Hidden Symmetries and Their Consequences in the t_{2g} Cubic Perovskites

The transition metal oxides have been the source of many fascinating physical phenomena such as high T_c superconductivity, colossal magnetoresistance, and orbiton physics [1]. These surprising and diverse physical properties arise from strong correlation effects in the *3d* bands. Most theoretical attempts to understand such systems are based on the Hubbard model. Here we report that for high symmetry transition metal oxides with threefold $\mathbf{t_{2g}}$ bands, this model possesses several novel hidden symmetries with many surprising consequences on the ground state properties [2, 3].

We consider cubic $3d^1$ perovskites (*i.e.*, ABO_3) where the five initially degenerate 3*d* states are split into a two-fold $\mathbf{e_g}$ manifold and a lower-energy threefold $\mathbf{t_{2g}}$ manifold with wavefunctions $d_{yz} \equiv X$, $d_{xz} \equiv Y$, and $d_{xy} \equiv Z$ (see Fig. 1). Keeping only the $\mathbf{t_{2g}}$ states, we base our discussion on the following generic three-band Hubbard Hamiltonian:

$$H = \sum_{i,\alpha,\sigma} \varepsilon_{i,\alpha} c^{+}_{i,\alpha,\sigma} c_{i,\alpha,\sigma} + \sum_{<ij>} \sum_{\alpha,\beta,\sigma} t_{i\alpha,j\beta} c^{+}_{i,\alpha,\sigma} c_{j,\beta,\sigma}$$
$$+ \sum_{i,\alpha,\beta,\sigma,\eta} U_{i\alpha,i\beta} \left(1 - \delta_{\alpha,\beta}\delta_{\sigma,\eta}\right) c^{+}_{i,\alpha,\sigma} c_{i,\alpha,\sigma} c^{+}_{i,\beta,\eta} c_{i,\beta,\eta}$$

Here $c^{+}_{i,\alpha,\sigma}$ creates a $\mathbf{t_{2g}}$ electron (or hole) on the i^{th} ion in the α spatial orbital (*i.e.*, $\alpha = X$, Y or Z) with spin σ, and $\varepsilon_{i,\alpha}$ is the on-site energy of the orbital at site i of a simple cubic lattice. $U_{i\alpha,i\beta}$ is the on-site Coulomb repulsion between orbitals α and β at site i. $t_{i\alpha,j\beta}$ is the effective hopping parameter from the α orbital at site i to the β orbital at its nearest neighbour site j.

As shown in Fig. 2, for cubic perovskites where the metal-oxygen-metal (*M-O-M*) bond is linear, the hopping parameter $t_{i\alpha,j\beta}$ is diagonal in the orbital indices α and β. This suggests that the total number of electrons in each orbital is a good quantum number. Furthermore $t_{i\alpha,j\beta}$ is zero along the "inactive" axis perpendicular to the orbital plane α, due to symmetry (Fig. 2). In other words an α-electron can only hop in α-plane. Thus, for the n^{th} plane perpendicular to the α-axis, the total number N_{n_α} of electrons in the α-orbital is conserved, *i.e.*, it is a good quantum number. Hence, one can consider the three dimensional lattice as a superposition of interpenetrating planes perpendicular to the *x*, *y*, and *z*-directions, each having a constant number of *X*, *Y*, and *Z* electrons, respectively, which are good quantum numbers (see Fig. 3(a)).

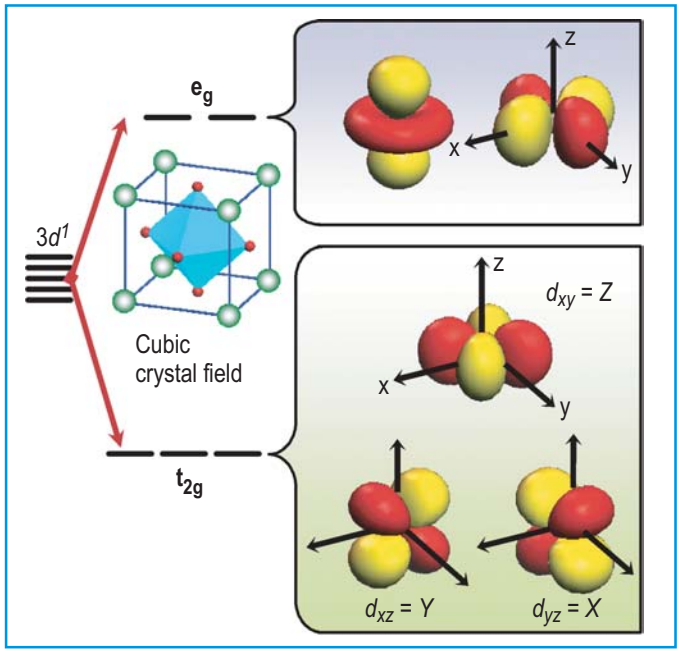

Fig. 1. A schematic view of the splitting of the five-fold *3d* orbitals under cubic crystal field. The transition metal is located at the center of the oxygen octahedra (shown in blue).

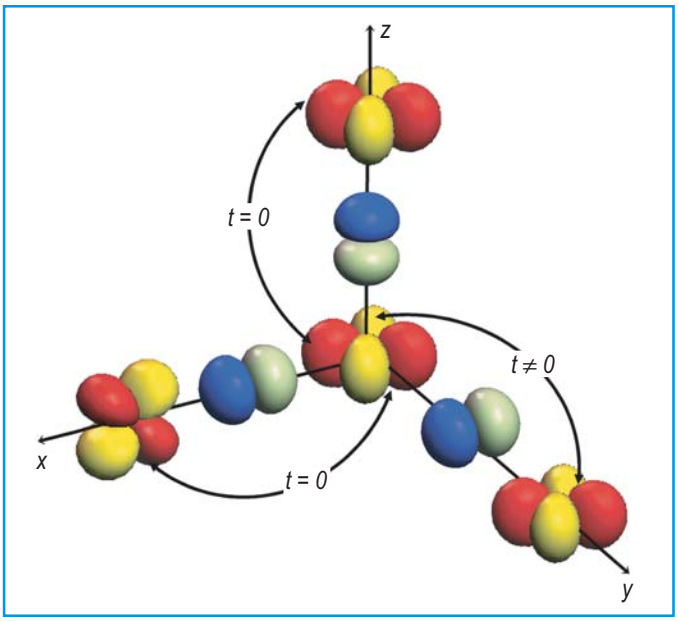

Fig. 2. A schematic view of the symmetry of the hopping parameter *t* via intermediate oxygen *p*-orbitals. Note that there is no hopping between different *d*-orbitals and no hopping along the *z*-axis for *Z*-orbitals due to symmetry.

In Ref. [3] we also show that the global rotation of the spins of α-orbital electrons *in any given plane* perpendicular to the α-axis leaves the Hubbard Hamiltonian given in Eq. (1) invariant. As a consequence of this rotational symmetry, one may conclude that both the Hubbard model and its 2nd order perturbation at order of t^2/U, the Kugel-Khomskii (KK) Hamiltonian, *cannot* support any long range spin order: if one *assumes* long-range spin order, the spins associated with α-orbitals within any given plane can be rotated at zero cost in energy, thereby destroying the supposed correlations among planes and/or among orbitals, and therefore the long-range order [2, 3]. The crucial conclusion here is that any credible theory of spin-ordering in these systems *cannot* be based solely on the KK Hamiltonian, as currently done in the literature.

The hidden symmetries discussed here are very useful in simplifying the exact numerical studies of small clusters. For example, to treat the simpler KK Hamiltonian for a cube of eight sites even using the conservation of the total spin (a widely used symmetry) requires the diagonalization of a matrix of dimensionality on the order of ½ million. Using the conservation laws applied to each face of the cube (see Fig. 3(a)), there is an astonishing numerical simplification. The ground state can be found from a Hamiltonian matrix within a manifold of just 16 states!! As seen in Fig. 3(b-d), these states are all products of four dimer states in each of which two electrons are paired into a spin zero singlet state. In this model a very unusual phenomenon occurs: when the electrons hop from site to site along active axes, they retain their membership in the singlet they started in. An example of this transformation is seen by comparing Figs. 3(c) and 3(d): pairs of electrons are tied together, as if by quantum mechanical rubber bands!

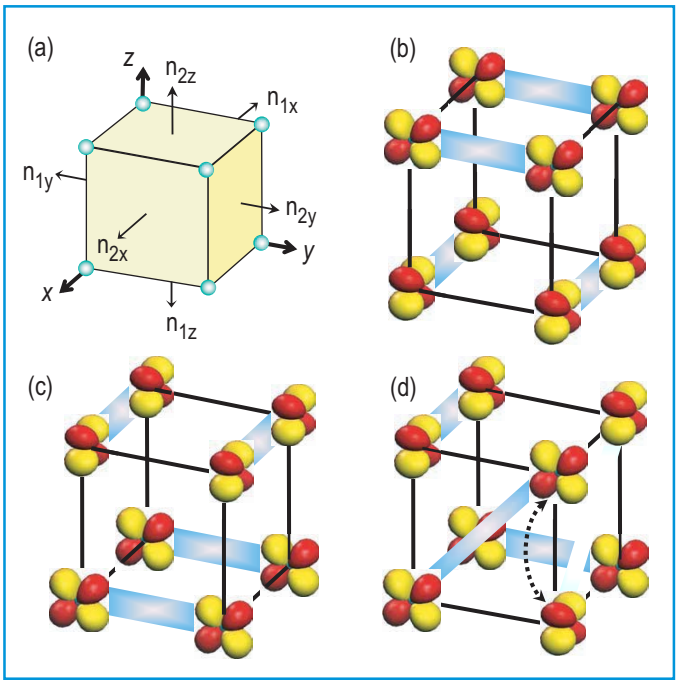

Fig. 3. (a) Six conserved quantum numbers as identified in the text, (b)-(c) Spin and orbital configurations for a cube of eight sites, indicating singlet spin dimers (as shown by thick blue lines) along the *x*-axis for *Y*-electrons and along *y*-axis for *X*-electrons. Configurations in (b) and (c) are the dominant ones in the ground state wavefunction. The less dominant configuration (d) is obtained from (c) by allowing the interchange of two *x*- and *y*- electrons along the *z*-axis, retaining their membership in the spin singlets.

In conclusion, we uncovered several novel symmetries of the Hubbard model for orthogonal $\mathbf{t_{2g}}$ systems. Using these symmetries, we rigorously showed that both the original Hubbard Hamiltonian [2] and the KK effective Hamiltonian [1] (without spin-orbit interactions) do not permit the development of long-range spin order in a three dimensional orthogonal lattice at nonzero temperature. It is important to take proper account of the symmetries identified here and to recognize that the observed long-range spin order can only be explained with the Hubbard or KK Hamiltonian providing suitable symmetry breaking terms are included. Such perturbations therefore play a crucial role in determining the observed behavior of these transition metal oxides. We hope that these results will inspire experimentalists to synthesize new $\mathbf{t_{2g}}$ transition metal oxides with tetragonal or higher symmetry. Such systems would have quite striking and anomalous properties.

References

[1] Y. Tokura and N. Nagaosa, Science **288**, 462 (2000) and references therein.

[2] A. B. Harris, T. Yildirim, A. Aharony, O. Entin-Wohlman, and I. Ya. Korenblit, Phys. Rev. Lett. (in press, 2003)(cond-mat/0303219).

[3] A. B. Harris, T. Yildirim, O. Entin-Wohlman, and A. Aharony, Phys. Rev. B (cond-mat/0307515).

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