Hidden Symmetries and Their Consequences in the Hubbard Model of t_{2g} Electrons*

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* **Phys. Rev. B *69*, 094409 (2004) and *69*, 035107 (2004).**

Outline

- Motivations: *High T_c oxides, CMR materials…*
- d-electrons in transition metal oxides
- Hubbard Model of the t_{2g} electrons
- Novel Hidden Symmetries
- Consequences

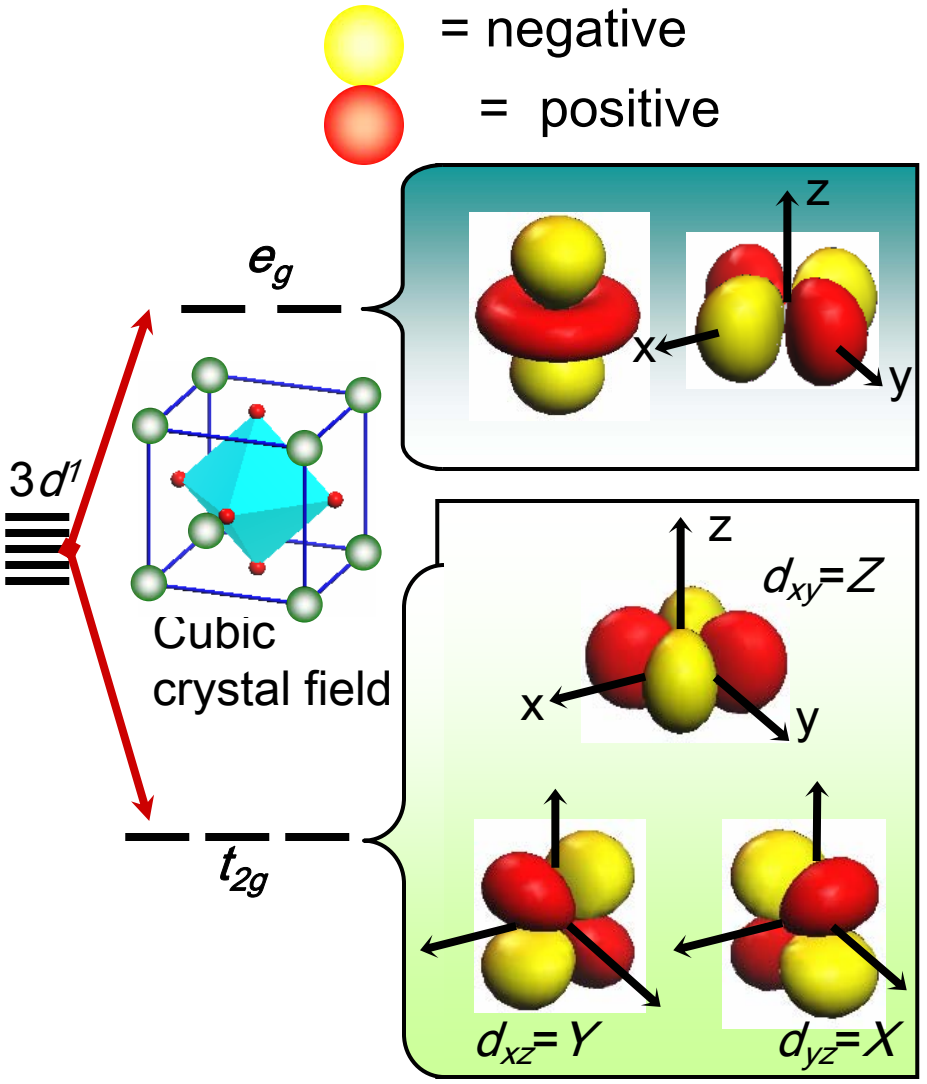
1. Absence of long-range spin order in the Kugel-Khomskii (KK) Hamiltonian
2. Extraordinary simplifications in numerical exact diagonalization studies
3. Gapless excitation spectrum even with spin-orbit interactions

Motivations

- *High temperature superconductivity* and *colossal magnetoresistance* sparked much recent interest in the magnetic properties of strongly correlated systems (i.e. transition metals), particularly those with orbital degeneracy.
- In most of the transition metal oxides (such as $LaTiO_3$), one has to deal with not only the spin degrees of freedom but also the orbital degrees of freedom of the strongly correlated electrons.
- Recent studies indicate that superexchange interactions between ions with spin and orbital degrees of freedom is a fascinating problem and suggest the possibility of exotic ground states with strong interplay between spin and orbital sectors.

d-electrons in transition metal oxides

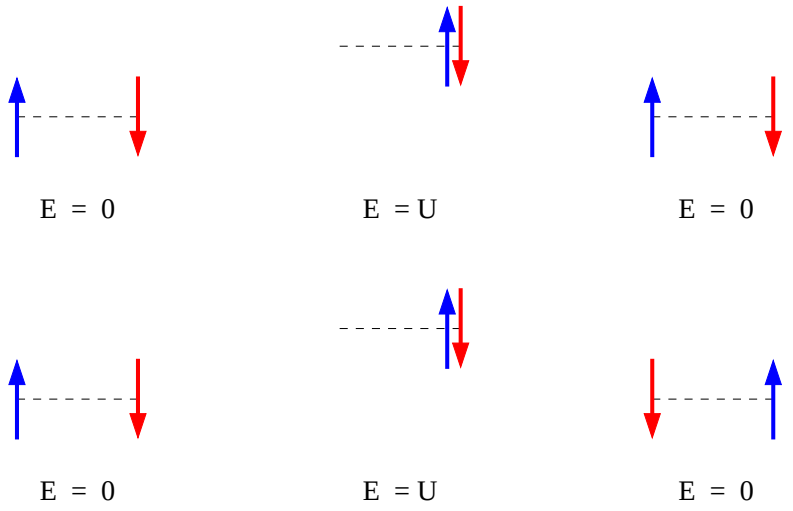
- For an ion with a single 3d electron the cubic crystal field gives rise to a two-fold degenerate e_g and a three-fold degenerate t_{2g} manifold.



Single-band Hubbard model Heisenberg Hamiltonian

- We first review the case when the on-site Coulomb interaction, U, is very large and there is one electron per site.

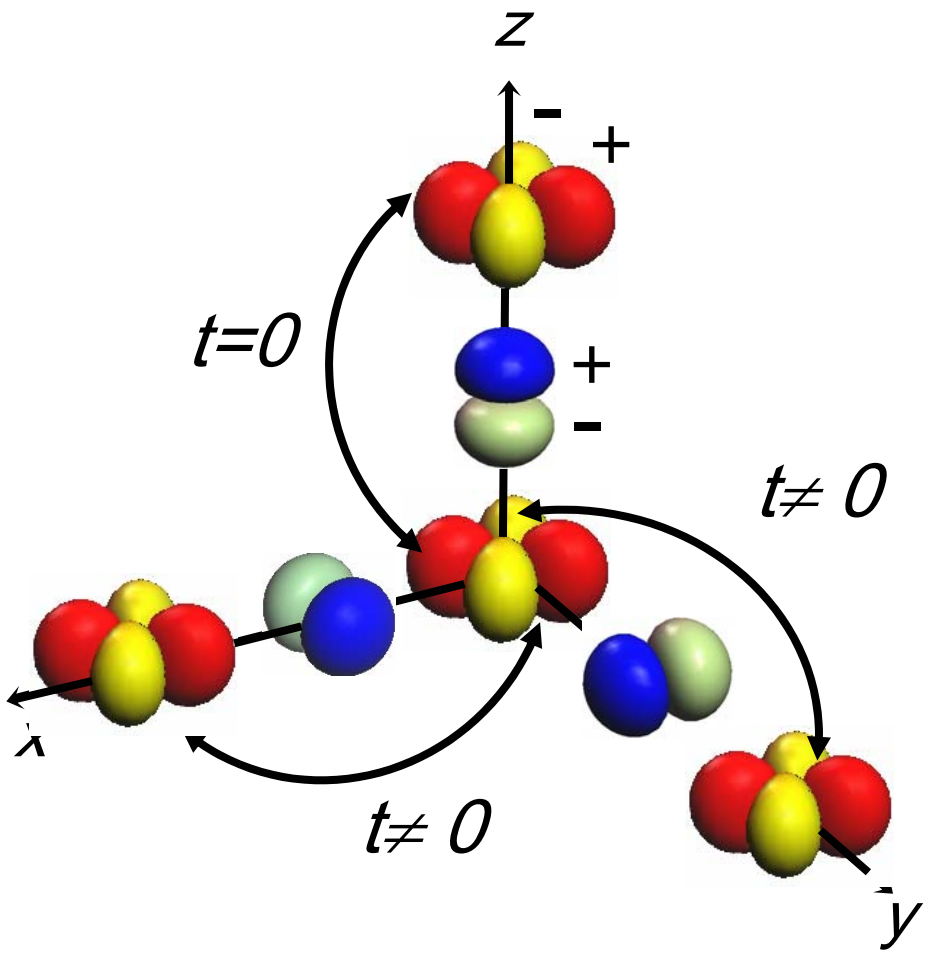
$$H = \sum_{i,j} t_{i,j} c_i^{+} c_j \; + \; U \sum_i n_{i\uparrow} n_{i\downarrow}$$



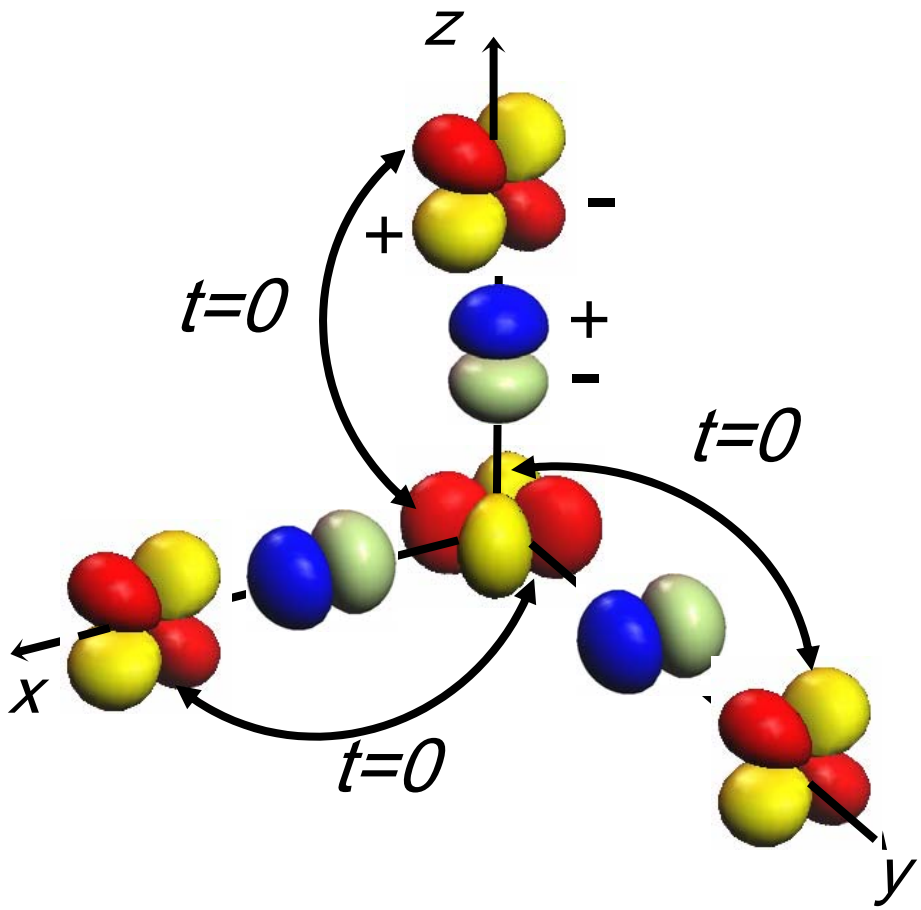
To leading order in t/U

$$H = \frac{t^2}{U}\left(4\vec{S}\cdot\vec{S} - 1\right)$$

Perturbation processes



Z (which is an xy wavefunction) can hop (via oxygen ions) to neighbors along either the x-axis or the y-axis, but NOT along the z-axis. The z-axis is called the ``inactive axis'' for orbital ``flavor'' Z (xy).



A Z-flavor orbital can not hop into a different flavor (here we show Z trying to hop into Y).

Hubbard Hamiltonian

Hubbard Hamiltonian: $H = H_{hop} + H_C$

$$H_{hop} = \sum_{<ij>} \sum_{\alpha\sigma} t_{ij}^{\alpha} c_{i\alpha\sigma}^{+} c_{j\alpha\sigma}$$

$$H_C = \frac{1}{2} \sum_{i} \sum_{\alpha\beta} U_{\alpha\beta} N_\alpha(i) N_\beta(i),$$

$$N_\alpha(i) = \sum_{\sigma} c_{i\alpha\sigma}^{+} c_{i\alpha\sigma}$$

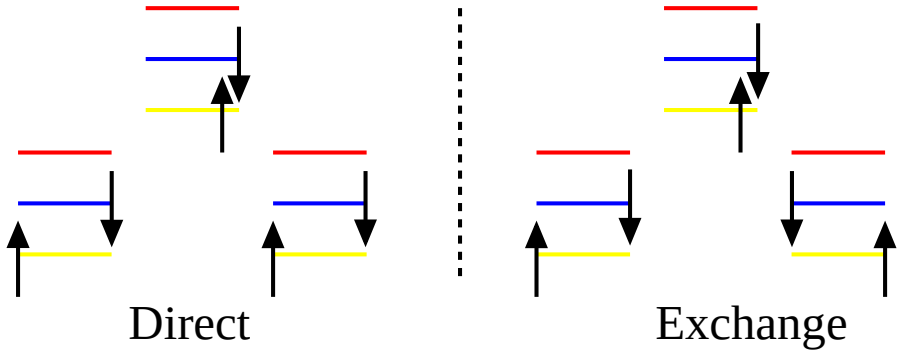
$c_{i\alpha\sigma}^{+}$ creates an electron at site *i* in orbital α with spin σ

KUGEL – KHOMSKII (1975)

$$H = \sum_{\langle ij \rangle} \sum_{\alpha\sigma} t^{\alpha}_{ij}\, c^{\dagger}_{i\alpha\sigma}\, c_{j\alpha\sigma} + \sum_{i\alpha\beta\sigma\eta} U\; c^{\dagger}_{i\alpha\sigma}\, c_{i\alpha\sigma}\, c^{\dagger}_{i\beta\eta}\, c_{i\beta\eta}$$

$$H = H_x + H_y + H_z$$

Red Axis is Inactive



$$H_x = \sum_{i<j} J_x \left(4\vec{S}_i \cdot \vec{S}_j - 1\right)$$

$$J_x = \sum_{\alpha\,\beta \neq x} \sum_{\sigma\eta} c^{\dagger}_{i\alpha}\, c_{i\beta}\, c^{\dagger}_{j\beta}\, c_{j\alpha}$$

``*Inconsistencies between experimental data and theoretical models need to be resolved.''*

Paraphrasing a reminiscence of R. Shull concerning the philosophy of his Nobel Laureate father.

Papers appear in PRL that explain properties Of LaTiO using exactly this model.

If experiments agree with the theoretical analysis of the model, DO WE DECLARE VICTORY?

Only if both are correct!!

ROTATIONAL INVARIANCE

If terms are invariant when the coordinate axes of the spin are rotated, then they are invariant when the spin is rotated. (We will obtain a remarkable spin symmetry.)

Simple example: the number of electrons of a given flavor, say X, is the sum of the number of ``up'' spins of that flavor plus the number of ``down'' spins of the flavor. But the directions of ``up'' and ``down'' don't matter.
So N_X is a rotational invariant.

Hubbard Hamiltonian

$$H_C = \frac{1}{2}\sum_i \sum_{\alpha\beta} U_{\alpha\beta} N_\alpha(i) N_\beta(i), \qquad N_\alpha(i) = \sum_\sigma c^+_{i\alpha\sigma} c_{i\alpha\sigma}$$

So since N is a rotational invariant, H_c is invariant against rotation of the spin of α-flavor electrons.

In fancier language: the operator which rotates the spin of α-flavor electrons commutes with H_c.

Now consider $$H_{hop} = \sum_{<ij>} \sum_{\alpha\beta\sigma} t_{ij}^{\alpha} c_{i\alpha\sigma}^{+} c_{j\alpha\sigma}$$

This is also a rotational invariant PROVIDING we rotate α-flavor electron spins on site i and those on site j IN THE SAME WAY.

Normally, all sites are coupled, so this means that rotational invariance only happens when ALL spins are rotated the same way. Here due to the inactive axes, d_{xy} electrons can only hop within an x-y plane, so we get rotational invariance when we rotate together all the d_{xy} spins in any single x-y plane (and similarly for other flavors).

MERMIN-WAGNER PROOF

In d=2 dimensions thermal excitations of spin-waves destroy long-range order.

The number of thermal spin excitations is

$$N_{\text{magnon}} = \sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle_T = \sum_{\mathbf{k}} \frac{1}{e^{\beta\ e_{\mathbf{k}}} - 1} \quad = \int \frac{k^{d-1}\, dk}{e^{\beta c k^2} - 1} \approx \int \frac{k^d\, dk}{k^3}$$

This diverges for d=2: the ground state is unstable to thermal excitation

Can we trust this heuristic argument??

MERMIN-WAGNER PROOF

We have constructed the analogous rigorous proof that there is no long range spin order in any flavor orbital at nonzero temperature. (PRB 69, 035107)

Although each orbital flavor has two dimensional dynamics, this system is really three dimensional.

It is very unusual for thermal fluctuations to destroy long-range order in a three dimensional system. But it happens for this special model.

Any small deviations from cubic symmetry invalidate this analysis.

MEAN-FIELD THEORY

THERE IS NO WAVEVECTOR SELECTION

$$F = \frac{1}{2}\sum_{\mathbf{k}} \chi^{-1}(\mathbf{k}) x(\mathbf{k}) x(-\mathbf{k})$$

The spin susceptibility for z-flavor orbitals is

$$\chi_z^{-1}(\mathbf{k}) = 12kT + 4\varepsilon[\cos(k_x a) + \cos(k_y a)] \qquad \varepsilon = \frac{t^2}{U}$$

This has an instability to order in antiferromagnetic planes which are active:

$k_x = k_y = \pi / a$ k_z = anything

ROTATIONAL SYMMETRY

Because we have rotational invariance FOR EACH FLAVOR separately

THE TOTAL SPIN, AS WELL AS ITS z-COMPONENT, FOR EACH FLAVOR, SUMMED OVER ALL SPINS IN THE ACTIVE PLANE OF THIS FLAVOR, ARE BOTH GOOD QUANTUM NUMBERS.

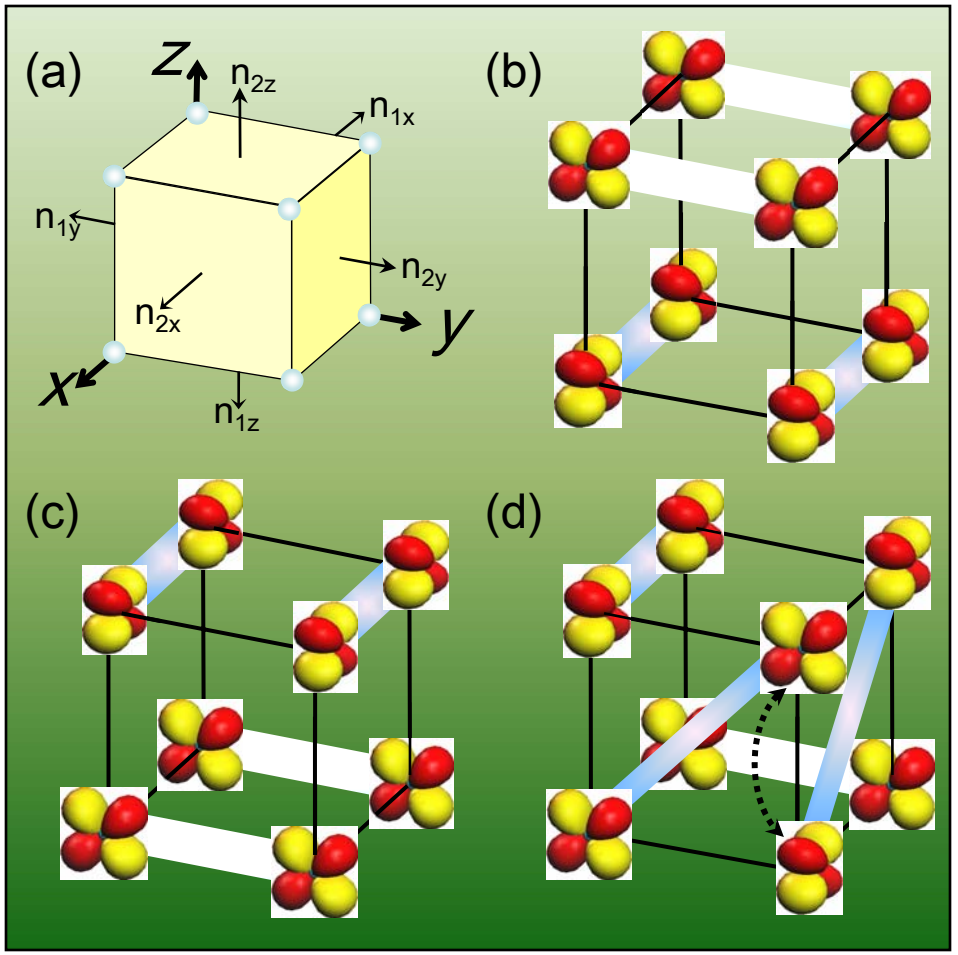
The spin at any given site is the sum over the spins of each orbital flavor (X, Y, and Z).

Consequences of the Novel Hidden Symmetries of t_{2g} Hubbard Hamiltonian

An i-j singlet wavefunction:

$$|(ij)_x> \equiv |(ji)_x> =$$
$$2^{-1/2}[c^+_{ix\uparrow}c^+_{jx\downarrow} - c^+_{ix\downarrow}c^+_{jx\uparrow}]\text{vac}>$$

The exact ground state is a sum of 16 dimer states, which can be obtained from the dominant configurations (c) and (b) by hopping as in panel (d).



Symmetry reduces 1.7 million to 16!!

$La\ Ti\ O_3$ B. Keimer *et al*

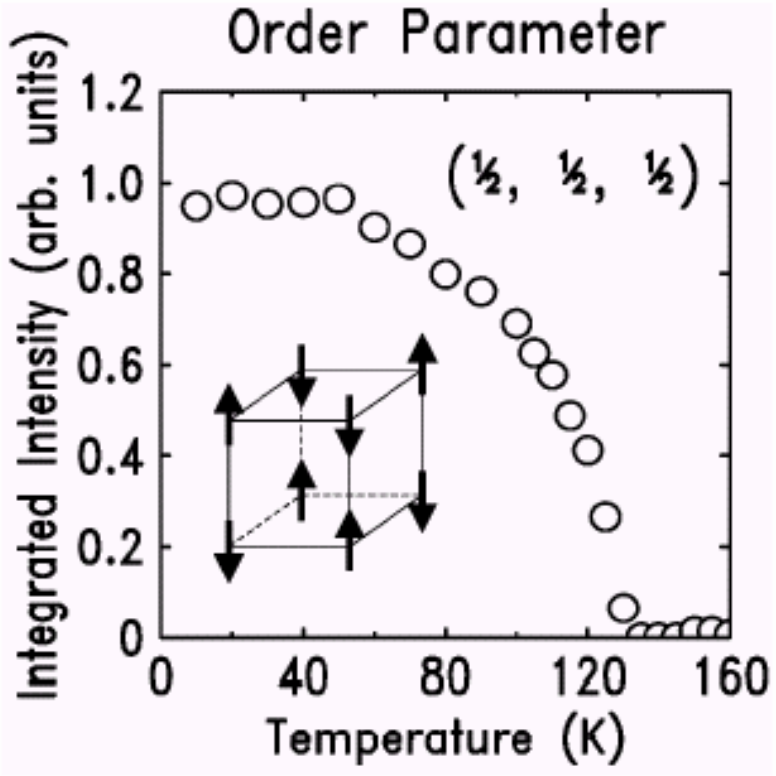


FIG. 1. Integrated intensity of the (0.5,0.5,0.5) AF Bragg reflection as a function of temperature. The inset shows the G-type spin structure.

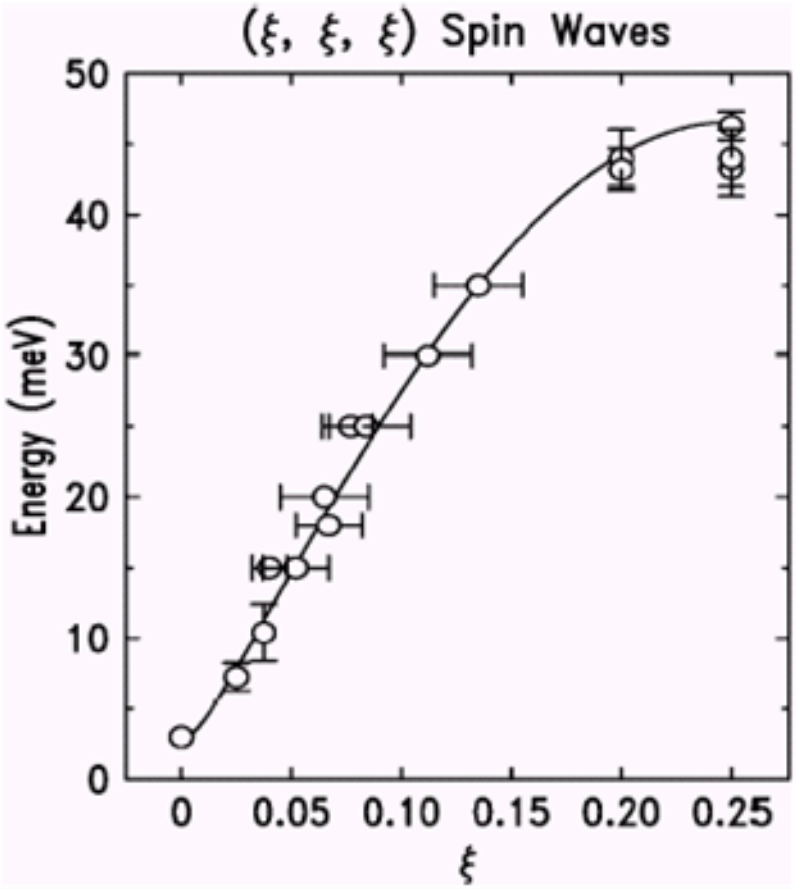


FIG. 4. Fitted spin wave peak positions in the (1,1,1) direction of reciprocal space. The line is the magnon dispersion curve described in the text.

J = 15.5 meV

Gap = 3.3 meV → D = 1.1 meV

Reduced moment = 0.45 μ_B (= μ_B for S = ½)

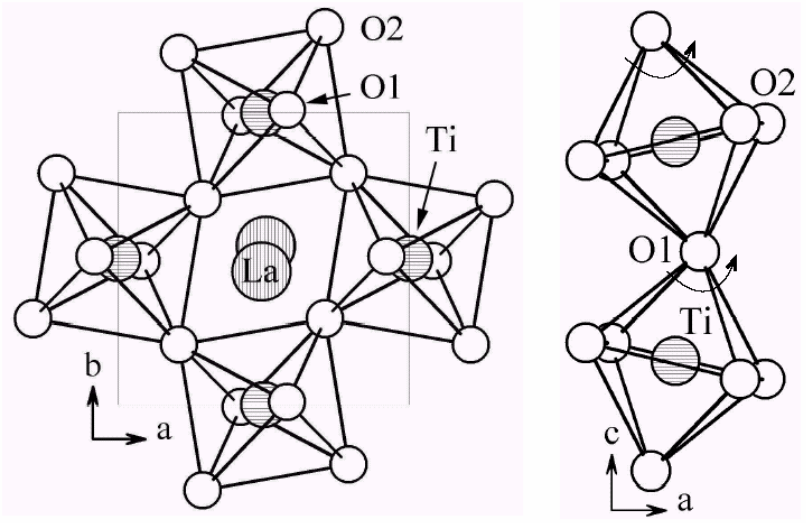
``*Inconsistencies between experimental data and theoretical models need to be resolved.''*

Paraphrasing a reminiscence of R. Shull concerning the philosophy of his Nobel Laureate father.

But suppose the experimental measurements are correct and the theory analysis of the model is accurate, but they disagree, THEN WHAT?

THE MODEL IS WRONG!!

In LaTiO the octahedra are rotated, so there are no inactive axes and this system is much like any other antiferromagnet.



But if a system more closely approximating the KK model could be fabricated, it would have very unusual properties: quasi 2d spin fluctuations, for example.

Almost any coupling will give rise to wave vector selection: if different flavors interact, they will all want to condense simultaneously, which can only happen at k = (pi, pi ,pi)/a.

For instance, if one adds spin-orbit Interactions, then the spins of all three orbital flavors simultaneously condense, but the spins of the different flavors are NOT parallel. this might explain large zero-point spin deviation.

SPIN-ORBIT INTERACTIONS

With spin-orbit interactions one would think that the spin knows where the crystal axes are -> we expect anisotropy

WRONG!!

$$V_{S-O} = \lambda \sum_{i} \sum_{\alpha\beta\gamma} < a \mid L_{\gamma} \mid \beta > [\sigma_{\gamma}]_{\mu,\nu} c^{+}_{i\alpha\mu} c_{i\beta\nu}$$

$$c_{i\alpha\sigma} = \sum_{t} V^{(a)}_{\sigma,\tau} \tilde{c}_{i\alpha\tau} \quad \text{with} \quad V^{(\alpha)} = \sigma_{\alpha} U \sigma_{\alpha}$$

Consequences of the Novel Hidden Symmetries of t_{2g} Hubbard Hamiltonian

- A global rotation of spins in a plane means that we CAN NOT have a long-range magnetic ordering at non-zero temperature (see Mermin and Wagner (PRL 13,1133,1966)).
- This conclusion also applies to the Kugel-Khomskii Hamiltonian which is obtained at second order perturbation (i.e. t^2/U):
- KK Hamiltonian – contrary to the general belief in the literature -does not support 3D magnetic ordering without additional terms such as spin-orbit interaction or allowing octahedral rotation!
- Inclusion of spin-orbit coupling allows such ordering but even then the excitation spectrum is gapless due to a continuous symmetry.

Therefore a consistent theoretical explanation of a real transition metal oxides must include other terms to the Hubbard or KK model

We hope that these results will inspire experimentalists to synthesize new t2g oxides with tetragonal or higher symmetry. Such systems would have quite striking and anomalous properties.

CONCLUSIONS

- For the first-time we uncovered several novel symmetries of the Hubbard Hamiltonian for a cubic t_{2g} system.
- **It is surprising that the Hubbard model has been widely used in the study of transition metal oxides for a long time but yet its remarkable symmetry properties were missed until now!**
- **Using these symmetries, we rigorously showed that the Hubbard model (and also KK model) without spin-orbit interaction does not permit the development of long-range spin order in three dimensional cubic lattice at non zero temperature.**
- **Finally,these symmetries reduce 1.7 million by 1.7 million matrix to 16x16 matrix for a cube of Ti cluster!**