Strongly correlated electron systems: superconductivity in Fe-As compounds.

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1. Background and purpose of proposed research period

The main topic that we proposed to study during my stay at IMR is that of the recently discovered family of Fe-pnictide superconductors which includes the much studied LaFeAs(O_{1-x}F_x). By replacing La by Sm the superconducting (SC) critical temperature has reached 55K, well above the MacMillan limit of 39K. This fact together with various experimental results points to an unconventional pairing. The crystal structure of these compounds presents layers of Fe-As which may play a similar role as Cu-O layers in cuprate superconductors. As in the cuprates, the undoped parent compound LaFeAsO presents a magnetic order but it is not an insulator but a bad metal. There are also various experimental results indicating the presence of strong correlations in these materials. There are other similitudes and differences between cuprates and Fe-As superconductors and hence we hope that understanding these new materials could shed light to pairing mechanisms of electronic origin in general.

Another topic we have considered for research involves heterostructures, particularly as a component of spintronics devices. For example, we have studied recently with Prof. S. Yunoki (RIKEN) various possible heterostructures involving LaSrMnO with different compositions as magnetic tunnel junctions.

2. Proposed plan

Specifically, the main issues to be investigated are:

i) To determine the minimal effective model involving the relevant Fe orbitals to properly describe these compounds at least at a qualitative level. In addition, such effective models could include spin-orbit effects or As-orbitals polarization as well.

ii) To find the mechanism of pairing and symmetry of the SC gap. There have been claims of fully gapped SC in LaFeAsO but of a gap with nodes in the isostructural compound LaFePO.

iii) To make models of heterostructures involving materials with different properties such as insulators, ferromagnetic metals, ferroelectrics and to study them by numerical techniques.

3. Results and discussions

Most experimental results point to nodeless superconductivity, favouring a s-wave mode and weak coupling physics. However our point of view is that the two-orbital effective model for Fe-ions, which due to its simplicity allows for numerical exact calculations, contains many essential ingredients of the real compounds and the pairing symmetry in this model is a well-posed question.

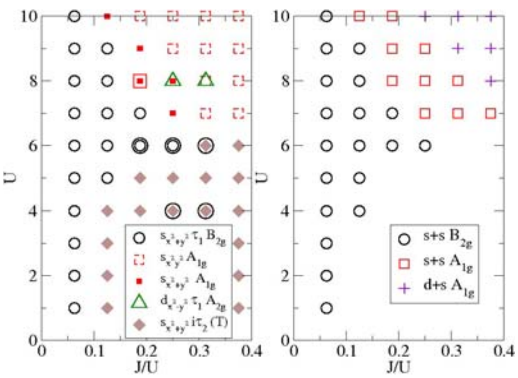

Fig. 1: Pairing phase diagram of the two-orbital model for Fe ions obtained by exact diagonalization on the 8-(small symbols) and 10-site (large symbols) clusters.

Taking advantage of the computational facilities at Maekawa Laboratory, we studied the pairing correlations for the two-orbital model. In addition following suggestions in the literature we studied combined pairs involving nearest neighbors and next nearest neighbor sites. These studies confirmed earlier results obtained for 8-site clusters (Fig. 1) pointing to a B2g symmetry for the parameters of interest. This analysis was extended to an effective J1-J2 model in the strong coupling limit where again in the region of the phase diagram where in the undoped case a stripe phase is present, a B2g pairing symmetry is dominant. Some of these results were presented at the ICC-IMR International Workshop "Physics on transition metal based superconductors", which took place during june 24-26, 2009.

We started to model heterostructures formed by manganites LaSrMnO3 and ferroelectrics BaTiO3 which could work as multiferroic tunnel junctions (Fig. 2).

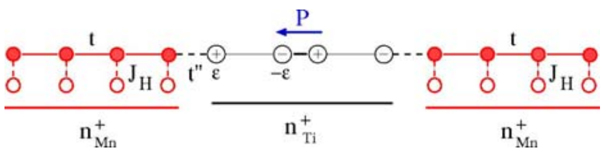

Fig. 2: A multiferroic tunnel junction formed by a central piece of ferroelectric surrounded by manganites.

This model allows for a study in one-dimension which we started to do using the DMRG technique. Preliminary results are encouraging (Fig. 3) and this study will be supplemented by Monte Carlo calculations performed by Seiji Yunoki's group at RIKEN, Tokyo.

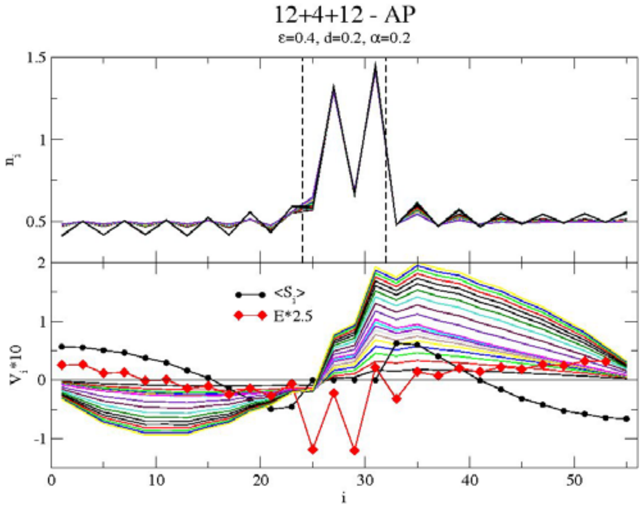

Fig. 3: DMRG results for the model shown in Fig. 2 showing the potential on the manganite leads for various iterations and the relationship between the electric field on the ferroelectric slab and the spin polarization at the interfaces on the manganite sides.

4. Summary and perspective

The research program around superconductivity in iron pnictides was not very strong partly due to the above-mentioned reason also because of the important research around spintronics at Maekawa Laboratory. In fact, during my three-month stay at this laboratory I tried to develop a project including some mechanism involved in the creation of spin-polarized charge carriers and taking advantage of my expertise on strongly correlated electron physics and related computational techniques. One such mechanism that allows the manipulation of spins by electric fields solely is that of the spin-orbit coupling (SOC). In addition, there are materials and heterostructures where SOC is present and at the same time electron correlations are important. Hence I started to investigate a Hubbard model with a Rashba spin-orbit coupling. A preliminary result we obtained is that the Hubbard coupling enhances the spin polarization induced by the SO coupling. I also found a complex dependence of the conductance on the Hubbard coupling, the SOC and the electron filling. I hope to continue working on this problem in collaboration with Professor S. Maekawa.