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Single-particle spectrum of the flux phase in the FM Kondo model

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Abstract

We investigate the 2D ferromagnetic Kondo lattice model for manganites with classical corespins at Hund's rule coupling $J_{\mathrm{H}}=6$, with antiferromagnetic superexchange $0.03 \leqslant J' \leqslant 0.05$. We employ canonical and grand canonical unbiased Monte Carlo simulations and find paramagnetism, weak ferromagnetism and the flux phase, depending on doping and on J'. The observed single-particle spectrum in the flux phase differs from the idealized infinite lattice case, but agrees well with an idealized finite lattice case with thermal fluctuations.

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The ferromagnetic Kondo lattice model is believed to describe the electronic degrees of freedom of compounds such as manganites. In these materials the spins of the itinerant electrons have a strong ferromagnetic coupling to localized corespins $\mathbf{S}_i$, leading to an effective spinless fermion (ESF) Hamiltonian [1]

$$\hat{H} = -\sum_{\langle i,j\rangle} t_{i,j}^{\uparrow\uparrow} c_i^\dagger c_j - \sum_{i,j} \frac{t_{i,j}^{\uparrow\downarrow}\, t_{j,i}^{\downarrow\uparrow}}{2J_{\mathrm{H}}} c_i^\dagger c_i + J' \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (1)$$

where $c_i^\dagger$ creates an electron at site i with its spin parallel to $\mathbf{S}_i$, and $J_{\mathrm{H}}=6$ throughout this work. The hopping of these spinless fermions is modulated by the factor $t_{i,j}^{\uparrow\uparrow} = \cos(\vartheta_{ij}/2)\mathrm{e}^{\mathrm{i}\psi_{ij}}$, which depends on the relative angles ϑ_{ij} of the two neighboring corespins and carries a complex phase ψ_{ij}. On a two-dimensional lattice, this complex phase leads to the so-called "flux phase" around half-filling of the lower Kondo band (doping $x=50\%$) [2]. While the system is ferromagnetic at half-filling for $J' \lesssim 0.025$, the flux phase has been shown [2] to be the ground state at half-filling for larger values of J'.

We performed canonical and grand canonical unbiased Monte Carlo simulations [3]. The

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magnetic phases can be observed in the corespin structure factor which is depicted in Fig. 1 for $J' = 0.05$. In the polaronic regime with high compressibility at $x \approx 18\%$ holes [3], only an AFM signal is visible. At $x \approx 24\%$, the compressibility is suddenly much reduced and the system becomes homogeneous but a small AFM peak persists. At $x \approx 28\%$ no magnetic structure at all is visible. The flux phase appears at $x \approx 44\%$ and $x = 50\%$ with signals at $(\pi, 0)$ and $(0, \pi)$. The only FM signal exists, weakly, at even larger doping $x \approx 62\%$.

Fig. 2 shows the normalized FM corespin moment $S(q=0) = |\sum_i \mathbf{S}_i|/L$ as a function of doping, where L is the number of lattice sites. It is expected to vanish in the flux phase. One sees that the doping range of the flux phase becomes smaller at smaller J'. The lattice then is weakly ferromagnetic at slightly lower doping $x \approx 40\%$. All our data are compatible with the existence of a flux phase in the region where $S(q=0) \simeq 0$.

The corespin structure in an idealized flux phase is depicted in Fig. 3(a). While all corespins are drawn parallel to the xy-plane for better visibility, a global rotation in spin space leads to equivalent configurations. In such corespin configurations, $|t_{i,j}^{\uparrow\uparrow}| = 1/\sqrt{2}$ is constant. However, the hopping carries a complex phase ψ_{ij}. Diagonalizing the ESF Hamiltonian for the four-site unit cell of the flux phase leads to the dispersion relation

$$\varepsilon(k_x, k_y) = -\frac{1}{J_\mathrm{H}} \pm \sqrt{2(\cos^2 k_x + \cos^2 k_y)}. \qquad (2)$$

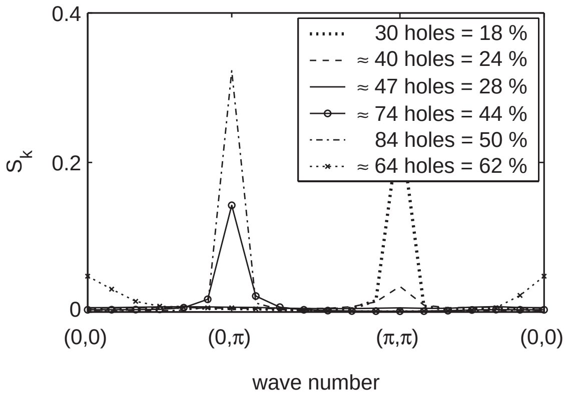

Fig. 1. Corespin structure factor for $J_\mathrm{H} = 6, \beta = 50$, $J' = 0.05$ and various doping levels. Simulations were done on a 12×14 lattice, i. e. for $L = 168$ lattice sites.

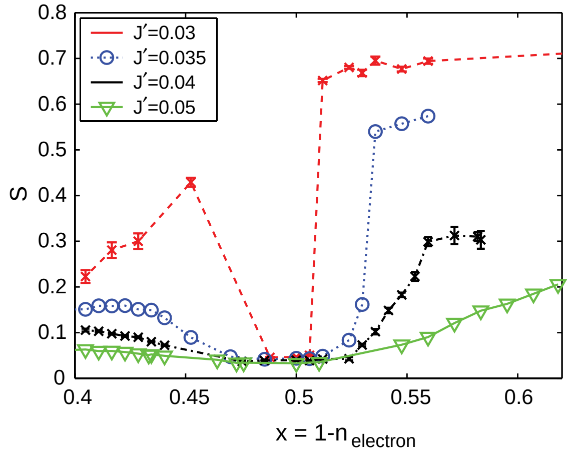

Fig. 2. FM corespin moment $S(q=0)$ as a function of doping for various values of J', remaining parameters as in Fig. 1.

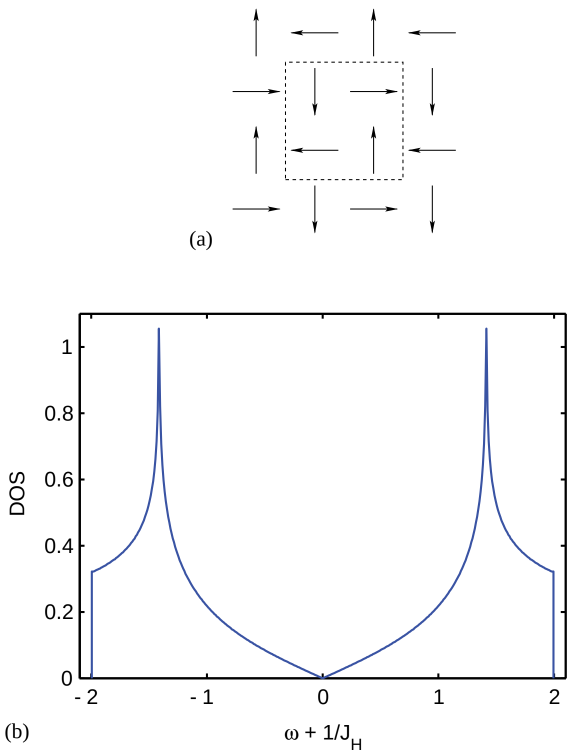

Fig. 3. Perfect flux phase: (a) schematic plot of the corespin configuration. The dashed square delimits the unit cell. All spins are drawn parallel to the xy-plane; (b) electronic DOS for the ESF Hamiltonian with $J_\mathrm{H} = 6$ on an infinite lattice.

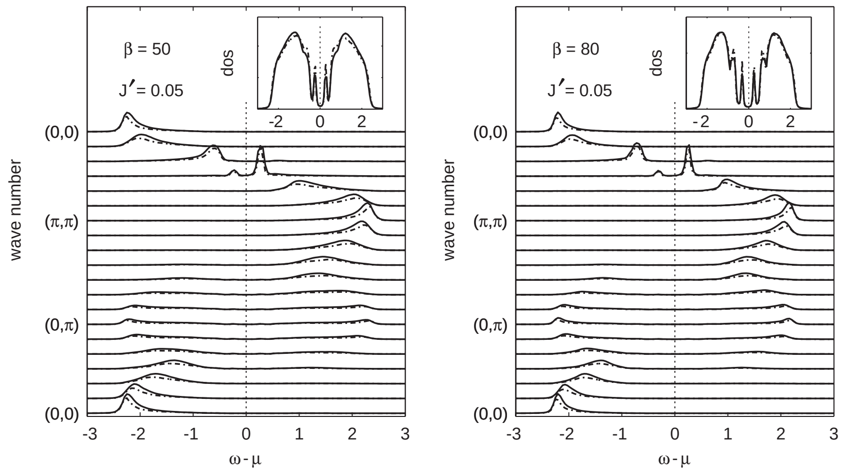

Fig. 4. Spectral density for the flux phase at half-filling for $J' = 0.05$, $\beta = 50$ (left) and $\beta = 80$ (right) on a 14×12-lattice. Dashed lines: MC results for the ESF model. Solid lines: ideal flux phase with random deviations.

The one-particle DOS of these bands for the infinite lattice with the corespins aligned in the perfect flux phase is depicted in Fig. 3(b); it features a pseudogap at half-filling. The dispersion and the DOS of the full Kondo model and for $J_H \to \infty$ can be found in Ref. [2].

The spectral density of the flux phase is subject to strong finite size effects, which are caused by the fact that only a very small part of the Brillouin zone contributes to the few states around the pseudogap at $(\pi/2, \pi/2)$. In order to ascertain that we did indeed observe the flux phase, we therefore compared our MC results to a model system. We started from a perfect flux phase configuration of the corespins on a finite lattice, added random perturbations, and diagonalized the resulting ESF Hamiltonian. The amount of fluctuations was chosen to fit the width of the peaks in the full MC results. Fig. 4 compares the average spectral density and the DOS thus obtained to MC simulations for the ESF model exhibiting almost perfect agreement, while there is a notable difference between the DOS in Fig. 4 and the idealized case in Fig. 3(b). The system can thus indeed be well described by thermal fluctuations about the flux phase on a finite lattice.

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References

[1] W. Koller, A. Prüll, H.G. Evertz, W. von der Linden, Phys. Rev. B 66 (2002) 144425.

[2] H. Aliaga, B. Normand, K. Hallberg, M. Avignon, B. Alascio, Phys. Rev. B 64 (2001) 024422;
D.F. Agterberg, S. Yunoki, Phys. Rev. B 62 (2000) 13816;
M. Yamanaka, W. Koshibae, S. Maekawa, Phys. Rev. Lett. 81 (1998) 5604.

[3] M. Daghofer, W. Koller, H.G. Evertz, W. von der Linden, J. Phys.: Condens. Matter 16 (2004) 5469.