Orbital ordering in $e_g$ orbital systems
Ground states and thermodynamic of the 120º model

Simon Trebst
Microsoft Station Q
UC Santa Barbara

IFW Dresden       June 2010
Orbital ordering in $e_g$ orbital systems
Ground states and thermodynamic of the $120^\circ$ model

Andre van Rynbach
UCSB physics

Synge Todo
University of Tokyo

IFW Dresden           June 2010
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)

| 3$d$ | $\begin{array}{c} e_g \\ \uparrow \quad \uparrow \\ t_{2g} \end{array}$ |

orbital degree of freedom

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

| LaMnO$_3$ | KCuF$_3$ (d$^4$) |
| Rb$_2$CrCl$_4$ | LiNiO$_2$ (d$^9$) |
| KCrF$_3$ | }
Orbital degrees of freedom

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

\[ |x^2 - y^2\rangle \quad |3z^2 - r^2\rangle \]
Orbital degrees of freedom

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

<table>
<thead>
<tr>
<th>spins</th>
<th>feature</th>
<th>orbitals</th>
</tr>
</thead>
<tbody>
<tr>
<td>weak</td>
<td>coupling to lattice</td>
<td>strong</td>
</tr>
<tr>
<td>high continuous</td>
<td>symmetry of Hamiltonian</td>
<td>orbital frustration</td>
</tr>
<tr>
<td>often gapless</td>
<td>excitations</td>
<td>almost always</td>
</tr>
<tr>
<td>sometimes</td>
<td>frustration</td>
<td>always</td>
</tr>
</tbody>
</table>
Orbital exchange

**Jahn-Teller interactions**

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

**classical** orbital model

![Diagram showing Jahn-Teller distortions](image)

**Kugel-Khomskii type interactions**

induced by **magnetic superexchange**

**quantum** orbital model

![Diagram showing Kugel-Khomskii interactions](image)
The 120 degree model

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

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

Jahn-Teller distortions
pseudospins are classical O(2) spins

Kugel-Khomskii type superexchange
pseudospins are quantum SU(2) spins
The 120 degree model

Both types of orbital exchanges give rise to the same Hamiltonian for the e\text{g} orbital degrees of freedom.

\[ H_{120} = -i, \quad \gamma = x, y \]

\[ J_z T_z^i + \gamma + \frac{3}{2} J_{mix} (T_z^i T_x^i + \gamma + T_x^i T_z^i) \]

\[ -i J_z T_z^i T_z^i + \gamma + \frac{3}{2} J_{mix} (T_z^i T_x^i + \gamma + T_x^i T_z^i) \]

\[ |\theta\rangle = \cos(\theta/2)|3z^2 - r^2\rangle + \sin(\theta/2)|x^2 - y^2\rangle \]

\[ = (T_z^i, T_x^i) \]

Jahn-Teller distortions

Kugel-Khomskii type superexchange

pseudospins are classical O(2) spins

pseudospins are quantum SU(2) spins

pseudospin representation

\[ |3y^2 - r^2\rangle \]

\[ |x^2 - y^2\rangle \]

\[ |z^2 - x^2\rangle \]

\[ |3z^2 - r^2\rangle \]

\[ |y^2 - z^2\rangle \]

\[ T_{i+z}^z \]
The 120 degree model

Our approach: explore 120° model in an extended parameter space

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

\[ \pm \sqrt{3} J_{\text{mix}} (T_i^z T_{i+\gamma}^x + T_i^x T_{i+\gamma}^z + \gamma) \]

symmetric model for equal-coupling

\[ J_x = J_z = J_{\text{mix}} \]

\[ H_{120} = -J \sum_{i, \gamma = x, y, z} (\tau_i \cdot e^\gamma)(\tau_{i+\gamma} \cdot e^\gamma) \]

\[ \tau_i = \left( [T_i^z + \sqrt{3} T_i^x]/2, [T_i^z - \sqrt{3} T_i^x]/2, T_i^z \right) \]
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 $120^\circ$ model

Pseudospins are classical $O(2)$ spins
Zero temperature: degenerate ground states

Emergent symmetries: U(1) and $Z_2$ symmetries

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

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

Low temperatures: Order by disorder


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

Symmetric 120° model

\[
\begin{align*}
|3y^2 - r^2\rangle &\quad |y^2 - z^2\rangle \\
|x^2 - y^2\rangle &\quad |3z^2 - r^2\rangle \\
|3x^2 - r^2\rangle &\quad |z^2 - x^2\rangle
\end{align*}
\]
Moving away from symmetric point

Emergent symmetries: U(1) and Z$_2$ symmetries

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

$$D = 2^{3L} \rightarrow D = 2^L$$
Low temperatures: Order by disorder

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

$J_x = J_z$

$J_{\text{mix}} / J_z$

Free energy $F(\theta^*)$

Angle $\theta^*$

$J_{\text{mix}} = 0$
$J_{\text{mix}} = 0.6$
$J_{\text{mix}} = 0.8$
$J_{\text{mix}} = 0.9$
$J_{\text{mix}} = 0.95$
$J_{\text{mix}} = 1$
Low temperatures: Order by disorder

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

$$J_x = J_z$$

$$J_{mix} / J_z$$

Truncated 120º model

$$F(\theta^*) = \frac{(|3z^2 - r^2| + |x^2 - y^2|)}{2}$$

$$\frac{|3z^2 - r^2| - |x^2 - y^2|}{2}$$
Thermal phase transitions

Specific heat \( C_v(T) \)

Temperature \( T / J_z \)

Order parameter \( M(T) \)

- 120° model
- Truncated model (\( J_{mix} = 0 \))

\[ M = \max(M_{xy}, M_{xz}, M_{yz}) \]

\[ M_{xy} = \sum_z \sum_{x,y} T_{x,y,z} \]
Moving back to the symmetric point

**Finite temperature:** A line of continuous thermal phase transitions.

**Zero temperature:** First-order transition to ‘mixed state’.

\[ J_x = J_z \]

\[ J_{\text{mix}} / J_z \]

- mixed state
  - xz / yz plane ordering
  - \( \theta_1, \theta_1 + 180^\circ \)

\[ T / J_z = 0.05 \]

\[ J_{\text{mix}} / J_z \]

\[ E(T) \]
Summary: classical 120° model

Considering the 120° 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 \( T_c \) away from symmetric point.
The quantum 120° model

pseudospins are quantum SU(2) spins
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 ($J_x=J_z$)

- a) specific heat
- b) magnetization
- c) Binder cumulant

Orbital ordering

[Diagram showing temperature vs. specific heat, magnetization, and Binder cumulant for different system sizes ($L=4, 6, 8, 10, 12, 16, 20$).]
Zero-temperature phase transition

$\frac{T}{J_z} = 0.15$

$\frac{J_x}{J_z}$

QMC

perturbation theory
(2nd order)

energy $E(T)$
1/S expansion


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

Zero-point energy to linear order in $S$

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

does not explicitly include mixing terms

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

mixing terms
1/S expansion

Zero-point energy to linear order in $S$

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

$E_0/N$ as a function of the angle for different values of $J_{mix}$.
‘Orbiton’ excitations

\[ |3z^2 - r^2\rangle \leftrightarrow |x^2 - y^2\rangle \]

orbital ordering

perturbation theory
(3rd order)

orbital ordering

QMC

QMC
Thermal phase transitions

A line of continuous thermal phase transitions.
Approaching the quantum 120° model

Going off into the $J_{\text{mix}} > 0$ plane

**orbiton condensation**

phase boundaries of gapped, polarized states
Phase diagram from orbiton condensation
The symmetric 120° model

\[ J_x = J_z \]

\[ J_{\text{mix}} / J_z \]

120° ground states

six ground states

twelve ground states
Summary

• Mott insulators with partially filled $3d$-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 $120^\circ$ 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.