What causes an energy barrier between (π,0) and (0,π) magnetic orders in Fe pnictides

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Abstract

Most of undoped parent compounds for FeAs-based superconductors undergo a transition into a magnetically ordered state with stripe-like antiferromagnetic (AFM) order. Two possible collinear stripe structures with AFM Fe chains running along x or y direction, i.e., with ordering vectors (π,0) or (0,π), can be continuously transformed one into another via non-collinear states in which magnetizations of two sublattices formed by second Fe neighbours are rotated by an arbitrary angle. In a classical Heisenberg model all these states are degenerate. Band structure calculation show, however, that in Fe arsenides the degeneracy is lifted already at the mean-field level and that (π,0) and (0,π) AFM orders are separated by an energy barrier [1], with the highest energy calculated when the angle between the Fe moments on two sublattices is 90°. In order to find out the origin of the barrier, we consider for some Fe arsenides band structures corrected for magnetic double counting as proposed in Ref. [2]. Their analysis shows that the energy barrier appears because gaps at the Fermi surface, which open due to formation of stripe AFM order, partially close in the 90° structure. The results for Fe arsenides are compared to $BaMn_2As_2$ and hypothetical KFe_2Se_2 for which we found that the 90° spin structure is more favorable than the collinear stripe one. A doping dependence of the barrier is also discussed.

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[1] A. N. Yaresko, G.-Q. Liu, V. N. Antonov, and O. K. Andersen, Phys. Rev. B **79**, 144421 (2009).

[2] O. Andersen and L. Boeri, Annalen der Physik **523**, 8 (2011).