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Spin-orbital entanglement due to dynamical Jahn-Teller effect

JOJI NASU, SUMIO ISHIHARA, Department of Physics, Tohoku University — Quantum spin liquid (QSL) state is one of the fascinating themes in correlated electron systems. Recently, a new candidate of the QSL state is experimentally reported in a layered copper oxide $\text{Ba}_3\text{CuSb}_2\text{O}_9$. In this material, a Cu^{2+} has the e_g orbital degree of freedom and the dynamical Jahn-Teller effect (DJTE) is suggested to play a key role for the emergence of the QSL state. Motivated from the recent experiments in $\text{Ba}_3\text{CuSb}_2\text{O}_9$, we study the DJTE in the spin-orbital coupled system and examine a possibility of the QSL state in a spin-orbital system with lattice vibrations. In particular, we focus on the competitive or cooperative phenomena between the superexchange (SE) interaction and the DJTE. A SE interaction Hamiltonian is derived from the $d-p$ type Hamiltonian and the DJTE Hamiltonian for the low-lying vibronic states is represented by the orbital pseudo-spin and the lattice vibration. We analyze the model, where these two interactions are taken into account on a honeycomb lattice, by using the cluster mean-field approximation with the exact diagonalization (ED) method and the combined method of the quantum Monte-Carlo method and ED method. We find that magnetic orders are unstable in a wide parameter region and a spin-singlet dimer state associated with an orbital order is realized. With increasing the DJTE, the orbital order is strongly suppressed and a resonance state of the spin-orbital dimers appears. We confirm that the spin and orbital degrees of freedom are strongly entangled with each other in this resonance state.

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