31 Spin-Polarons in the FM Kondo Model

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Abstract. We show that holes doped into the FM Kondo model form independent FM spin-polarons with single holes inside, instead of showing phase separation. As a consequence there is a pseudogap in the DOS, which has been observed experimentally. Phase separation does appear at vanishing coupling J_{AF} of the corespins, where we also observe stripe-like configurations. At large J_{AF} and large doping, a flux phase appears. We present the phase diagram of this model in 2d.

Manganite compounds like $La_{1-x}Sr_xMnO_3$ and $La_{1-x}Ca_xMnO_3$ exhibit a very complex phase diagram involving, e.g., ferromagnetic (FM) metallic, FM insulating and different combinations of FM and AF behaviour in different lattice directions. They have been at the forefront of both experimental and theoretical research for a number of years [1]. One of the most striking effects is the so-called "Colossal Magneto-Resistance" (CMR), a fast change of resistivity as a function of magnetic field which occurs in part of the phase diagram and may lead to technical applications. The manganites have a perovskite lattice structure, similar to cuprates. The rich phase diagram is due to a complicated interplay of kinetic, spin, orbital, Coulomb, and Jahn-Teller lattice degrees of freedom, and has been a tremendous challenge for theoretical descriptions.

In Mn^{3+} the 3d orbitals are relevant. Three of them, called t_{2g}, are lower in energy and effectively form a spin-$\frac{3}{2}$ "corespin". Only one of the two higher e_g-orbitals is occupied. The simplest model which captures an essential part of the relevant physics is the FM Kondo model (double exchange model)

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - J_H \sum_i \hat{s}_i \cdot \hat{S}_i + J_{AF} \sum_i \hat{S}_i \cdot \hat{S}_i \tag{31.1}$$

in which lattice couplings and the second e_g-orbital have been neglected. The first term describes hopping of e_g electrons, the second is the Hund coupling to corespins, and the third the AF coupling among corespins. Because of strong Hund coupling J_H, the e_g-spins like to be almost parallel to the corespins which therefore tend to align ferromagnetically in the doped case. In the undoped case ($n = 1$) the corespins are AF. This model has been extensively investigated in the past, and has been claimed to show phase separation into a conducting hole-rich FM region and an AF insulator [1,2]. After consideration

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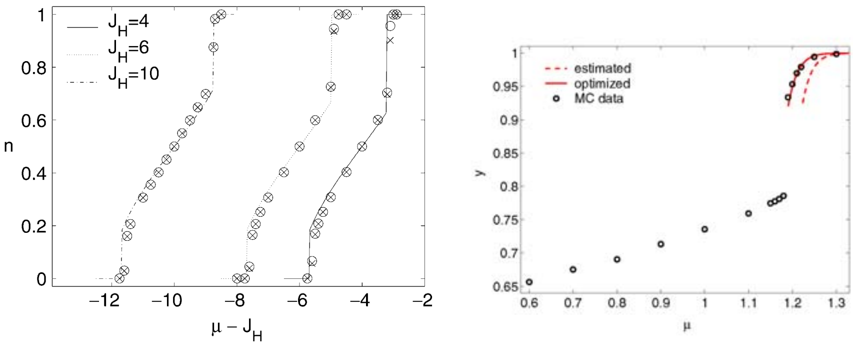

Fig. 31.1. Electron filling $n(\mu)$ for 1d (*left*) and 2d (*right*). The symbols denote MC-results

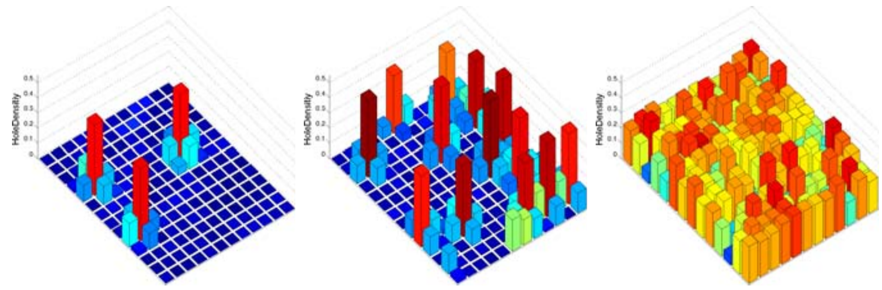

Fig. 31.2. MC snapshots of hole-density in 2d. AF-region (*left*), gap-region (*middle*), and the weakly FM-region (*right*)

of long range Coulomb repulsion, this gives rise to a model of "nanoscale phase separation" at the root of CMR [1,3]. We have, however, shown recently [4,5], that in 1d and 2d within physically relevant parameter ranges, there is instead a separation of individual holes into tiny FM regions, so-called spin-polarons, even without long-range Coulomb forces.

In our calculations, we first integrate out the high energy state in which the e_g electron has spin opposite to the corespin [6–8]. This is similar to the derivation of the tJ model from the Hubbard model. It results in an effective coupling $J_{\text{eff}} = J_{AF} + \frac{1}{2J_H}$. We can thus include effects of finite J_H without extra effort, instead of setting it to infinity as is often done. We treat the corespins as classical, which is justified because of their size [9,10]. $\hat{H}$ is then bilinear in e_g electrons and can be integrated. What remains is a classical Monte Carlo simulation over corespin configurations [2], for which we have used suitable updates and taken care to treat autocorrelations correctly [4,5,8]. In the following, we show results for physically relevant parameter values $\beta = 50, J_{AF} = 0.02$, and $J_H = 6$, with t as our unit of energy. The calculations were performed on a lattices of size 50 in 1d and 12×14 in 2d.

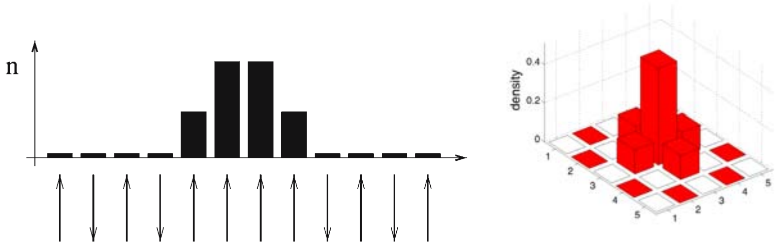

Fig. 31.3. Simple model for single-hole polarons in 1d (*left*) and 2d (*right*)

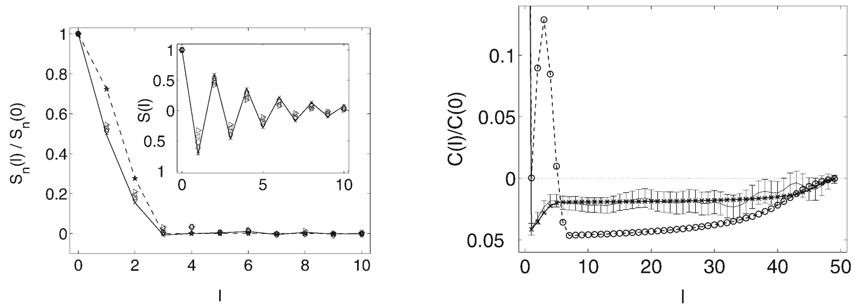

Fig. 31.4. *Left*: Dressed corespin-correlations for $1\ldots5$ holes in 1d. *Lines*: model polarons with perfect order (*dashed*) and in UHA (*solid*). *Inset*: spin-spin-correlation. *Right*: density correlations in 1d

In grand canonical simulations a jump in the electron filling $n(\mu)$ appears close to $n = 1$ (Fig. 31.1). This is usually interpreted as the above mentioned phase separation [2]. There are, however, strong indications against this interpretation, as we will now demonstrate.

One piece of evidence is the distribution of fermion occupation numbers in the simulations, which is smooth and broad in the FM region below the gap, but which is strongly peaked at integer electron occupations within the gap-region. Indeed, MC snapshots within the gap region (and above) do not show phase separation, but instead separated individual holes in a small FM corespin region, in which (in 2d) a single corespin is flipped with respect to the AF configuration (Fig. 31.2). These FM spin-polarons do not attract each other, but appear to occur at random positions.

We developed a simple model to describe such objects, as depicted in Fig. 31.3. Each polaron here contains a single hole and 3–5 FM corespin sites, embedded in an AF corespin background. In the simplest case, FM and AF order are taken to be perfect. This can be improved by the so-called Uniform Hopping Approximation (UHA) [8,11,12], wich uses constant angles between corespins in the FM resp. AF phases. Within this model, single-hole polarons

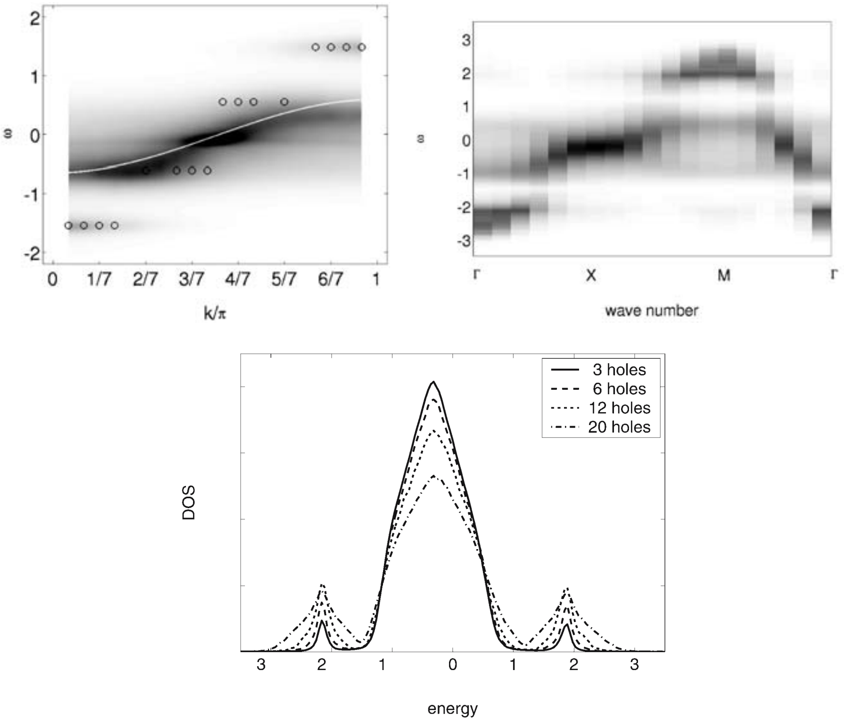

Fig. 31.5. Spectral function in 1d with 1 hole (*left*) and in 2d with 20 holes in the gap region (*middle*). *Right*: DOS in 2d for different dopings

turn out to be energetically favored over larger objects, except at very small J_{AF} (see below). At the critical chemical potential μ_c, the addition of another polaron costs no energy, which results in large fluctuations of the number of holes and can explain the jump in $n(\mu)$. We generated ensembles of such model polarons in random locations. Comparison with MC snapshots shows strikingly good agreement [5].

More quantitative evidence for *single*-hole polarons is shown in Fig. 31.4. On the left, the corespin-correlations $n_i^{\text{hole}}\ S_i \cdot S_j$ around a hole are seen to be almost independent of the number of holes. This is similar in 2d. On the right, the MC-data (bars) are perfectly described by single-hole polarons (solid line), but do not match at all the behavior of a bipolaron with two holes (dashed line).

The single-hole polaron of typically 4 sites in 1d is like a quantum mechanical well with just 4 states. The outermost of these states lie outside the band of the AF background (Fig. 31.5 left). Thus as a consequence of the small polaron, a symmetric *pseudogap* appears in the density of states, which has also been observed experimentally [13–16] and in previous calcula-

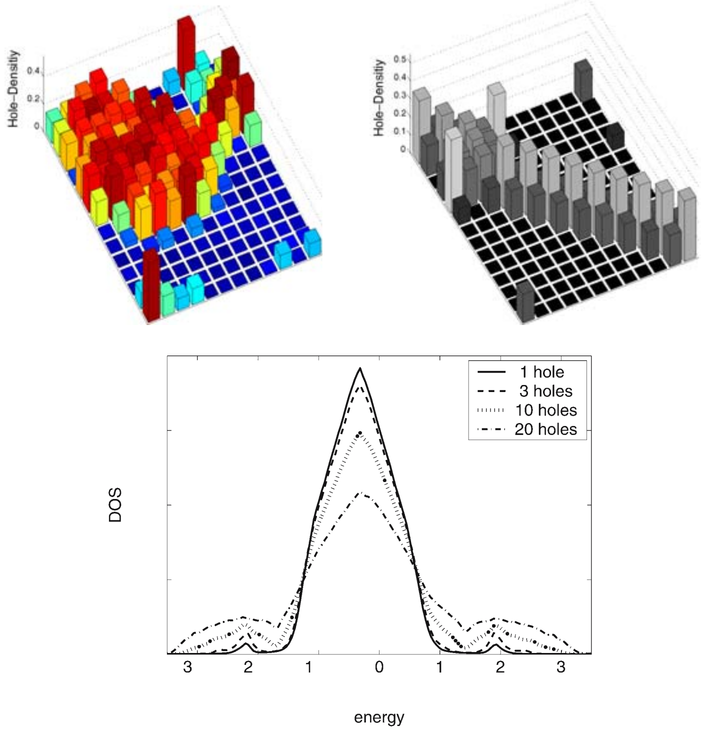

Fig. 31.6. $J_{AF} = 0$. Snapshots with phase separation (20 holes, *left*) and a stripe (11 holes, *middle*) at $\beta = 80$, both in the gap region. Closing of the pseudogap in the DOS (*right*, $\beta = 50$)

tions [1]. In 2d, the situation is similar. Additional holes go into more small polarons, and the pseudogap remains, independent of the number of holes, until the FM region is reached (Fig. 31.5 right). In fact, the transition from polaronic to FM behavior occurs when there is no more space for individual polarons.

The situation is different for $J_{AF} = 0$ (unphysical for the manganites), when there is less resistance to phase separated FM domains of corespins. We still see individual polarons, but at larger filling phase separation can occur now. As a consequence, the pseudogap fills up when the number of holes increases (Fig. 31.6). In addition, other exotic configurations occur at low temperature, like the stripe depicted in Fig. 31.6.

We have determined the phase diagram of the FM Kondo model in 2d (Fig. 31.7) at $\beta = 50$ and $\beta = 80$. For large J_{AF}, a so-called flux phase appears around $x = 1 - n = 0.5$ [17–19]. In the interesting doping range below about 20%, but with small J_{AF}, there is coexistence of polarons and

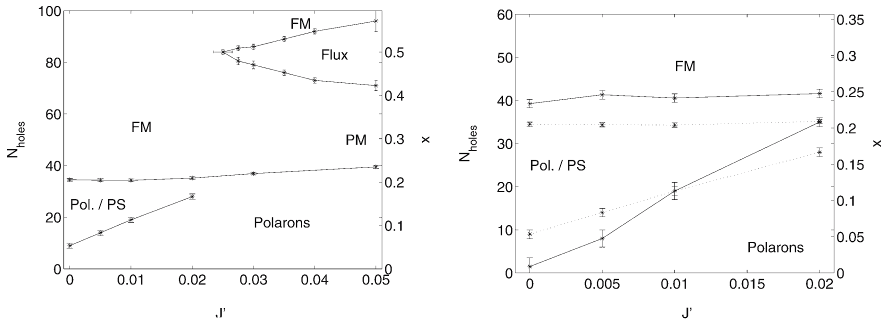

Fig. 31.7. Phase diagram in 2d, as a function of doping x (*right scale*) and AF coupling $J' \equiv J_{AF}$. *Left*: $\beta = 50$. *Right*: $\beta = 50$ (*dashed*) and $\beta = 80$ (*solid*) in a smaller range of parameters

phase separation, with strenghened phase separation for low temperature. For the likely physically relevant range $J_{AF} = 0.02 \ldots 0.05$, however, polarons become even stronger when the temperature is reduced. At the same time, the ferromagnetism of corespins in the FM/PM phase becomes weaker as J_{AF} rises.

In summary, we have shown strong evidence, from MC simulations of the FM Kondo model with classical corespins, that holes doped into the model do not phase separate, but instead form small individual FM polarons. This effect becomes even stronger at lower temperatures in the relevant range of couplings.

References

1. E. Dagotto, T. Hotta, A. Moreo: Phys. Rep. **344**, 1 (2001)
2. S. Yunoki *et al.*: Phys. Rev. Lett. **80**, 845 (1998)
3. T. Wu *et al.*: Phys. Rev. Lett. **86**, 5998 (2001)
4. W. Koller, A. Prüll, H.G. Evertz, W. von der Linden: Phys. Rev. B **67**, 174418 (2003)
5. M. Daghofer, W. Koller, H.G. Evertz, W. von der Linden: cond-mat/0312394, and in preparation
6. S. Yarlagadda, C.S. Ting: Int. J. Mod. Phys. B **15**, 2719 (2001)
7. S.-Q. Shen, Z.D. Wang: Phys. Rev. B **61**, 9532 (2000)
8. W. Koller, A. Prüll, H.G. Evertz, W. von der Linden: Phys. Rev. B **66**, 144425 (2002)
9. N. Furukawa, in: *Physics of manganites*, 1. edn. (Kluwer Academic Publishing, New York 1998)
10. E. Dagotto *et al.*: Phys. Rev. B **58**, 6414 (1998)
11. J. van den Brink, D. Khomskii: Phys. Rev. Lett. **82**, 1016 (1999)
12. W. Koller, A. Prüll, H.G. Evertz, W. von der Linden: Phys. Rev. B **67**, 104432 (2003)

13. D.S. Dessau *et al.*: Phys. Rev. Lett. **81**, 192 (1998)
14. T. Saitoh *et al.*: Phys. Rev. B **62**, 1039 (2000)
15. Y.-D. Chuang *et al.*: Science **292**, 1509 (2001)
16. J.H. Park *et al.*: Phys. Rev. Lett **76**, 4215 (1996)
17. H. Aliaga *et al.*: Phys. Rev. B **64**, 024422 (2001)
18. D.F. Agterberg, S. Yunoki: Phys. Rev. B **62**, 13816 (2000)
19. M.Y.W. Koshibae, S. Maekawa: Phys. Rev. Lett. **81**, 5604 (1998)