Journal of Magnetism and Magnetic Materials 125 (1993) 368–370
North-Holland

The thermodynamic density of states of the Emery model

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The charge transfer gap caused by electron–electron correlation and the phase diagram of the Emery model is calculated within the Gutzwiller approximation. Contrary to the one-particle DOS the thermodynamic DOS shows the oxygen-like states detected in experiments.

1. Introduction

Due to its high degree of abstraction, the Emery model [1], developed for the description of the electronic structure of the CuO_2-plane in high-T_c superconductors, may serve as starting point to the understanding of electron–electron correlation in transition metal chalcogenides. In these materials Zaanen, Sawatzky, and Allen [2] stated a new kind of metal–insulator transition (MIT), which is of charge transfer type. Their phase diagram was confirmed by other authors [3]. On the contrary, Oleś and Zaanen [4], by applying the Gutzwiller approximation (GA), doubted the existence of a charge transfer gap at infinite U. Therefore, we first recalculated the phase diagram, coming from both the metallic and the insulating side to the transition, and second, we derived the thermodynamic density of states (TDOS), which is different from the one-particle DOS for correlated systems and gives an instructive insight to the MIT.

2. The Emery model in GA

We consider the following class of models:

$$H = -\Delta \sum_k \sum_\sigma d^+_{k\sigma} d_{k\sigma} + U \sum_i n_{\mathrm{D}i_\uparrow} n_{\mathrm{D}i_\downarrow} + t \sum_k \sum_\sigma V_k (d^+_{k\sigma} c_{k\sigma} + \mathrm{h.c.}), \qquad (1)$$

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where the $d^+_{i\sigma}$ and $c^+_{i\sigma}$ describe the creation of a hole at a d- and p-orbital respectively. Having in mind the Cu–O chains and plains found within the high-T_c cuprates, we associate the d-orbital with copper and the p-orbital with oxygen, and take for the k-dependence of the hybridization $V_k = -2\sin(k_x)$ and $V_k = 2(\sin^2 k_x + \sin^2 k_y)^{-1/2}$ respectively. The lattice constant is set to 1. After applying the GA, the diagonalization of the effective Hamiltonian

$$H_{\mathrm{eff}} = -\tilde{\Delta} \sum_k \sum_\sigma d^+_{k\sigma} d_{k\sigma} + t\sqrt{q} \sum_k \sum_\sigma V_k (d^+_{k\sigma} c_{k\sigma} + c^+_{k\sigma} d_{k\sigma}) \qquad (2)$$

remains, where the effective hopping matrix element is reduced by the square root of a factor q, which is

$$q = \frac{(n_{\mathrm{D}}/2 - d)\left(\sqrt{1 - n_{\mathrm{D}} + d} + \sqrt{d}\right)}{(n_{\mathrm{D}}/2)(1 - n_{\mathrm{D}}/2)}. \qquad (3)$$

Furthermore a renormalization $\tilde{\Delta} = \Delta + \lambda$ of the copper level has been introduced to fix the number of copper holes n_{D}. The diagonalization of H_{eff} yields

$$\langle H_{\mathrm{eff}} \rangle = 2 \sum_k^{\mathrm{occ.}} \sum_\nu E_\nu(k) \text{ with}$$

$$E_{1,2} = -\tilde{\Delta}/2 \mp \left(\tilde{\Delta}^2/2 + t^2 q V_k^2\right)^{1/2}. \qquad (4)$$

The number of occupied states and the number

of d-holes n_D can be determined from

$$n = \sum_{k}^{\text{occ.}} \sum_{\nu} 1 \quad \text{and} \quad n_D = -\left(\frac{\partial}{\partial \lambda} K\right). \tag{5}$$

The ground state energy can then be found via minimization of the energy $E = \langle H_{\text{eff}} \rangle + \lambda n_D + Ud$ with respect to n_D and d, yielding

$$\lambda = -\left(\frac{\partial}{\partial n_D} q\right)_d \left(\frac{\partial}{\partial q} K\right)_\lambda \quad \text{and}$$
$$n_D = -\left(\frac{\partial}{\partial d} q\right)_n \left(\frac{\partial}{\partial q} K\right)_\lambda . \tag{6}$$

By solving this system of equations we found a MIT due to vanishing d at $n_D = 1$. Such a transition occurs either at $n = 1$ or $n = 3$. To get the phase diagram, we look for a solution at $n = 1$ and small q. Expansion of eqs. (5) and (6) for $1 - n_D \ll 1$ and $d \ll 1$ gives the critical values Δ_c and U_c in dependence of the parameter $\nu = d/(1 - n_D)$:

$$\Delta_c = t\sqrt{B}\left(\sqrt{1+\nu} + \sqrt{\nu} + \frac{1}{\sqrt{1+\nu}}\right),$$
$$U_c = t\sqrt{B}\left(\frac{1}{\sqrt{\nu}} + \frac{1}{\sqrt{1+\nu}}\right). \tag{7}$$

Figure 1 shows the phase diagram. The critical values for $n = 3$ one gets from particle–hole symmetry. Since the Gutzwiller method is a variational procedure to give ground state properties like energy and densities, the effective one-particle Hamiltonian (2) should be considered as an

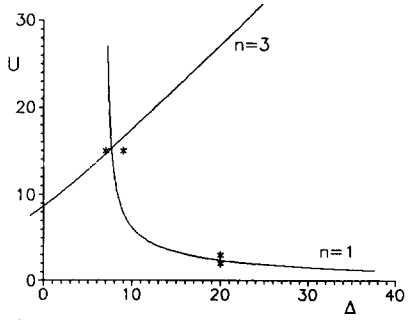

Fig. 1. Phase diagram for the Emery model. The energy unit is the p–d hopping integral.

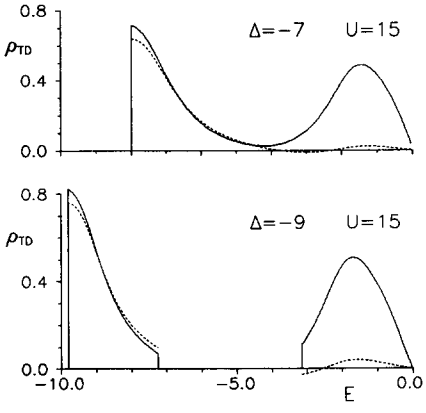

Fig. 2. TDOS (full line) and partial TDOS for d-holes (broken line) below and above the charge-transfer critical Δ_c for $U = 15$.

intermediate result and is not directly related to the one-particle density of states. It gives every time only two bands, independently if a correlation gap exists or not, also the correlation gap E_g is not visible in eq. (2). But it is possible to calculate the so called thermodynamic density of states (TDOS) ρ_{TD}, which is defined via the ground state energy E and the total electron density n by means of $\rho_{TD} = dn/d\mu$, with $\mu = dE/dn$. The TDOS coincides with the one-particle DOS if there is no electron interaction, but can differ from it up to a large amount in the general case. The correlation gap will be shown by the TDOS in a correct way. In the case of doping the Cu–O system, it is of interest, whether the additional holes go to oxygen or copper sites. To answer this question, we calculate the quantity $\rho_{d,TD} = dn_D/d\mu$, which has the dimensions of a DOS and therefore should be called a "partial TDOS". Figures 2 and 3 show the two different ways in which the MIT will take place. For this end we calculated ρ_{TD} and $\rho_{d,TD}$ at the points marked by stars in fig. 1, for the CuO_2 plane. For the one-dimensional case we refer to ref. [5]. Below the transition, shown in fig. 2, we find a broad band. The states at the bottom of this band are nearly d-like whereas the states at the top are mainly of p-character. In the midst of the band, where the TDOS is relatively low, the partial TDOS of the d-holes becomes negative. It

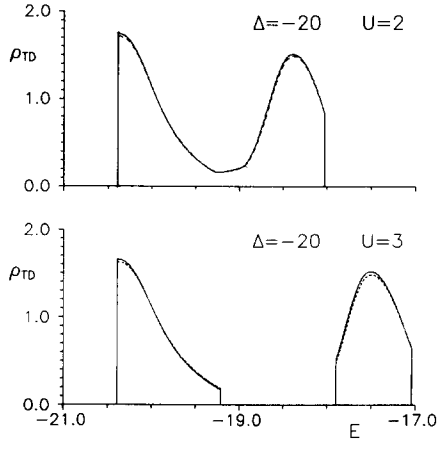

Fig. 3. TDOS (full line) and partial TDOS for d-holes (broken line) below and above the critical U_c for $\Delta_c = 20$.

looks like a gap smeared out with oxygen states. Also in the isolating region, if the lower band is filled with holes and we dope further, the next holes go to the oxygen sites. This agrees well with experimental results [6]. It seems that the GA reflects the singlet states predicted by alternative investigations of eq. (1), but in the smeared form of a tail below the main oxygen band. For larger values of Δ the correlation splitting is like that of the Hubbard model. This is demonstrated in fig. 3, where the opening of the Hubbard–Mott gap is illustrated.

3. Conclusion

It seems that the GA describes the crossover from the charge transfer to the Hubbard–Mott regime quite well, and also some spectroscopical data may be understood. Nevertheless the GA results have to be handled with care, due to the reasons discussed in ref. [5]. Especially the critical values are much higher than usually accepted for the cuprates. Recent Monte Carlo calculations predict a critical value Δ_c between $2t$ and $3t$ for $U = 6t$ [7]. This discrepancy may be due to the mean field character of the GA, since an analogous situation is well known from other mean field theories. Last we want to mention the negative partial TDOS of the d-states in fig. 2, which hints to an instability of the d-subsystem. In our case a negative $\rho_{d,TD}$ means that with increasing chemical potential the number of states in the d-subsystem will be reduced, since due to renormalization effects it will become more efficient for the whole system to fill the weak correlated p-like states instead of increasing the number of strongly correlated d-like holes.

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