Modeling of Fe pnictides: the Magnetic Order and Pairing Channels

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We use numerical methods - exact diagonalization and the variational cluster approach - to study a two-orbital model for Fe-pnictide superconductors, including onsite Coulomb interaction $U$ and Hund’s rule coupling $J$ [1]. Robust next-nearest neighbor hoppings stabilize the spin “striped” AF order for undoped clusters, in agreement with neutron scattering data. The ordered magnetic moment depends on $U$ and $J$, and we find a bad metal with small ordered moment at intermediate $U$, as observed experimentally. By adding two electrons to the undoped cluster, we identify three different pairings channels: An inter-orbital triplet at small $U$, which transforms as the $A_{2g}$ representation of the $D_{4h}$ group, an inter-orbital singlet transforming as $B_{2g}$ at the most realistic intermediate $U$, and an intra-orbital $A_{1g}$ singlet at large $U$. We compare the results to a three-orbital model including the $xy$ orbital in addition to the $xz$ and $yz$ orbitals. [1] M. Daghofer et al., arXiv:0805.0148, to appear in PRL.

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