Orbital Frustration and Entanglement with Spin and Lattice Degrees of Freedom

Sumio Ishihara[A], and Joji Nasu[B]
Department of Physics, Tohoku University[A],
Department of Applied Physics, University of Tokyo[B]
ishihara@cmpt.phys.tohoku.ac.jp

Orbital degree of freedom in correlated electron systems is one of the central themes in recent solid state physics. Essence of the orbital degenerate system is the directional nature and the intrinsic frustration effect due to the unique exchange interaction which explicitly depends on the bond direction [1]. Once we consider the orbital configuration which minimizes the bond energy in one direction, this does not minimize the bond energy in other directions. Due to this intrinsic frustration effect, a macroscopic number of degeneracy exists in the classical orbital configuration in some orbital models. This degeneracy is sometime lifted by the thermal and quantum fluctuations, as seen in the frustrated spin system, i.e. order by disorder mechanism.

We have studied several orbital models where the intrinsic orbital frustration plays essential roles. i) The Ring-exchange interaction in Mott insulator with doubly degenerate e_g orbitals.[2] Hamiltonian for the RE interaction is derived by the perturbational calculation. A remarkably weak ring-exchange interaction destroys the orbital order caused by the order-by-fluctuation mechanism in the nearest-neighbour exchange-interaction model. A long range order of magnetic octupole moment, i.e. complex orbital wave functions, appears. ii) The orbital compass model in a checkerboard lattice [3]. The orbital degeneracy is lifted by the thermal and quantum fluctuations, and a tricritical point appears due to the coexistence of the orbital frustration and the geometrical frustration.

In addition, we talk about an orbital system with the dynamical Jahn-Teller (DJT) coupling in a honeycomb lattice. The cooperative JT effect controls orbital order and structural phase transition in several transition-metal compounds. On the other hand, little is known about the dynamical aspect of the JT effect, i.e. the dynamical JT effect in correlated electron solids. Motivated from the recent exotic magnetic state, where the long-range spin and orbital order does not appear down to very low temperatures in $Ba_3CuSb_2O_9$ [4], we study theoretically the DJT effects in an orbital degenerate low dimensional magnet [5]. The derived low-energy effective model describes tunneling motions of the lattice vibrations during the potential minima. The cooperation / competition between the superexchange interaction and the dynamical JT effect are focused on. The effective model in a honeycomb lattice for $Ba_3CuSb_2O_9$ is analyzed by the mean-field approximation, a spin-wave method, quantum Monte-Carlo simulation, and the exact-diagonalization method associated with the mean fields. It is found that long-range magnetic order does not appears and a spin-orbital resonant state is stabilized by the DJT effect. A possible scenario for the spin liquid state discovered in $Ba_3CuSb_2O_9$ will be presented.

[1] S. Ishihara, in "The Jahn-Teller effect - Fundamentals and Implications for Physics and Chemistry", Springer Series in Chemical Physics, Vol. 97, H. Koppel, D. R. Yarkony, H. Barentzen (Eds.) Springer-Verlag (2010).
[2] J. Nasu, S. Todo, and S. Ishihara, Phys. Rev. B 85, 205141 (2012).
[3] J. Nasu and S. Ishihara, Europhys. Lett. 97, 27002 (2012) .
[4] S Nakatsuji, *et al.* Science, **336,** 559 (2012).
[5] J. Nasu and S. Ishihara arXiv:1209.0239.