Magnetism in parent Fe-chalcogenides.

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The analysis of magnetism in parent compounds of iron-based superconductors (FeSCs) plays an important role for understanding superconductivity in these materials upon doping. In most Fe-pnictides, magnetism can be reasonably well understood within itinerant scenario. The locations of the Fermi surfaces (FSs) select two possible momenta for the order – $(0, \pi)$ and $(\pi, 0)$ – in the Fe-only Brillouin zone (BZ). Electron-electron interaction and the shape of the FSs further reduce the ground state manifold to single-momentum states with either $(0, \pi)$ or $(\pi, 0)$. In each of these two states spins are ordered in a stripe fashion – ferromagnetically along one direction in 2D Fe-plane and antiferromagnetically in the other. Upon doping, long-range order is lost, but magnetic fluctuations evolve smoothly and remain peaked at or near $(0, \pi)$ and $(\pi, 0)$ even beyond optimal doping.

There is one family of FeSCs - 11 Fe-chalcogenides $Fe_{1+y}Te_{1-x}Se_x$, in which smooth evolution between parent and optimally doped compounds does not hold. Magnetism in these materials changes considerably between $x = 0$ and $x \sim 0.5$, where the T_c is the largest. Near optimal doping magnetic fluctuations are peaked at or near $(0, \pi)$ and $(\pi, 0)$, as in Fe-pnictides, while magnetic order in a parent compound $Fe_{1+y}Te$ has very different momenta $\pm(\pi/2, \pm\pi/2)$ [1–5]. Upon doping, the spectral weight at $\pm(\pi/2, \pm\pi/2)$ decreases, and the spectral weight at $(0, \pi)$ and $(\pi, 0)$ increases.

In order to study magnetic order in $Fe_{1+y}Te$, we apply the localized electron scenario and verify whether the observed commensurate $\pm(\pi/2, \pm\pi/2)$ order can be obtained in a Heisenberg model with exchange interactions up to third neighbors [6]. Classically, $\pm(\pi/2, \pm\pi/2)$ order is unstable with respect to a spiral order for any non-zero first neighbor exchange, unless one artificially breaks C_4 symmetry and sets interactions to be spatially anisotropic. We analyze the isotropic quantum Heisenberg model and show that quantum fluctuations do stabilize a commensurate $\pm(\pi/2, \pm\pi/2)$ order in some range of parameters. However, this stabilization does not uniquely determine spin configuration as a generic $\pm(\pi/2, \pm\pi/2)$ order is a superposition of two different $Q-$vectors: $\mathbf{Q}_1 = (\pi/2, -\pi/2)$, and $\mathbf{Q}_2 = (\pi/2, \pi/2)$.

Previous works (for review, see [7]) argued that spin order is a single-Q state (either Q_1 or Q_2). Such an order breaks rotational C_4 symmetry and order spins into a double diagonal stripe. We show [6] that quantum fluctuations actually select another order – a double Q plaquette state with equal weight of Q_1 and Q_2 components, which preserves C_4 symmetry but breaks Z_4 translational symmetry. We argue that the plaquette state is consistent with recent neutron scattering experiments on $Fe_{1+y}Te$.

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