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Study of the Multiorbital Hubbard Model for the Fe-Superconductors Beyond Weak Coupling

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A variety of experimental and theoretical investigations indicate that the pnictides and chalcogenides are materials with on-site Hubbard repulsion intermediate between weak coupling, where simple nesting ideas apply, and strong coupling where the spins are localized. For this reason, it is desirable to broaden the range of couplings theoretically studied as well as the many-body models and techniques employed. In this talk, an extensive analysis of model Hamiltonians for the Fe-based superconductors is presented. The multiorbital Hubbard models with two, three, and five orbitals are studied, via the Hartree-Fock approximation and exact diagonalization techniques. The main topics to be discussed are: magnetic ordering tendencies [1], range of realistic Hubbard repulsion and Hund couplings [2], orbital-weight redistribution at the Fermi surface and comparison with photoemission data [3], low-temperature transport properties [4], and competing pairing channels [5]. The possible magnetic states of the $\sqrt{5} \times \sqrt{5}$ Fe-vacancy arrangement will also be presented [6]. The experimental reports of local moments at room temperature leads to our most recent efforts employing a three-orbital spin-fermion model, analyzed via Monte Carlo simulations, to study the temperature dependence of the (anisotropic) conductance [7]. It is concluded that considerable progress has been made in the understanding of these materials in spite of their difficult range of intermediate couplings. However, the existence of several open problems will also be discussed.

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