

energy to the doublet but this, even if its population reduced from 6/5 by the crystal field, has larger critical U because of its degeneracy, certainly above the realistic value of the Coulomb repulsion in these materials. The other bands are pushed at still lower energies and will probably be populated by more than 6/5 particles.

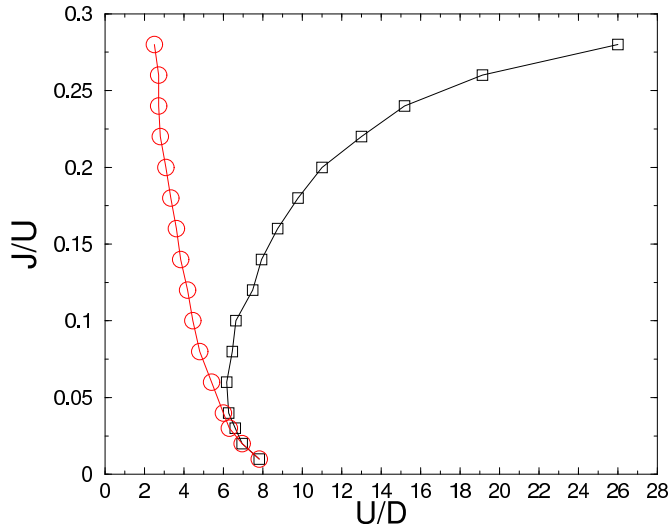


Fig. 2 Phase diagram (Slave-spin mean-field), as a function of U and J , of a 5-band model with four bands degenerate and one lifted by the crystal field so to be always half-filled. The other bands host the remaining 5 electrons. D is the half-bandwidth.

We did not enter in the realistic calculation with all the details of the crystal field splitting, this is left for further work. We only show here (figure 2) the phase diagram of the system with four degenerate bands and one lifted by the crystal field in the (1,5) populated phase. It is easy to see that as predicted the OSMP is more easy to trigger than in the previous case (Fig. 1 of Ref. [6]) due to the increased proximity to half-filling. Indeed a smaller critical J is found and also a smaller crystal field is enough to enter the OSMP.

We also notice that within our naive model and crude approximation the values estimated for the local interaction in the pnictides ($U \sim 2.7D$, $J/U \sim 0.1 \div 0.2$) fall very close to the border of the OSMT. In this regime, even if the zero-temperature transition has not happened yet, the renormalization of the electronic properties differs very strongly between the bands, the almost localized one having a very low coherence temperature compared to the others. Thus even if pnictides are not strictly in the zone of the phase diagram showing a selectively localized ground state (and even this has to be confirmed by more accurate methods in more realistic models), most probably they lie in a regime of selective localization at finite temperature.

4 Magnetic properties and comparison with experiments

A key quantity for the individuation of the OSMT in materials is the local spin susceptibility χ_{loc} . Indeed while the itinerant electrons will dominate the transport properties, the presence of a localized component will show up, thanks to the magnetic moments that form.

Dynamical mean-field theory allows a reliable calculation of this quantity. However the 5-band model under examination here requires a tremendous numerical effort to be tackled reliably by this technique. Here we just want to show some general features of the local magnetic susceptibility of a selectively localized phase, namely the dependence of the size of the local moment on the Hund's coupling J . In Fig.3 we show this dependence in a much simpler model, paradigmatic for the OSMT, of two bands with different bandwidth ($W_2 = 0.15W_1$), in which the narrower one gets localized by correlations while the wider one remains itinerant.

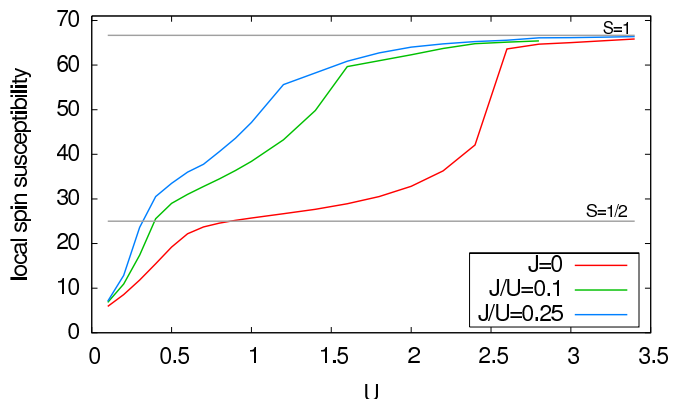


Fig. 3 Local magnetic susceptibility in the "classic" model for OSMT (2 bands of unequal bandwidth), as a function of U/D , for different strength of the Hund's coupling. It is easily seen that when $J > 0$ the local magnetic moment that develops in the selectively localized phase is bigger than the expected $S = 1/2$, and grows with J .

When a band gets localized the susceptibility goes from a Pauli-like to a Curie-like behaviour indicating the formation of free moments. As expected for an OSMT in Fig. 3 one sees a two stage saturation of the χ_{loc} signaling the partial localization followed by the complete Mott insulating state with magnetic moments corresponding to the high-spin atomic state.

One could naively expect that the value at which the χ_{loc} saturates upon entering the selective phase be the one for a local $S = 1/2$ moment. However the free moments in the OSMP are coupled to the itinerant electrons by the exchange interaction. As a result we see