Two-orbital quantum spin model of magnetism in the iron pnictides

CHEN LIU, Boston University, DAO-XIN YAO, Sun Yat-Sen University, ANDERS SANDVIK, Boston University — We study a two-orbital spin model to describe \((\pi, 0)\) stripe antiferromagnetism in the iron pnictides. The “double-spin” model has an on-site Hund's coupling and inter-site interactions extending to second neighbors on the square lattice. Using a variational method based on a cluster decomposition, we optimize wave functions with up to 8 cluster sites (up to \(2^{16}\) variational parameters). We focus on the anomalously small ordered moments in the stripe state of the pnictides. To account for it, and large variations among different compounds, we show that the second-neighbor cross-orbital exchange constant should be ferromagnetic, which leads to “partially hidden” stripe order. In a different parameter region, we confirm a canted state previously found in spin-wave theory.

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