

MAR11-2010-001103

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Computational studies of models for the magnetism and superconductivity in iron pnictides

ADRIANA MOREO, University of Tennessee and Oak Ridge National Lab

The properties of multiorbital electronic model Hamiltonians for the pnictides are explored using a variety of many-body techniques. Via mean-field approximations, a regime where the undoped system develops $(\pi, 0)$ magnetic order while remaining metallic is found at intermediate values of the Hubbard repulsion U . Comparison of our results against ARPES and neutron scattering data allows us to determine a range of realistic values for the parameters in the models [1]. The orbital spectral weight redistribution that occurs near the Fermi surface in the $(\pi, 0)$ magnetic state without long-range orbital order is also discussed [2]. The two-orbital “ t - U - J ” Hubbard model at intermediate U , with magnetic order and pairing tendencies enhanced by the addition of Heisenberg terms that arise from the strong coupling expansion, is studied via exact diagonalization. At intermediate couplings and considering two extra electrons added to the undoped system, an A_{1g} bound state is found compatible with the “extended $s\pm$ ” pairing discussed in the RPA approximation. Bound states with B_{2g} symmetry, involving intra- and inter-band components, are also stable in portions of the phase diagram, while states with B_{1g} symmetry are close in energy, suggesting that small changes in parameters may render any of the three channels stable [3]. Finally, using the real-space Hartree-Fock approximation on finite clusters the presence of charge stripes at intermediate U is also observed for electron-doped systems. The patterns of charge, spin, and orbital order, as well as the influence of quenched disorder will be discussed [4].

[1] Q. Luo *et al.*, Phys. Rev. B **82**, 104508(2010). See also R. Yu *et al.*, Phys. Rev. B **79**, 104510 (2009).

[2] M. Daghofer *et al.*, Phys. Rev. B **81**, 180514(R) (2010).

[3] A. Nicholson *et al.*, preprint. See also M. Daghofer *et al.*, Phys. Rev. Lett. **101**, 237004 (2008), and A. Moreo *et al.*, Phys. Rev. B **79**, 134502 (2009).

[4] Q. Luo *et al.*, preprint.