MAR15-2014-020155

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Generic spin model for the honeycomb iridates with trigonal distortion

JEFFREY G. RAU, University of Waterloo

Recently, realizations of Kitaev physics have been sought in the A_2IrO_3 family of honeycomb iridates, originating from oxygen-mediated exchange through edge-shared octahedra. However, for the j = 1/2 Mott insulator in these materials exchange from direct d-orbital overlap is relevant, and it was proposed that a Heisenberg term should be added to the Kitaev model. Here we provide the generic nearest-neighbour spin Hamiltonian when both oxygen-mediated and direct overlap are present, containing a bond dependent off-diagonal exchanges in addition to Heisenberg and Kitaev terms. We analyze this complete model using a combination of classical techniques and exact diagonalization. Near the Kitaev limit, we find new magnetic phases, 120 degree and incommensurate spiral order, as well as extended regions of zigzag and stripy order. By including a small amount of trigonal distortion, as found in Na_2IrO_3, we show that such a zigzag phase can be stabilized near the ferromagnetic Kitaev limit. Decreasing the distortion destabilizes the zigzag phase toward a spiral phase that may be relevant for Li_2IrO_3. Using semi-classical spin-wave calculations we show that this regime is qualitatively consistent with experimentally known features of the dynamical structure factor in Na_2IrO_3 and speculate on implications for Li_2IrO_3.