Temperature dependence of uniform magnetic susceptibility of iron pnictides from dynamical mean-field theory

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The discovery of superconductivity in ferropnictides has sparked tremendous interest to the new class of superconducting materials. In addition to rather high critical temperatures the iron pnictides demonstrate unusual magnetic properties. Namely, in some cases the paramagnetic susceptibility shows unusual non-Pauli and non-Curie-Weiss temperature dependence. Therefore understanding of the microscopic mechanism for such an unusual temperature evolution of the susceptibility is a challenging task. In our work we present the LDA+DMFT (method combining Local Density Approximation with Dynamical Mean-Field Theory) results for magnetic properties of the parent superconductors LaFeAsO, BaFe2As2 and KFe2As2 in the paramagnetic phase. Calculated uniform magnetic susceptibility demonstrates quasilinear increase at low temperatures followed by a maximum and decrease at higher T. The increase is detected experimentally for LaFeAsO and BaFe2As2 while the increase, maximum and the decrease are observed in hole-doped KFe2As2. The calculated susceptibility curves and their evolution with doping are in agreement with experimental data. We show that the microscopic origin of this anomalous behavior is connected with thermal excitation of the states forming the peak of the spectral function located approximately 100 meV below the Fermi level. This peak is due to the weak dispersion of the two-dimensional bands associated with layered crystal structure of the pnictides. Our results demonstrate that the unusual temperature dependence of the static magnetic susceptibility in the pnictide superconductors is connected with their spectral properties and can be understood without invoking intersite magnetic fluctuations.