Local and non-local magnetic properties of iron and pnictides

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Investigations of ferromagnetism of iron attracts a lot of attention in spite of both, theoretical and practical interest to this substance. To explain physical properties of iron it is important to answer the question whether local moments exist in this material. We consider this problem within the ab initio LDA+DMFT approach with continuous-time quantum Monte Carlo solver (Ising symmetry of the Hund exchange), considering in particular orbitally-resolved contributions to one- and two-particle properties. For alpha-iron we find that at low temperatures eg and t2g states almost equally contribute to the formation of local magnetic moment (in contrast to earlier suggestion of Mott and Goodenough that the local moment is formed solely by eg electrons), and emphasize the important role of hybridization between eg and t2g states. We show that at low temperatures in the paramagnetic phase the subsystem of t2g states is close to the spin freezing transition, which accompany earlier found non-quasiparticle form of eg states. In gamma- (fcc) iron [3] we find that the magnetic properties at not too low temperatures T>1000K can be described in terms of temperature-dependent effective local moments, yielding relatively narrow peaks in the real part of the local dynamic magnetic susceptibility, which static part fulfills the Curie-Weiss law. At the same time, at low temperatures gamma-iron (which is realized in precipitates) is better described in terms of itinerant picture. In particular, the nesting features of the Fermi surfaces yield maximum of the static magnetic susceptibility at the incommensurate wave vector, belonging the direction X-W in agreement with the experimental data. In both cases from our calculations in paramagnetic phase, we extract the magnetic exchange integrals, which are in reasonable agreement with existing theoretical results and experimental data. We also compare these results with the calculations of local magnetic properties of iron pnictide compound LaFeAsO.