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Model for frustrated spin-orbital chains: application to CaV2O4

NATALIA PERKINS, University of Wisconsin, Madison, GIA-WEI CHERN, chern@physics.wisc.edu — Motivated by recent interest in quasi-one-dimensional compound CaV2O4, we investigate the physics of frustrated vanadium chains in which the interplay of geometrical frustration, spin-orbital couplings, Jahn-Teller effect, and enhanced quantum fluctuations leads to a rich phase diagram. Contrary to its spinel cousins, V ions in CaV2O4 are arranged in zigzag chains of edge-sharing VO6 octahedra. Antiferromagnetic interaction on zigzag chains consisting of triangular loops is subject to geometrical frustration as well. The rather weak and frustrated inter-chain couplings make the vanadium chains quasi-1D systems susceptible to quantum fluctuations. To make progress toward an understanding of the ground-state structure and the nature of phase transitions in CaV2O4, we study the zero-temperature phase diagram of its building blocks, i.e. zigzag chains with S=1 spins and Ising orbital variables. We find that while orbital interaction governed by an Ising-like Hamiltonian favors an antiferro-orbital order, on-site coupling of orbitals to spins and phonons tends to destroy the long-range order. Depending on the underlying orbital configuration, magnetic properties of the zigzag chain is equivalent either to those of two weakly coupled S=1 chains, or of an unfrustrated spin-1 ladder. In the presence of large spin-orbit coupling, the zigzag chain can be viewed as a spin-2 chain with anisotropic interaction.

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