On the Dual Role of the *d*-Electrons in Iron-Pnictides

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Introduction

Iron-pnictides are remarkable for the competition between superconductivity and magnetism. One unresolved issue concerns the dual role of the d-electrons that in these materials manifest themselves both as the localized moments formed on the Fe-sites and as the itinerant carriers. Recent Fe X-ray emission spectroscopy experiments unveiled the existence of sizable local moments at the room-temperature [1] almost for all the pnictides similar in magnitude to those reported in the low-temperature neutron scattering experiments (see also [2]). We studied the dual role of the *d*-electrons in the stoichiometric Fe-pnictides in *the paramagnetic phase* in the model of the local moments and the itinerant electrons interacting via the Kondo-type Hamiltonian.

Results and Discussion

At a moderate on-site Coulomb interaction the "bare" local moments become renormalized via the Kondo-like exchange interactions with itinerant electrons. In turn, the itinerant carriers scatter on the local moments that are disordered in the paramagnetic state. The latter mechanism explains the surprisingly high values of resistivity of the stoichiometric pnictides at the temperature of their transition into the antiferromagnetic phase. It was shown that instability to the SDW ordering is caused by the RKKY-interactions between the renormalized local moments via the exchange by the electron –hole pairs (the structural vector of the SDW phase is pre-determined by the positions of the electron- and the hole-pockets in the Brillouin zone). The dependence of the transition temperature, T_{SDW} on anisotropy and doping is found different from that one in the "nesting" scenario.
Generally, the assumed *intra-atomic* Hund's exchange is comparable or can even prevail over the Coulomb onsite repulsion. However, in the limit of strong Kondo-like exchange between the local moment and itinerant carriers the value of the local moment itself and the effective mean free time for carriers scattered on the moments tend to the finite values. The independence of the result on the strength of the on-site Coulomb repulsion was then justified by solving a simplistic model.
It is shown that at calculations of conductivity of iron-pnictides in the paramagnetic phase the multi-band character of the electronic spectrum in iron pnictides had to be taking into account; contributions from several electron- and hole-like pockets were then considered one by one.
All results were obtained owing to use of the new exact equations for the electronic Green functions in the real space.

Conclusions

The model of the d-electrons responsible both for formation of the local spins and the itinerant bands interacting via the Kondo-like exchange correctly describes properties of the stoichiometric iron pnictides in the paramagnetic phase [3] thus justifying studying the low temperature properties on the same terms.

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References

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