Orbital orders and orbital order driven quantum criticality

Zohar Nussinov



C. D. Batista, LANL arXiv:cond-mat/0410599 (PRB)

M. Biskup, L. Chayes, UCLA; J. van den Brink, Dresden arXiv:cond-mat/0309691 (Comm Math Phys); 0309692 (EPL)

E. Fradkin, UIUC arXiv:cond-mat/0410720 (PRB)

G. Ortiz, E. Cobanera, Indiana arXiv:cond-mat/0702377, 0801.4391, 0812.4309, 0907.0733 (Annals of Physics, EPL, PRB); PNAS 2009

Conclusions (new results)

- Orbital systems can order by thermal "order out of disorder" fluctuations even in their classical limit (no (1/S) zero point quantum fluctuations are necessary).
- Similar to charge and spin driven quantum critical behavior, it is theoretically possible to have orbital order driven quantum critical behavior. (Prediction.)
- Orbital systems can exhibit topological order and dimensional reductions due to their unusual symmetries (*exact or approximate*).
- A new approach to dualities.
- **Orbital nematic orders** (from symmetry selection rules) and related selection rules
- Orbital Larmor effects are predicted- periodic changes in the orbital state under the application of uniaxial strain.

- I. What are orbital orders?
- 2. Models for orbital order "Order by disorder" in orbital systems
- 3. Orbital order driven quantum criticality and glassiness Exact solutions as a theoretical proof of concept

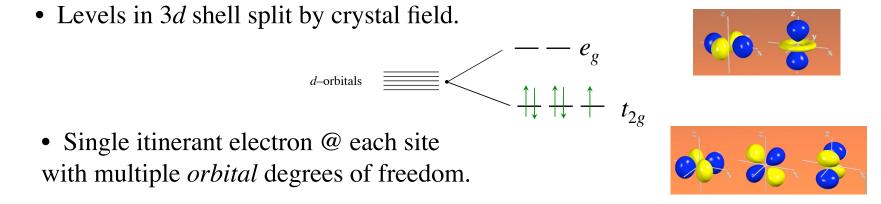
4. Symmetries and topological order Low dimensional gauge like symmetries and dimensional reductions; experimentally testable selection rules .What are orbital orders? (old)

2. Models for orbital order (old) "Order by disorder" in orbital systems (thermal fluctuations) (new)

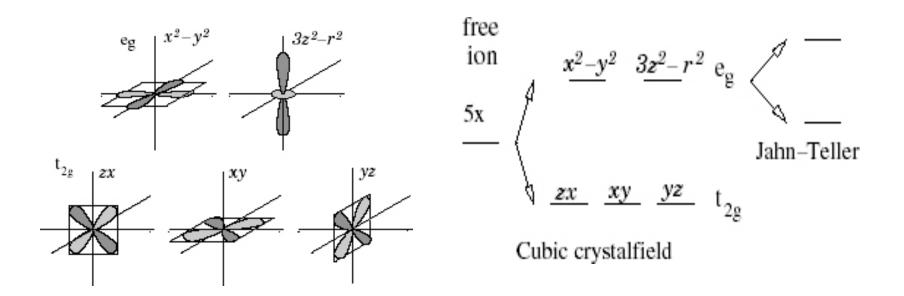
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4. Symmetries and topological order *Low dimensional gauge like symmetries and dimensional reductions; experimentally testable selection rules (new)*

Transition Metal Compounds



The 3d orbitals



The five 3d orbital states share the same radial Function. Their angular dependence:

$$|x^{2} - y^{2}\rangle = \left(\frac{Y_{2}^{2} + Y_{2}^{-2}}{\sqrt{2}}\right) |3z^{2} - r^{2}\rangle = Y_{2}^{0}$$
$$|xy\rangle = \left(\frac{Y_{2}^{-2} - Y_{2}^{2}}{\sqrt{2}}\right) |yz\rangle = \left(\frac{Y_{2}^{-1} + Y_{2}^{1}}{\sqrt{2}}\right) |zx\rangle = \left(\frac{Y_{2}^{-1} - Y_{2}^{1}}{\sqrt{2}}\right)$$

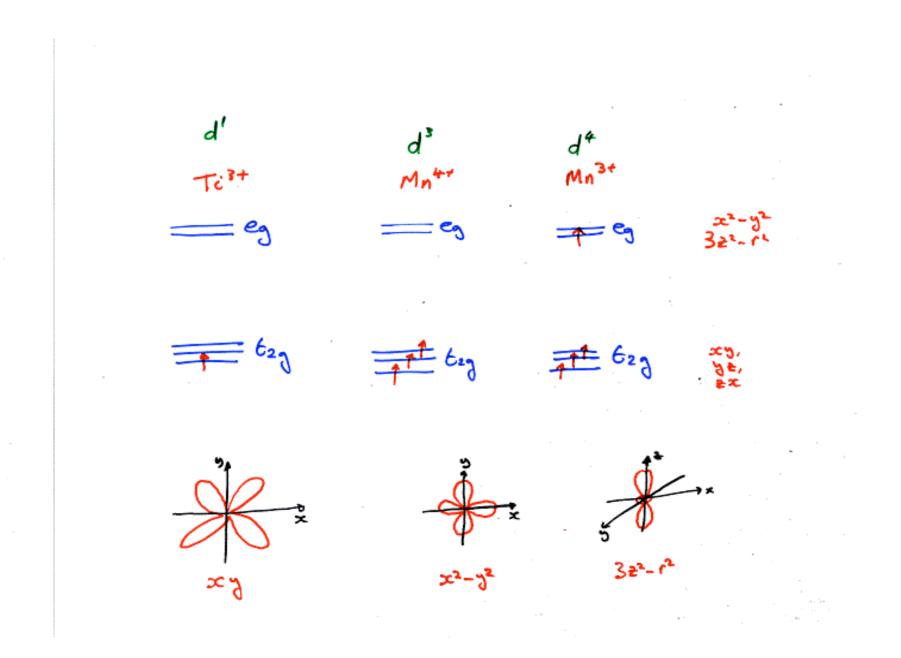
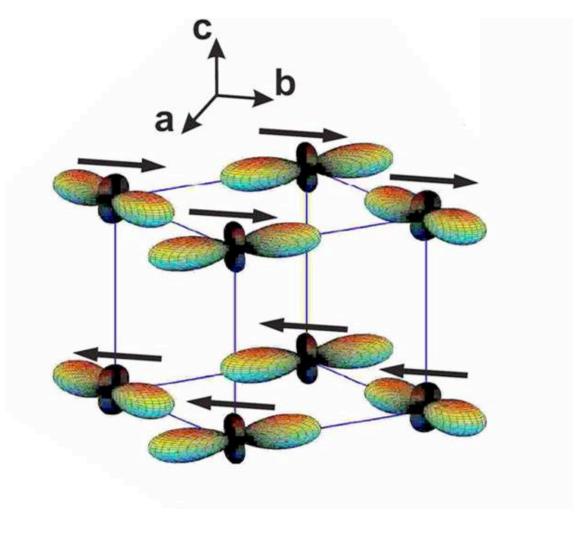
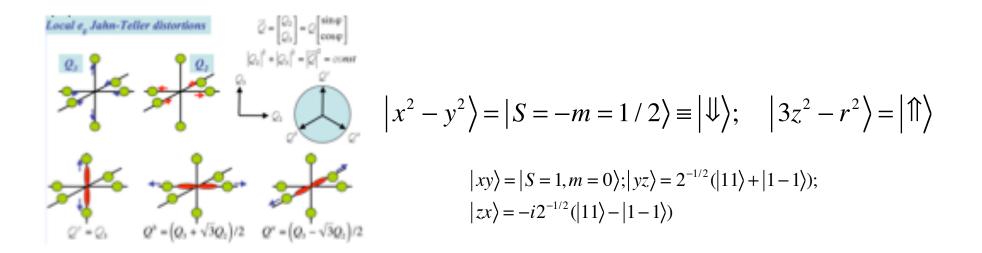


Illustration by R. Hill



LaMnO₃



The Hilbert space of the e_g orbitals is spanned by two states. The associated Jahn-Teller distortions can be expressed as vectors on a two dimensional unit disk (linear combinations of the two independent distortions $Q_{2,3}$). An effective pseudo-spin S=1/2 (or CP₁) representation. There is an angle of <u>120 degrees</u> between the three different cubic lattice symmetry related orbitals.

Similarly, the three t_{2g} orbitals can be represented by an effective S=1 representation. (In a Bloch sphere representation, there is an angle of <u>90</u> <u>degrees</u> between different point group symmetry related distortions.)

I.What are orbital orders? (old)

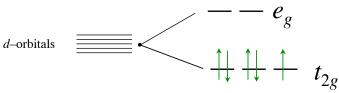
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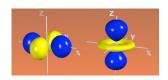
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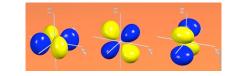
4. Symmetries and topological order *Low dimensional gauge like symmetries and dimensional reductions; experimentally testable selection rules (new)* Unlike spins, orbitals live in real space. The orbital interactions are <u>not</u> isotropic. Reduced symmetry and frustration.

Transition Metal Compounds

• Levels in 3*d* shell split by crystal field.







• Single itinerant electron @ each site with multiple *orbital* degrees of freedom.

Super-exchange approximation (and neglect of strain-field induced interactions among orbitals):

$$H = \sum_{\langle r,r' \rangle} H_{\text{orb}}^{r,r'} (\mathbf{s}_r \cdot \mathbf{s}_{r'} + \frac{1}{4}) \qquad \qquad H_{\text{orb}}^{r,r'} = J[4\hat{\pi}_r^{\alpha}\hat{\pi}_{r'}^{\alpha} - 2\hat{\pi}_r^{\alpha} - 2\hat{\pi}_{r'}^{\alpha} + 1]$$

$$\mathbb{W} = \text{direction of bond } r - r'$$

[Kugel-Khomskii Hamiltonian]

120°-model (e_g -compounds) V₂O₃, LiVO₂, LaVO₃,LaMnO₃,...

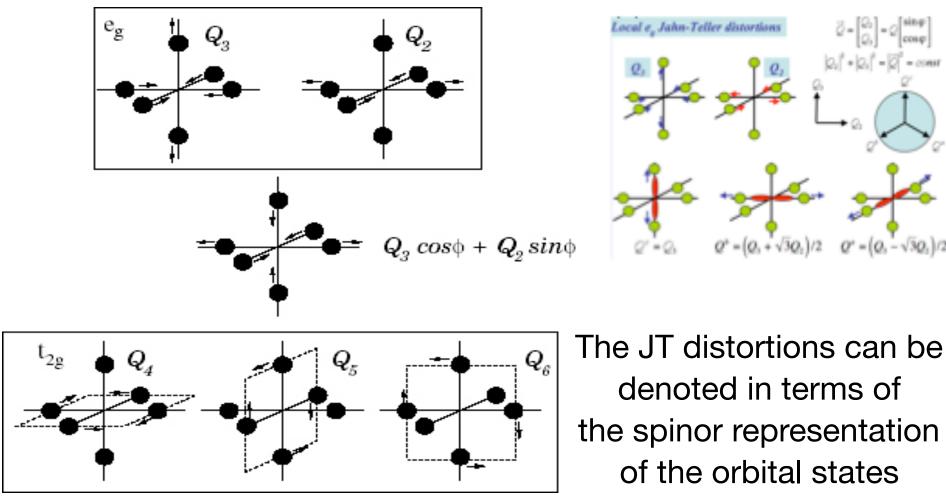
$$\hat{\pi}_r^x = \frac{1}{4} \left(-\sigma_r^z + \sqrt{3}\sigma_r^x \right) \quad \hat{\pi}_r^y = \frac{1}{4} \left(\sigma_r^z - \sqrt{3}\sigma_r^x \right)$$
$$\hat{\pi}_r^z = \frac{1}{2}\sigma_r^z$$

orbital compass-model (
$$t_{2g}$$
-compounds)
LaTiO₃, ...

$$\hat{\pi}_r^x = \frac{1}{2}\sigma_r^x \qquad \hat{\pi}_r^y = \frac{1}{2}\sigma_r^y$$
$$\hat{\pi}_r^z = \frac{1}{2}\sigma_r^z$$

Jahn-Teller distortions

The distortions preferred by different orbital states:



The orbital only interactions

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

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

• Orbital only approximation: Neglect spin degrees of freedom.

120° Hamiltonian:

$$H = J \sum_{r} \left(S_{r}^{[a]} S_{r+e_{x}}^{[a]} + S_{r}^{[b]} S_{r+e_{y}}^{[b]} + S_{r}^{[c]} S_{r+e_{z}}^{[c]} \right)$$

$$\vec{S}_r$$
 an XY-spin
 $S_r^{[a]} = \vec{S}_r \cdot \hat{a}$
similarly for $S_r^{[b]}$ & $S_r^{[c]}$,
 \hat{a}, \hat{b} and \hat{c}
unit vectors spaced @ 120°.

Orbital compass Hamiltonian:

$$H = J \sum_{r} \left(S_{r}^{[x]} S_{r+e_{x}}^{[x]} + S_{r}^{[y]} S_{r+e_{y}}^{[y]} + S_{r}^{[y]} S_{r+e_{z}}^{[z]} \right)$$

$$\vec{S}_r = (S_r^{[x]}, S_r^{[y]}, S_r^{[z]})$$

- usual Heisenberg spins.

The 120 degree model

$$\vec{S}_{r} \in S_{1}, \text{ write } \vec{S}_{r} = \left(S_{r}^{[x]}, S_{r}^{[y]}\right), \qquad S_{r}^{[a]} = \vec{S}_{r} \cdot \hat{a}.$$

$$H = J \sum_{r \in \Lambda_{L}} \left(S_{r}^{[a]} S_{r+e_{x}}^{[a]} + S_{r}^{[b]} S_{r+e_{y}}^{[b]} + S_{r}^{[c]} S_{r+e_{z}}^{[c]}\right)$$

$$= -\frac{J}{2} \sum_{r \in \Lambda_{L}} \left(\left(S_{r}^{[a]} - S_{r+e_{x}}^{[a]}\right)^{2} + \left(S_{r}^{[b]} - S_{r+e_{y}}^{[b]}\right)^{2} + \left(S_{r}^{[c]} - S_{r+e_{z}}^{[c]}\right)^{2}\right) + \text{ constant.}$$

Attractive couplings (ferromagnetic).

Couples in *x*-direction with projection along *a*-component. Couples in *y*-direction with *b*-component. Couples in *z*- direction with c-component

Clear: Any constant spin–field is a classical ground state. Ditto for the orbital compass model.

•U(1) symmetry emerges in the ground state sector of the large S theory*

Naïve spin-wave theory is a complete disaster

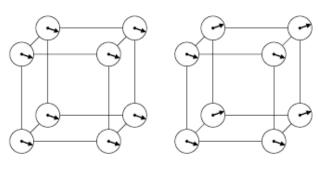
$$G(k,\omega=0) \quad \alpha \quad \frac{\Delta_a + \Delta_b + \Delta_c}{\Delta_a \Delta_b + \Delta_a \Delta_c + \Delta_b \Delta_c}$$

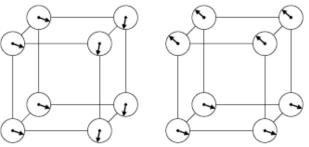
Fix k_z
$$G(k,\omega=0) \quad \alpha \quad \frac{1}{\Delta_a + \Delta_b}$$

Very IR divergent.

Lower Dimensional Symmetries

Z. Nussinov, M. Biskup, L. Chayes, and J. v. d. Brink 0309692 (EPL)

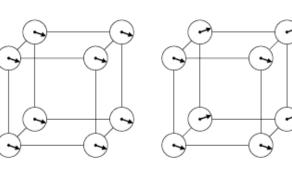




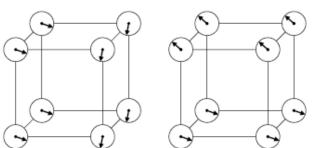
Ising-type discrete emergent symmetries of the classical 120 degree model

Lower Dimensional Symmetries

L x L x L lattice



Reflect all orbital pseudo-spins in entire planes.



Additional discrete degeneracy factor of 2^{3L} for the ground states

Order out of disorder-In the physics literature since the early 80's

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

E. F. Shender, *Antiferromagnetic Garnets with Fluctuationally Interacting Sublattices*, Sov. Phys. JETP **56** (1982) 178–184 .

C. L. Henley, Ordering Due to Disorder in a Frustrated Vector Antiferromagnet, Phys. Rev. Lett. **62** (1989) 2056–2059.

Really clarified matters; put things on a firm foundation in a general context.

Plus infinitely many papers (mostly quantum) in which specific calculations done. Earlier orbital order work focused on zero point 1/S fluctuations.

<u>Our result</u>: orbital order is robust and persists for infinite S. Zero point quantum fluctuations are not needed to account for the observed orbital order.

1) Weighting of various ground states must take into account more than just energetics:

• Fluctuations of spins will contribute to overall statistical weight.

2) These (spin–fluctuation) degrees of freedom will themselves organize into spin–wave like modes.

• Can be calculated (or estimated).

Spin wave free energy calculation

Expand about the uniform, state: $\theta_r = \theta^*$

$$\begin{split} \vartheta_{r} &\equiv \theta_{r} - \theta^{*} \qquad H_{SW} = \frac{J}{2} \sum_{r,\alpha} q_{\gamma}(\theta^{*}) (\vartheta_{r} - \vartheta_{r+e_{\alpha}})^{2} \\ q_{c}(\theta^{*}) &= \sin^{2} \theta^{*}, \quad q_{a,b}(\theta^{*}) = \sin^{2}(\theta^{*} \pm \frac{2\pi}{3}) \\ \log Z(\theta^{*}) &= -\frac{1}{2} \sum_{k \neq 0} \log \left(\sum_{\alpha} \beta J q_{\alpha}(\theta^{*}) \Delta(k_{\alpha}) \right) \end{split}$$

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

The free energy has strict minima at $\theta^* = n\pi/3$ Six uniform ground states: $S_r = \pm Se_{\alpha}$ **Stratified states:** $\theta_r = (-1)^x \theta^*$

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

$$\Pi_{k} = \begin{pmatrix} q_{1}\Delta_{1} + q_{+}\Delta_{+} & q_{-}\Delta_{-} \\ q_{-}\Delta_{-} & q_{1}\Delta_{1}^{*} + q_{+}\Delta_{+}^{*} \end{pmatrix}$$

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

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

$$q_{\pm} = \frac{1}{2}(q_{2} \pm q_{3})$$

$$\Delta_{\pm} = \Delta_{2} \pm \Delta_{3}$$

 $F(\theta^*) > F(0), \quad \theta^* \neq 0, \pi$

Low free energy states are not stratified.

Finite temperature order

Reflection Positivity (chessboard estimates): $P_{\beta}(A) \leq \left(\frac{z_{\beta}(A)}{z_{\beta}}\right)^{B^{3}}$

Interesting feature: Limiting behavior of model as *T* goes to zero is *not* the same as the behavior of the model @ T = 0.

Z. Nussinov, M. Biskup, L. Chayes, and J. v. d. Brink, arXiv: cond-mat/0309692

Nematic orbital order

For the t_{2g} orbital compass type models, uniform order cannot appear. By symmetry considerations, it is established tha $\langle S_r \rangle = 0$. Instead, an "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) can be proven to onset at sufficiently low yet finite temperatures. I.What are orbital orders? (old)

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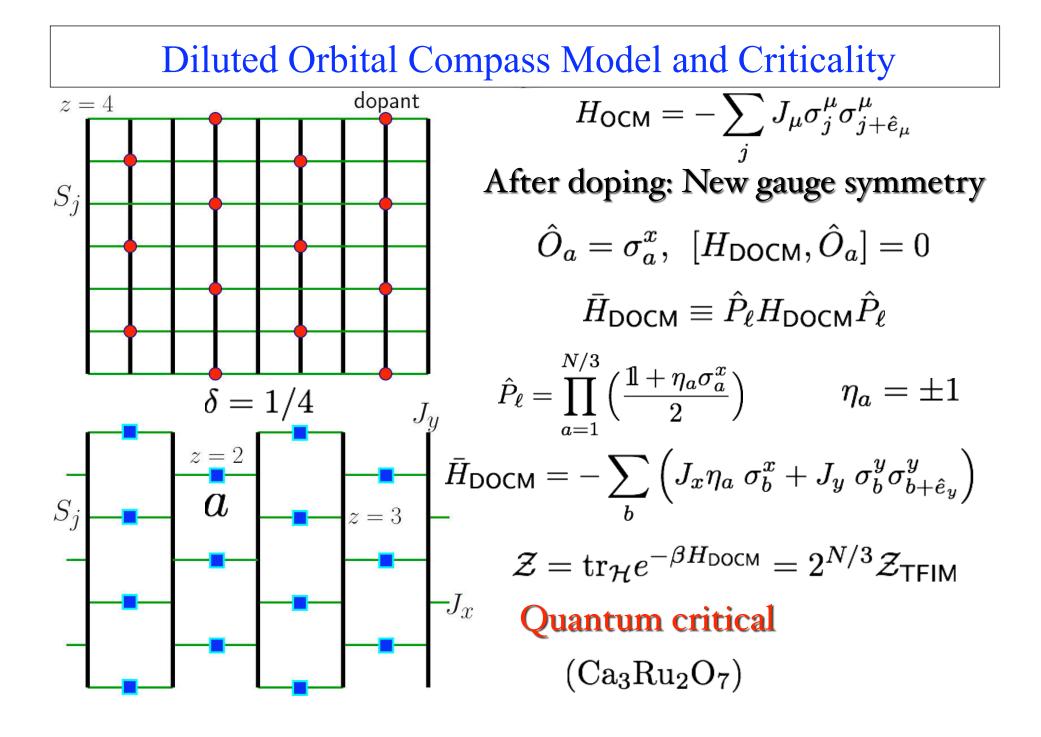
Orbital order driven quantum criticality

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

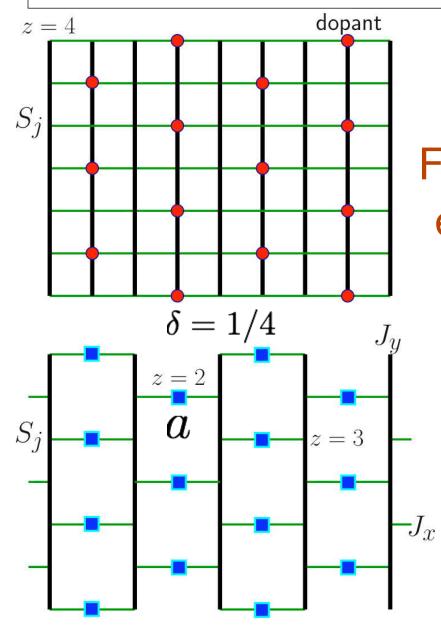
Question: Can there be an entirely new family of "orbital order driven quantum critical points"?

Answer: This is not forbidden and may occur theoretically. Indeed, in some simple yet exactly solvable models, there are orbital order driven quantum critical points (driven in the Hamiltonians by doping/dilution and/or uni-axial pressure). Orbital analogues of quantum spin glasses are similarly found. For these models, the associated CFTs are standard.

Z. Nussinov and G. Ortiz, arxiv:0801.4391



Diluted Orbital Compass Model and Criticality



 $H_{\mathsf{OCM}} = -\sum_{i} J_{\mu} \sigma^{\mu}_{j} \sigma^{\mu}_{j+\hat{e}_{\mu}}$ After doping: New gauge symmetry For a system with random exchange couplings J_{μ} , replicating the same steps mutatis mutandis leads to the Random **Transverse Field Ising** Model. Pressure plays the role of a transverse field.

Intermezzo: using the same idea, we can solve many other models using "Bond Algebras" (Z. Nussinov and G. Ortiz, 0812.4309) and derive a new exact self duality (E. Cobanera, G. Ortiz, and Z. Nussinov 0907.0733) for Z_N gauge theories in 3+1 dimensions (earlier conjectured not be self-dual). With 't Hooft ideas in mind, numerous authors studied of Wilson's action for Lattice Gauge Field Theories U_{kl}

 ${}^{\bullet}U_{_{jk}}$

 $U_{_{ij}}$

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

restricting the fields to Nth roots of unity (Z_N).

Specifically, the dual coupling is given by

$$K_{N}(\frac{1}{2g^{2}}) \equiv K \qquad 4g_{c}^{2}K_{N}(\frac{1}{2g_{c}^{2}}) = 1$$

•

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

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

Exact lattice relation! No Villain type nor any other approximation. E. Cobanera, G. Ortiz, and Z. Nussinov 0907.0733 The "Orbital Larmor Effect"

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 uniaxial pressure, the orbital state will change periodically in time.

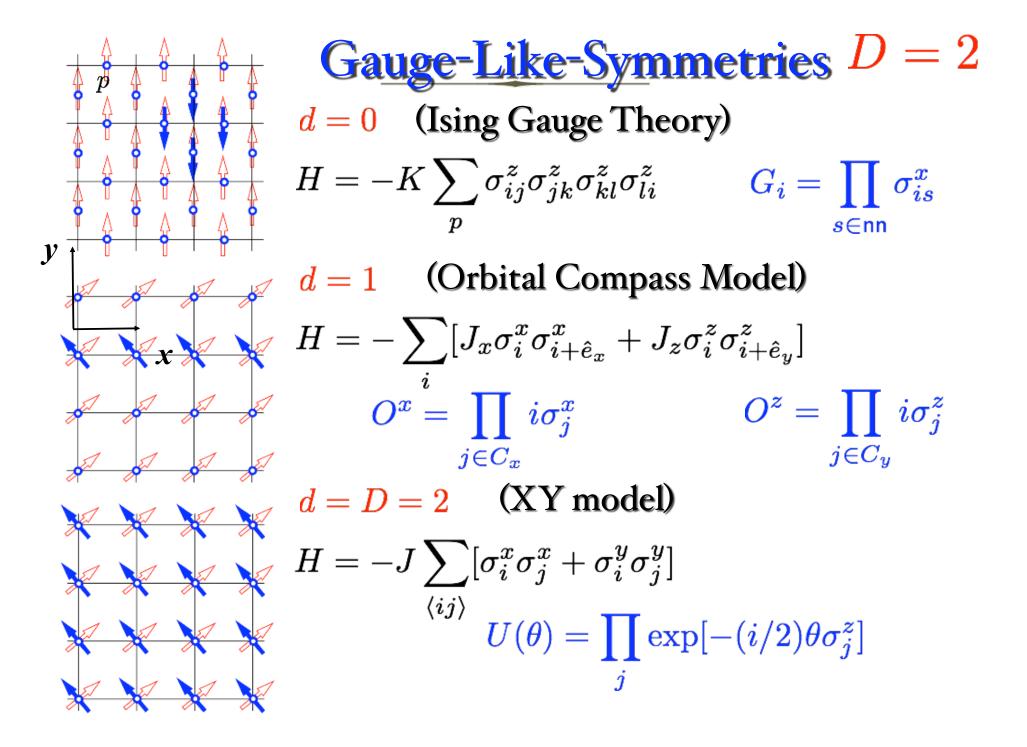
Z. Nussinov and G. Ortiz, arxiv: 0801.4391

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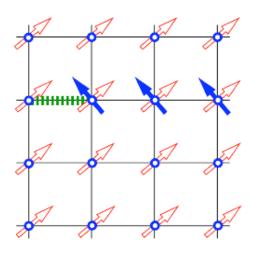
d-GLSs and Topological Phases

There is a connection between Topological Phases and the group generators of *d*-GLSs and its Topological defects

d = 1 (D=2 Orbital Compass Model) C_x : closed path

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

Symmetries are linking operators: $O^{\mu}|g_{lpha}
angle=|g_{eta}
angle$



Topological defect: C_+ : open path $D^x = e^{i\frac{\pi}{2}\sum_{j\in C_+} \sigma_j^x} = \mathcal{P}e^{i\int_{C_+} \vec{A}\cdot \vec{ds}}$ Defect-Antidefect pair creation Z. Nussinov and G. Ortiz, PNAS (2009)

Lower dimensional bounds

D-dim system with Hamiltonian H_D and d-GLS group \mathcal{G}_d

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

$$\mathcal{C}_{j} \ \phi_{i} = \left\{egin{array}{c} \eta_{i} \ \eta_{i} ext{ if } i \in \mathcal{C}_{j} \ \eta_{i} ext{ if } i \notin \mathcal{C}_{j} \ \psi_{i} ext{ if } i \notin \mathcal{C}_{j} \end{array}
ight.$$

$$|\langle f(\phi_i) \rangle_{H_D}| \le |\langle f(\eta_i) \rangle_{H_d}|$$

Dimensional reduction C. D. Batista, Z. Nussinov (cond-mat/0410599)

To Break or not to Break

Can we spontaneously break a *d*-GLS in a *D*-dim system ?

- From the Generalized Elitzur's Theorem: (finite-range and For non- \mathcal{G}_d -invariant quantities strength interactions)
 - 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 forbidden even at T=0

Transitions and crossovers are signaled by symmetry-invariant string/brane or Wilson-like loops

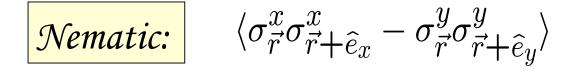
Example of application

Orbital Compass Model

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

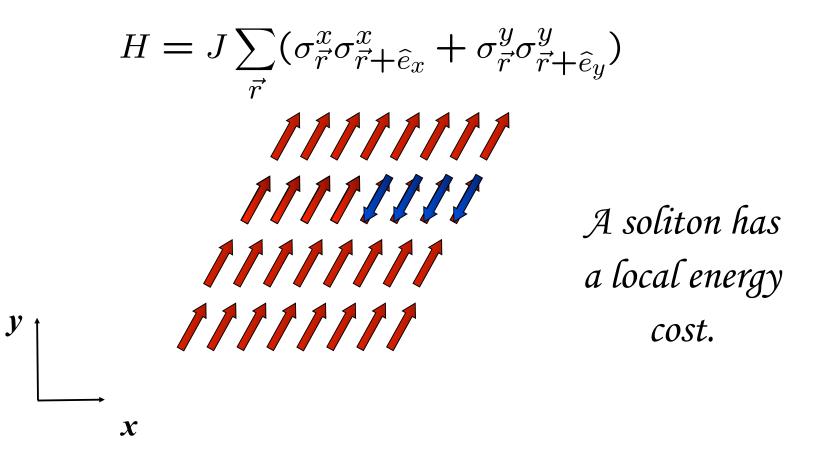
 $\begin{array}{c} \text{Rotation by } \pi \\ \text{around the y-axis} \end{array} \longrightarrow \\ y \end{array}$

x Lowest order allowed order parameter:

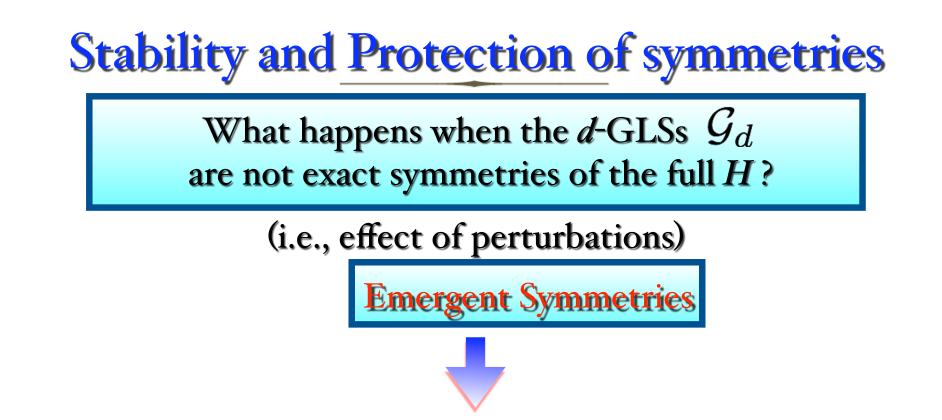


Intuitive Physical Picture

Orbital Compass Model



2D Orbital Compass Model dual to p+ip superconducting array. Z. Nussinov and E. Fradkin, cond-mat/0410720

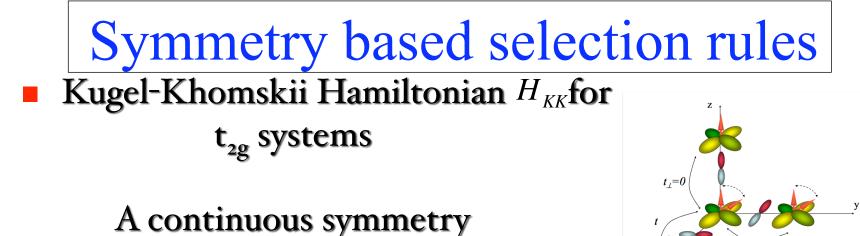


Case I: (Exact result) Continuous d < 2 emergent symmetry in a gapped system, results unchanged

Case II: Numerous systems with exact discrete *d*-GLSs are adiabatically connected to states where *d*-GLSs are emergent; results unchanged

Holographic Entropy

For independent d-GLSs with d=1, degeneracy is exponential in the surface area of the system.



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

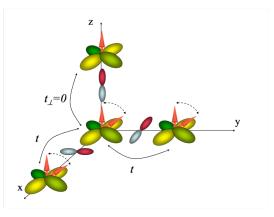
$$O_P^{\gamma} \equiv [\exp(i\vec{S}_P^{\gamma} \cdot \vec{\theta}_P^{\gamma}) / \hbar]$$
$$[H_{KK}, O_P^{\gamma}] = 0, \quad \vec{S}_P^{\gamma} = \sum_{r \in P} \vec{S}_r^{\gamma}$$

But a continuous d=2 symmetry cannot be broken, no long range order.

Symmetry based selection rules

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

For a system in ky> 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 thus have a separation along the direction orthonormal to the planes of z=0), the two point correlator is not invariant under a continuous d=2 symmetry. Other int. must be present to account for spin order. Similar considerations apply for kz> and kyz> order. In general, if the KK interactions are dominant

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

with a,b,c orthogonal axis is the largest when a,b, and c are along the crystalline axis. Nematic type parameters:

 $[2I(k_a,k_b,c,\omega) - I(k_b,k_c,a,\omega) - I(k_c,k_a,b,\omega)]$

Conclusions (new results)

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