_y}^{[b]} + S_r^{[c]} S_{r+e_z}^{[c]})$$

$\vec{S}$

simil

unit ve

Orbital compass Hamiltonian:

$$= J \sum_r (S_r^{[x]} S_{r+e_x}^{[x]} + S_r^{[y]} S_{r+e_y}^{[y]} + S_r^{[y]} S_{r+e_z}^{[z]})$$

$\vec{S}_r =$

— 1181

$$\vec{S}_r \in S_1, \text{ write } \vec{S}_r = (S_r^{[x]}, S_r^{[y]}).$$

$$S_r^{[a]} = \vec{S}_r \cdot \vec{e}_a$$

$$H = J \sum_{r \in \Lambda_L} (S_r^{[a]} S_{r+e_x}^{[a]} + S_r^{[b]} S_{r+e_y}^{[b]} + S_r^{[c]} S_{r+e_z}^{[c]})$$

$$\frac{J}{2} \sum_{r \in \Lambda_L} \left( (S_r^{[a]} - S_{r+e_x}^{[a]})^2 + (S_r^{[b]} - S_{r+e_y}^{[b]})^2 + (S_r^{[c]} - S_{r+e_z}^{[c]})^2 \right)$$

active couplings (ferromagnetic).

couplings in  $x$ -direction with projection along  $a$ -component.

couplings in  $y$ -direction with  $b$ -component.

couplings in  $z$ -direction with  $c$ -component

Remark: Any constant spin-field is a classical ground state.

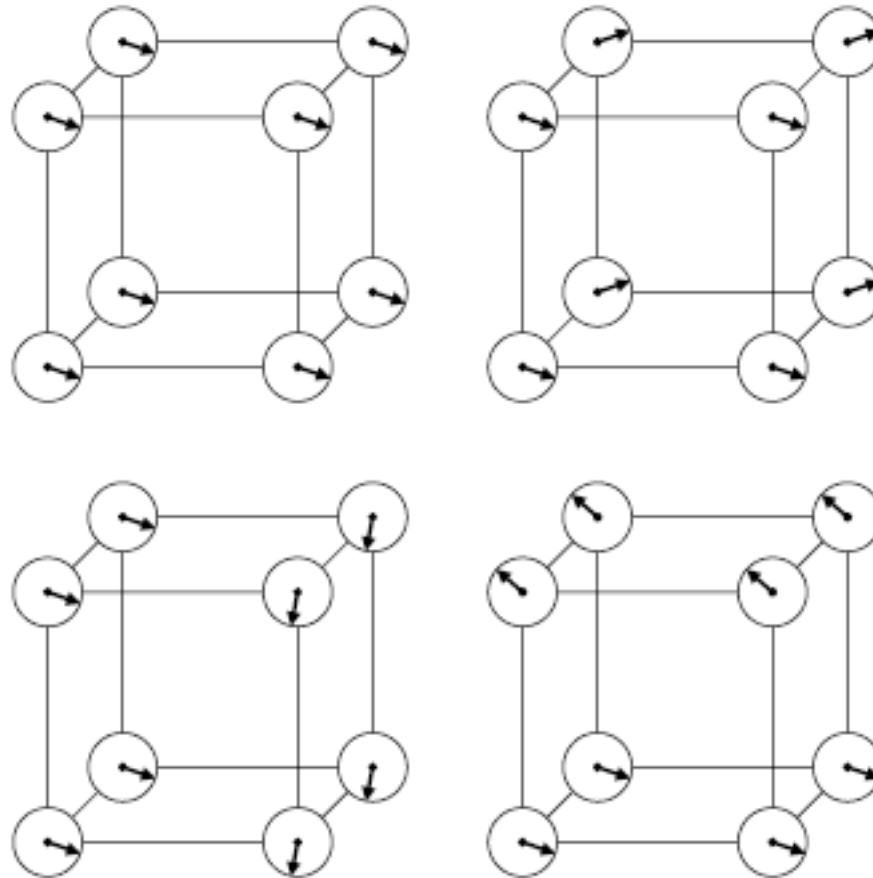
$$G(k, \omega = 0) \propto \frac{\Delta_a + \Delta_b + \Delta_c}{\Delta_a \Delta_b + \Delta_a \Delta_c + \Delta_b \Delta_c}$$

Fix  $k_z$

$$G(k, \omega = 0) \propto \frac{1}{\Delta_a + \Delta_b}$$

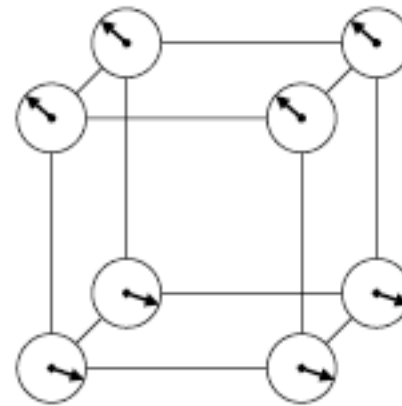
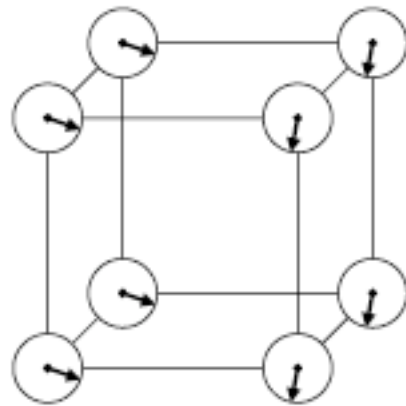
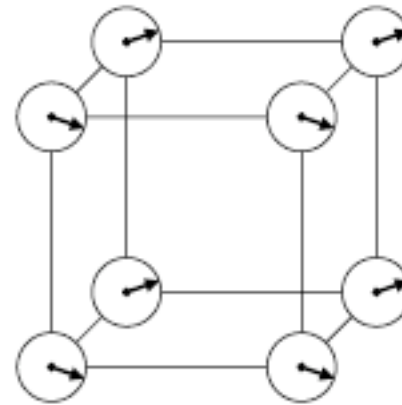
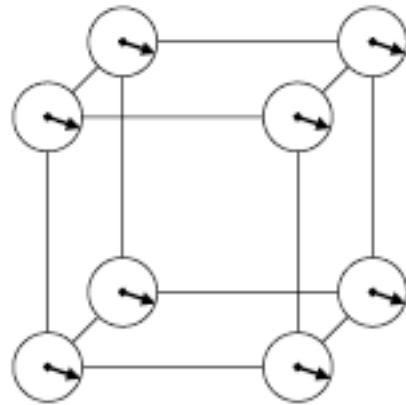
Very IR divergent.

ov, M. Biskup,  
and J. v. d. Brink  
(EPL)



Ising-type discrete emergent

$L \times L$   
lattice



Ref  
ps  
el

Additional discrete degeneracy fa



L. Bidaux, J. P. Carton and R. Conte, *Order as an Effect of*  
*Phys. (Paris)* **41** (1980), no.11, 1263–1272.

er, *Antiferromagnetic Garnets with Fluctuationally*  
*Sublattices*, Sov. Phys. JETP **56** (1982) 178–184 .

y, *Ordering Due to Disorder in a Frustrated Vector*  
*magnet*, Phys. Rev. Lett. **62** (1989) 2056–2059.



Really clarified  
firm foundation

itely many papers (mostly quantum) in which specific cal  
bital order work focused on zero point  $1/S$  fluctuations.

*It: orbital order is robust and persists for infinite  $S$ . Zero  
ns are not needed to account for the observed orbital ord*

Weighting of various ground states

take into account more than just energetics:

Fluctuations of spins will contribute to overall statist

and about the uniform state:  $\theta$

$$\vartheta_r \equiv \theta_r - \theta^* \quad H_{SW} = \frac{J}{2} \sum_{r,\alpha} q_\gamma(\theta^*) (\vartheta_r \pm \vartheta_{r+\alpha})^2$$

$$q_c(\theta^*) = \sin^2 \theta^*, \quad q_{a,b}(\theta^*) = \sin^2(\theta^* \pm \frac{\pi}{2})$$

$$\log Z(\theta^*) = -\frac{1}{2} \sum_{k \neq 0} \log \left( \sum_{\alpha} \beta J q_{\alpha}(\theta^*) \Delta(k_{\alpha}) \right)$$

$$\Delta(k_{\alpha}) = 2 - 2 \cos k_{\alpha}$$

the free energy has strict minima

$$F(\theta^*) = \int_{k \in B.Z.} \frac{d^3 k}{(2\pi)^3} \log \det(\beta J \Pi_k)$$

$$\Pi_k = \begin{pmatrix} q_1 \Delta_1 + q_+ \Delta_+ & q_- \Delta_- \\ q_- \Delta_- & q_1 \Delta_1^* + q_+ \Delta_+^* \end{pmatrix}$$

$$q_\alpha \equiv q_\alpha(\theta^*) \quad \Delta_\alpha \equiv \Delta_\alpha(k)$$

$$\Delta_\alpha^* = \Delta_\alpha(k + \pi e_\alpha)$$

$$q_\pm = \frac{1}{2}(q_2 \pm q_3)$$

$$\Delta_+ = \Delta_{\gamma} \pm \Delta_{\mathfrak{z}}$$

Reflection Positivity (chessboard estimates):  $P_\beta(A)$

Using Reflection Positivity along  
a Peierls argument, we readily establish  
that at sufficiently low temperatures,  
one of the six low free energy  
states is spontaneously chosen.

Interesting feature: Limiting behavior of

For the  $t_{2g}$  orbital compass type magnetic order cannot appear. By symmetry it is established that  $\langle S_r \rangle = 0$ . Instead

“orbital nematic order”

(e.g.,  $\langle (S_r^x S_{r+e_x}^x - S_r^y S_{r+e_y}^y) \rangle \neq 0$  in the 2D orbital compass model) can be proven to onset at sufficiently low yet finite temperatures.

Models for orbital order (old)

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*“Order by disorder” in orbital system  
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Orbital order driven quantum criticality

*Exact solutions as a theoretical proof of*

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Symmetries and topological order

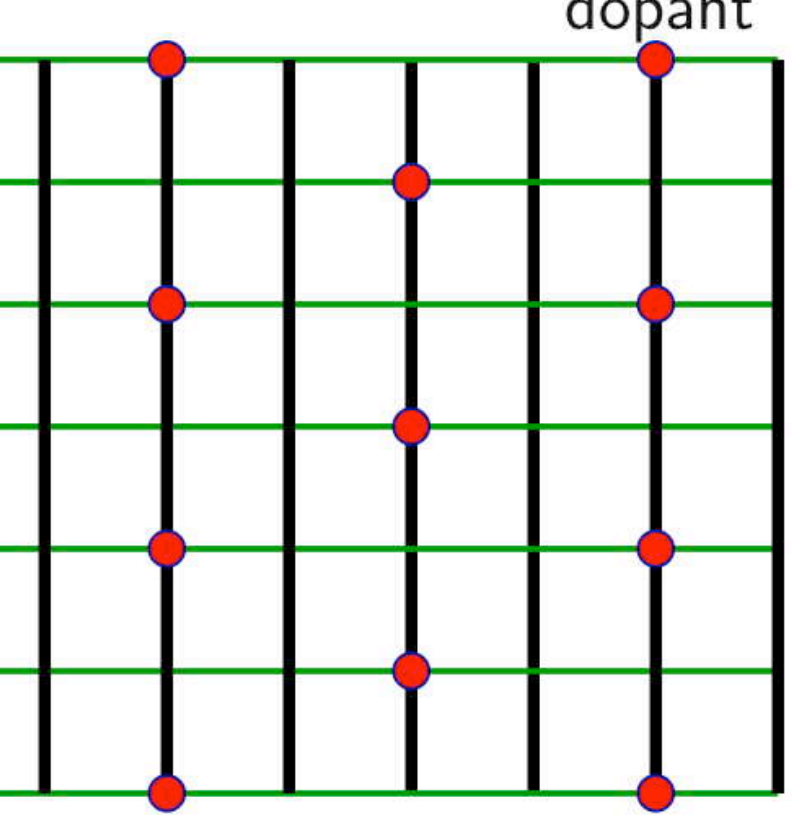
*n-dimensional gauge like symmetries and*

**Fact:** Quantum criticality can be associated with charge and spin driven orders. The transition metal oxides show an interplay of charge/superconducting, spin, and orbital orders.

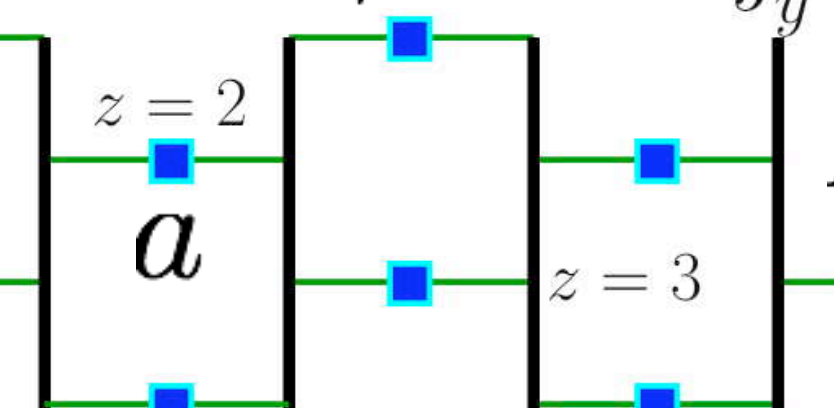
**Question:** Can there be an entirely new family of “orbital quantum critical points”? Glasses?

**Answer:** This is not forbidden and may occur theoretically. In some simple yet exactly solvable models, the orbital driven quantum critical points (driven in the presence of orbital order) can be driven to zero temperature by doping/dilution and/or uni-axial pressure.

~ ~ ~ ~ ~



$$\delta = 1/4$$



$$H_{\text{OCM}} = - \sum_j$$

After doping: New

$$\hat{O}_a = \sigma_a^x, \quad [H_{\text{DOCM}}, \hat{O}_a] = 0$$

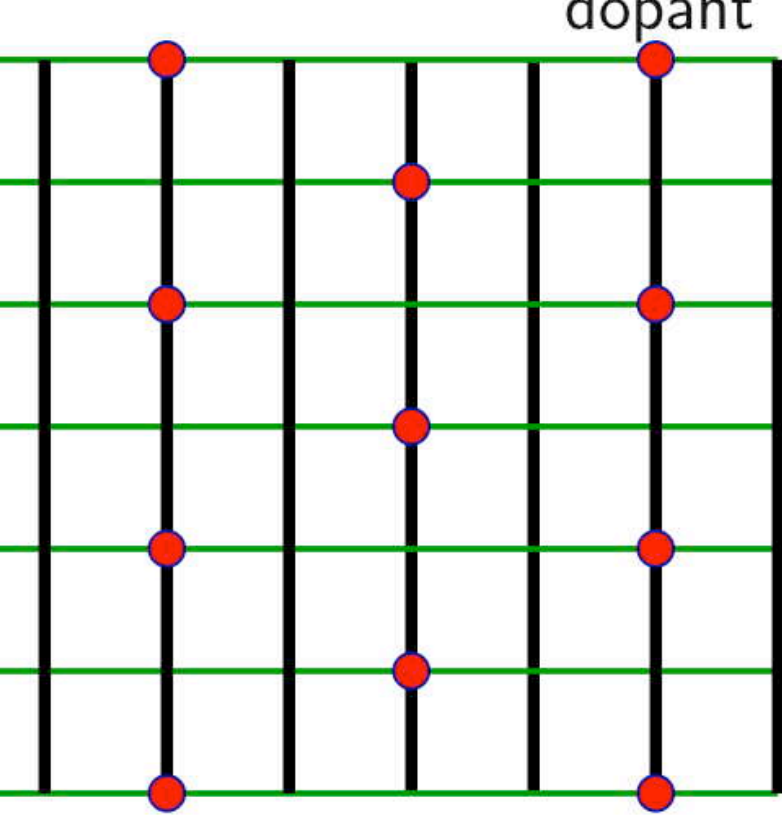
$$\bar{H}_{\text{DOCM}} \equiv \hat{P}_\ell$$

$$\hat{P}_\ell = \prod_{a=1}^{N/3} \left( \frac{\mathbb{1} + \eta_a \sigma_a^x}{2} \right)$$

$$\bar{H}_{\text{DOCM}} = - \sum_b \left( J_x \eta_a \sigma_a^x \right)$$

$$\mathcal{Z} = \text{Tr} e^{-\beta H_{\text{DOCM}}}$$

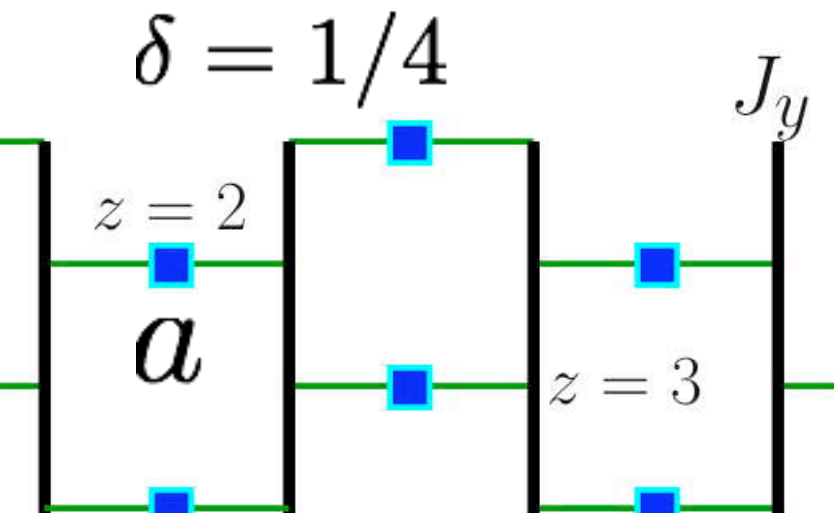




$$H_{\text{OCM}} = - \sum_j$$

After doping: New

For a system with  
exchange coupling  
replicating the  
steps mutatis  
leads to the  
Transverse F



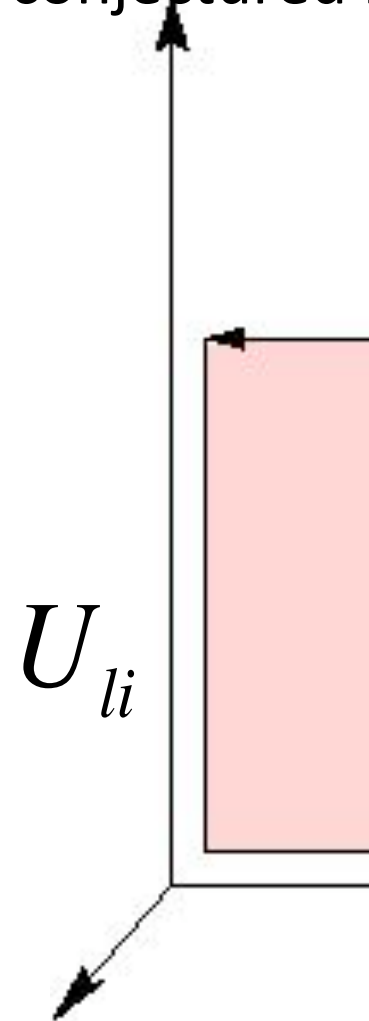
The exchange constants and magnetic field can vary with random dilution/pressure.

A uniaxial pressure (as we will discuss) and a magnetic field along the  $z$  direction. For uniaxial pressures- random longitudinal exchange.

By duality, the transverse field and the exchange can be interchanged with one another in a transverse field Ising chain. Random field in the vertical direction amounts to random longitudinal exchange. Random coupling

the 1990s, using the same idea, we can solve many other problems  
 "Cobanera" (Z. Nussinov and G. Ortiz, 0812.4309) and derive many  
 including a new exact self duality (E. Cobanera, G. Ortiz, and Z.  
 all  $Z_N$  gauge theories in 3+1 dimensions (earlier conjectured to be  
 self-dual). With 't Hooft ideas in mind,  
 numerous authors studied Wilson's action for  
 Lattice Gauge Field Theories

$$\frac{1}{g^2} \left( \sum \text{Re}(\text{Tr}(U_{ij} U_{jk} U_{kl} U_{li}) - 1) \right)$$



restricting the fields to  
 the roots of unity (Z)

Specifically, the dual coupling is given by

$$K_N\left(\frac{1}{2g^2}\right) \equiv K \qquad 4g_c^2 K_N\left(\frac{1}{2g^2}\right) = 1$$

$$\frac{1}{2} \frac{\partial F_N(K)}{\partial K} = \exp\left[-\frac{1}{2g^2} \left(1 - \cos \frac{2\pi}{N}\right)\right]$$

$$F_N(K) = \sum_{n=0}^{N-1} -2K \cos\left(\frac{2\pi n}{N}\right)$$

# Pressure effects:

$$H_P = \gamma \sum_j P_v \sigma_j^v$$

$$\frac{d\vec{\sigma}_i}{dt} = \gamma \vec{\sigma}_i \times \vec{P}_i$$

$$\vec{P}_i = P_{i,v} e_v$$

Prediction: In the presence of uniform pressure the orbital state will pre-

Models for orbital order (old)

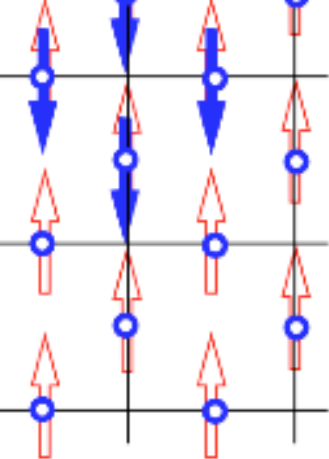
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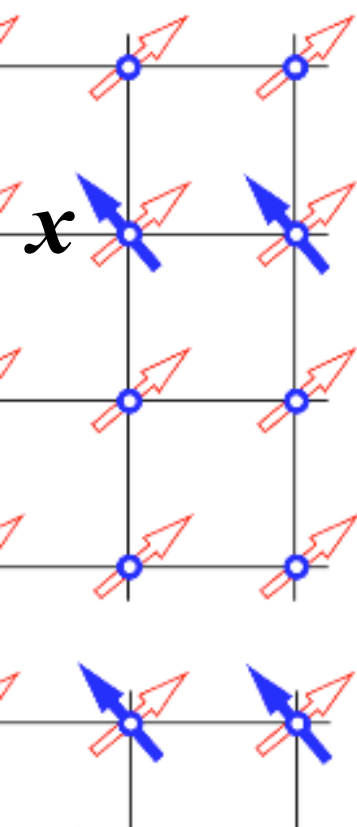
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Symmetries and topological order  
*n-dimensional gauge like symmetries an*



$d = 0$  (Ising Gauge Theory)

$$H = -K \sum_p \sigma_{ij}^z \sigma_{jk}^z \sigma_{kl}^z \sigma_{li}^z$$



$d = 1$  (Orbital Compass Model)

$$H = - \sum_i [J_x \sigma_i^x \sigma_{i+\hat{e}_x}^x + J_z \sigma_i^z \sigma_{i+\hat{e}_z}^z]$$

$$O^x = \prod_{j \in C_x} i \sigma_j^x$$

$d = D = 2$  (XY model)

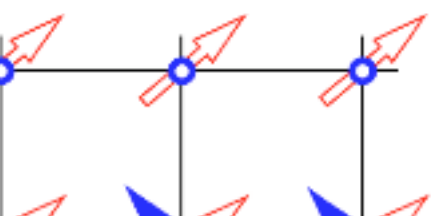
$$H = - \sum_{\langle ij \rangle} [J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y]$$

There is a connection between Topological Linking  
 group generators of  $d$ -GLSs and its Topological

( $D=2$  Orbital Compass Model)  $C_x$

$$O^x = e^{i\frac{\pi}{2} \sum_{j \in C_x} \sigma_j^x} = \mathcal{P} e^{i \oint_{C_x} \mathcal{A}}$$

symmetries are linking operators:  $O^\mu |g\rangle$



Topological defect:  $C_+ : \text{op}$

...

...



n system with Hamiltonian  $H_D$  and  $d$ -G

The absolute value of the average of any quantity  $f$  which is not invariant under  $d$ -G is bounded from above by the absolute value of the mean of the same quantity when this quasi-invariant quantity is computed with a  $d$ -dim  $H_d$  that is globally invariant under  $\mathcal{G}_d$  and preserves the structure of the interactions in the original  $D$ -dim system.

$\mathcal{C}_j$  |  $n_i$

$$|\langle f(\phi_i) \rangle_{H_d}| < |\langle f(n_i) \rangle_{H_D}|$$

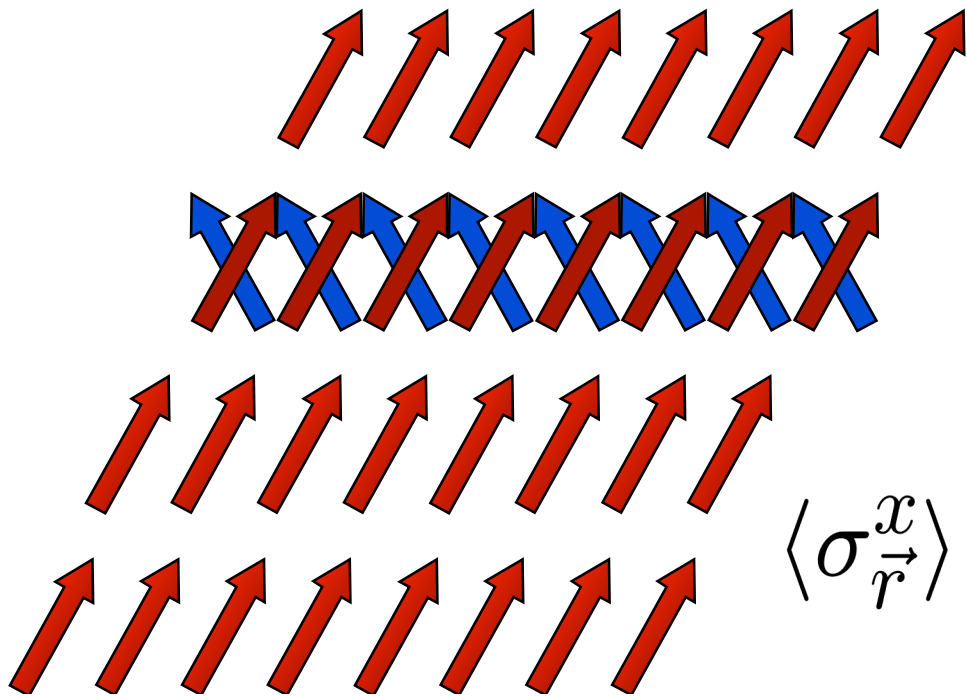
we spontaneously break a  $d$ -GLS in a  $D$

the Generalized Elitzur's Theorem: (for  
non- $\mathcal{G}_d$ -invariant quantities stren

- $d=0$  SSB is forbidden
- $d=1$  SSB is forbidden
- $d=2$  (continuous) SSB is forbidden
- $d=2$  (discrete) SSB may be broken
- $d=2$  (continuous with a gap) SSB is f

# Orbital Compass Model

$$H = J \sum_{\vec{r}} (\sigma_{\vec{r}}^x \sigma_{\vec{r}+\hat{e}_x}^x + \sigma_{\vec{r}}^y \sigma_{\vec{r}+\hat{e}_y}^y)$$

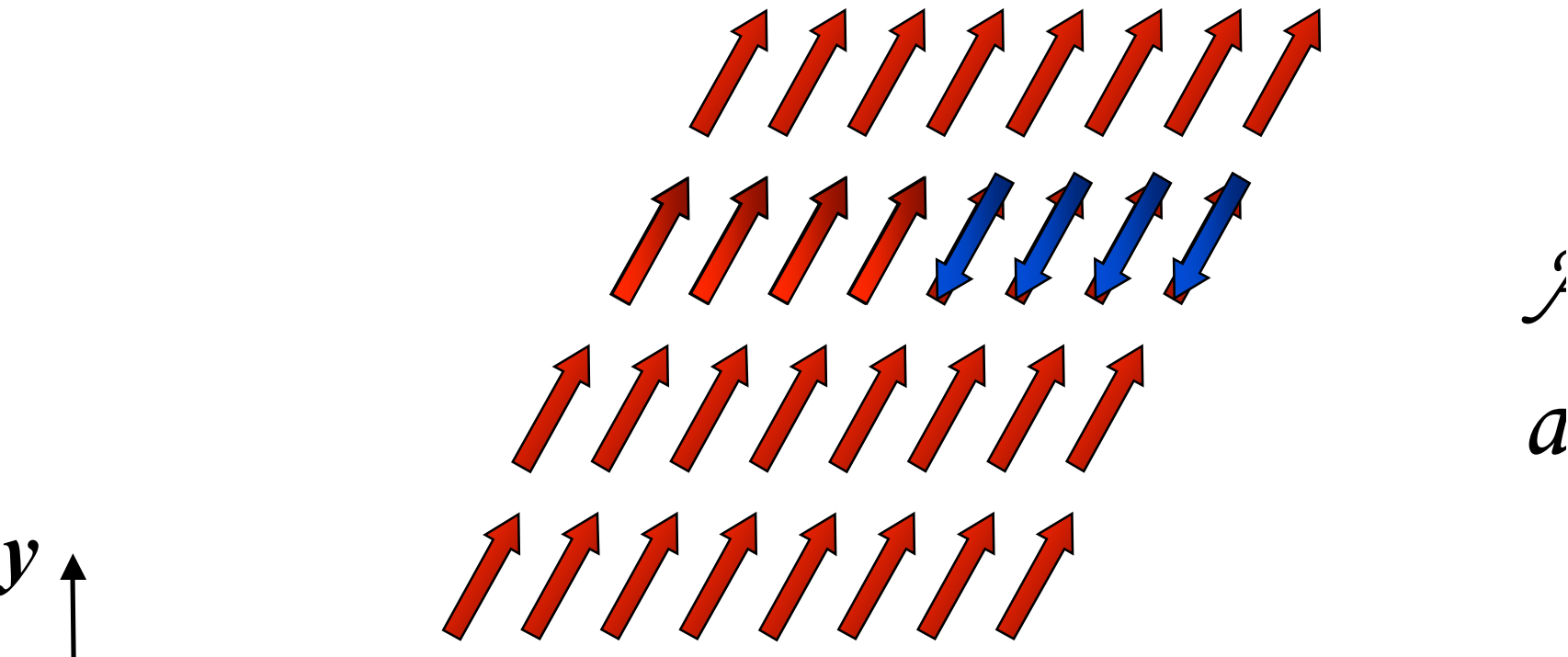


*Rotation by  
around the y-*

$$\langle \sigma_{\vec{r}}^x \rangle = \langle \sigma_{\vec{r}}^y \rangle = \langle \sigma_{\vec{r}}^z \rangle =$$

# Orbital Compass Model

$$H = J \sum_{\vec{r}} (\sigma_{\vec{r}}^x \sigma_{\vec{r}+\hat{e}_x}^x + \sigma_{\vec{r}}^y \sigma_{\vec{r}+\hat{e}_y}^y)$$



What happens when the  $d$ -GLSs  
are not exact symmetries of the full

(i.e., effect of perturbations)

**Emergent Symmetries**

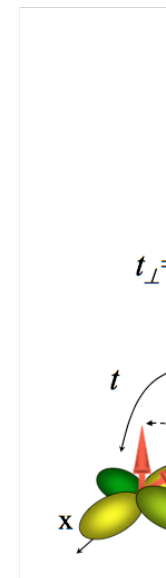


1: (Exact result) Continuous  $d < 2$  emergent  
in a gapped system, results

For independent d-GL  
with  $d=1$ , degeneracy  
is exponential in the surface  $\varepsilon$   
system.

# Jugel-Khomskii Hamiltonian $H_{KK}$ for $t_{2g}$ systems

A continuous symmetry  
Harris et al., PRL 91, 087206 (2003)



$$O_P^\gamma \equiv [\exp(i\vec{S}_P^\gamma \cdot \vec{\theta}_P^\gamma) / \hbar]$$

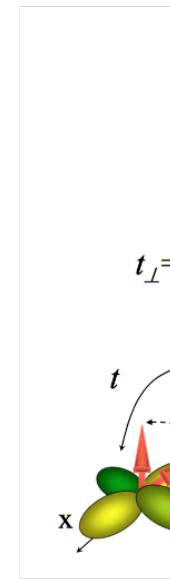
$$[H_{KK}, O_P^\gamma] = 0, \quad \vec{S}_P^\gamma = \sum_{r \in P} \vec{S}_r^\gamma$$

a continuous d=2 symmetry, c

# Kugel-Khomskii Hamiltonian $H_{KK}$ for $t_{2g}$ systems.

For a system in  $|xy\rangle$  state,

$$I(k_x, k_y, z, \omega) = \int dk_z e^{ik_z z} S(\vec{k}, \omega)$$



vanishes for non-zero  $z$ . This is so  
 as if two spins do not lie in the same plane (and  
 a separation along the direction orthonormal to the planes of  
 the correlator is not invariant under a continuous  $d=2$  sym-  
 metry. A discrete symmetry must be present to account for spin order. Similar considerations apply to  
 $|yz\rangle$  order. In general, if the KK interactions are d

$$[I(k_a, k_b, c, \omega) + I(k_b, k_c, a, \omega) + I(k_c, k_a, b, \omega)]$$



# Conclusions (new results)

Orbital systems can order by **thermal** “order-disorder” **fluctuations** even in their classical ( $1/S$ ) zero point quantum fluctuations are neglected.

Similar to charge and spin driven quantum critical behavior, it is theoretically possible to have **orbital driven quantum critical** behavior. (Predictions)

Orbital systems can exhibit topological order **dimensional reductions** due to their unusual symmetries (*exact or approximate*).

A new approach to dualities.

**Orbital nematic orders** (from symmetry breaking and related selection rules)

**Orbital Larmor effects** are predicted- periodicity in the orbital state under the application of an external magnetic field.

