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$_2$IrO$_3$ 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$_2$IrO$_3$, 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$_2$IrO$_3$. 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$_2$IrO$_3$ and speculate on implications for Li$_2$IrO$_3$. 