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The Magnetic Phase Diagram of the Emery Model within the Hartree-Fock Approximation

By

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The Hartree-Fock approximation is applied to investigate the ferromagnetic, antiferromagnetic, and paramagnetic phases of the Emery model. The phase diagram in dependence on copper correlation and hole doping is calculated by comparing the total energy in the one-dimensional case. The transition from the antiferromagnetic to the paramagnetic phase with increasing doping is only found for relatively small values of the correlation. In the other cases a transition to ferromagnetism is obtained.

Die Hartree-Fock-Näherung wird angewandt, um die ferro-, antiferro- und paramagnetischen Phasen des Emery-Modells zu untersuchen. In Abhängigkeit von der Kupferkorrelation und der Löcherdotierung wird das Phasendiagramm berechnet, indem die Gesamtenergie im eindimensionalen Fall verglichen wird. Der Übergang von der antiferromagnetischen zur paramagnetischen Phase mit zunehmender Dotierung wird nur für relativ kleine Werte der Korrelation gefunden. In anderen Fällen wird ein Übergang zum Ferromagnetismus erhalten.

1. Introduction

The discovery of high-T_c superconductors [1] stimulated a great amount of experimental and theoretical studies. Very soon after this discovery, Shirane et al. [2] found experimentally an antiferromagnetic ordering of the undoped materials. That is in contrast with ordinary band-structure calculations [3] which predict a metallic behaviour. The reason for this discrepancy is the strong electron correlation U at the copper sites. A realistic model to describe the highly correlated copper oxygen plane has been given by Emery [4]. Oleš and Zaanen [5] applied the Hartree-Fock approximation (HFA) and the Gutzwiller approximation to study the magnetic structure of this model. In qualitative agreement with the experiment they found a transition from the antiferromagnetic to the paramagnetic state with increasing doping.

The model proposed by Emery is an extended three-band Hubbard model. Its behaviour is believed to be similar to the original Hubbard model [6]. But there, besides the antiferromagnetic behaviour at half filling, we find a strong tendency towards ferromagnetism. That is mostly pronounced at $U \to \infty$ where already one electron away from half filling gives rise to a transition from the antiferromagnetic to the ferromagnetic phase according to the Nagaoka theorem [7]. This tendency is also displayed within the magnetic phase diagram of the one-band Hubbard model calculated within the HFA [8] or the Gutzwiller approximation [9]. Therefore, it is tempting to test this ferromagnetic phase also in the Emery model.

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In the present paper we fill this gap and calculate the magnetic phase diagram of the Emery model including the antiferromagnetic, ferromagnetic, and paramagnetic states. We calculate this phase diagram within the HFA by comparing the energy of these three phases. Like in every mean field approximation, one can expect that the results are not very sensitive to the dimension of the problem. Therefore, we restrict our calculation in the following to the one-dimensional model. But we expect similar results also in higher dimensions.

2. Hartree-Fock Approximation in the Antiferromagnetic Case

We consider the Emery model in the hole picture. The operator $d_{j\sigma}^{+}$ describes the creation of a hole in the copper d-orbital and the operator $c_{m\sigma}^{+}$ the creation of a hole in the oxygen p-orbital. The energy scale is chosen such that the energy level of the oxygen orbital ε_{P} is zero. The Hamiltonian has then the following form:

$$H = \varepsilon_{\mathrm{D}} \sum_{j=1}^{L} \sum_{\sigma} d_{j\sigma}^{+} d_{j\sigma} + t \sum_{\langle j,m \rangle} \sum_{\sigma} (d_{j\sigma}^{+} c_{m\sigma} + \text{h.c.}) + U \sum_{j=1}^{L} d_{j\uparrow}^{+} d_{j\uparrow} d_{j\downarrow}^{+} d_{j\downarrow} , \tag{1}$$

where $\langle j, m \rangle$ means the sum over next neighbours in the alternating chain of oxygen and copper. This chain has a length of $2L$ atoms. The undoped case corresponds to one hole in the elementary cell and we will consider hole numbers l between one and two.

We decouple the interaction term by using the HFA. But we get different one-particle problems if we assume the antiferromagnetic or the ferromagnetic state. In the antiferromagnetic state the magnetization at the copper sites alternates,

$$m = (-1)^{j} (\langle d_{j\uparrow}^{+} d_{j\uparrow} \rangle - \langle d_{j\downarrow}^{+} d_{j\downarrow} \rangle) . \tag{2}$$

That gives rise to an alternating effective potential with different signs for spin up and spin down. The effective one-particle Hamiltonian has the following form:

$$H_0 = \sum_{j=1}^{L} \sum_{\sigma} (\bar{\varepsilon}_{\mathrm{D}} + v_{j\sigma}) d_{j\sigma}^{+} d_{j\sigma} + t \sum_{\langle j,m \rangle} \sum_{\sigma} (d_{j\sigma}^{+} c_{m\sigma} + \text{h.c.}) \tag{3}$$

with

$$\bar{\varepsilon}_{\mathrm{D}} = \varepsilon_{\mathrm{D}} + \frac{U}{2} n , \qquad n = \langle d_{j\uparrow}^{+} d_{j\uparrow} \rangle + \langle d_{j\downarrow}^{+} d_{j\downarrow} \rangle$$

and

$$v_{j\sigma} = \sigma (-1)^{j} v , \qquad v = \frac{U}{2} m , \qquad \sigma = \pm 1 .$$

It is sufficient to consider only one spin component. For it the Hamiltonian (3) gets the following form after Fourier transformation:

$$H_0 = \sum_{k=-\pi/4}^{\pi/4} (d_{k\uparrow}^{+} c_{k\uparrow}^{+} d_{k+Q\uparrow}^{+} c_{k+Q\uparrow}^{+}) \begin{pmatrix} \bar{\varepsilon}_{\mathrm{D}} & v_k & v & 0 \\ v_k & 0 & 0 & 0 \\ v & 0 & \bar{\varepsilon}_{\mathrm{D}} & v_{k+Q} \\ 0 & 0 & v_{k+Q} & 0 \end{pmatrix} \begin{pmatrix} d_{k\uparrow} \\ c_{k\uparrow} \\ d_{k+Q\uparrow} \\ c_{k+Q\uparrow} \end{pmatrix} \tag{4}$$

with

$$v_k = 2t \cos k \quad \text{and} \quad Q = \pi/2 ,$$

the distance between neighbouring atoms has been chosen to be unity. In (4) the sum over the possible k-values goes from $-\pi/4$ to $\pi/4$, since the elementary cell consists of four atoms due to the magnetic structure. To calculate the magnetization m and the copper occupancy n self-consistently we look for the minimum of the total energy E with respect to these two parameters,

$$\frac{\partial E}{\partial n} = 0\,, \qquad \frac{\partial E}{\partial m} = 0\,. \tag{5}$$

The total energy E contains a contribution from the sum over all occupied eigenvalues of (4) $\langle H_0 \rangle$ and an operatorless contribution proportional to U,

$$\frac{E}{L} = \frac{2}{L}\langle H_0 \rangle - \frac{U}{4}(n^2 - m^2)\,. \tag{6}$$

From the conditions (5) one finds with (4) and (6) the following fix-point equations for the values of n and m:

$$n = \frac{4}{L}\left\{\sum_{k=0}^{\pi/4}((\varphi_{k11})^2 + (\varphi_{k13})^2) + \sum_{k=k_F}^{\pi/4}((\varphi_{k21})^2 + (\varphi_{k23})^2)\right\},$$

$$m = \frac{4}{L}\left\{\sum_{k=0}^{\pi/4}(-2\varphi_{k11}\varphi_{k13}) + \sum_{k=k_F}^{\pi/4}(-2\varphi_{k21}\varphi_{k23})\right\}, \tag{7}$$

where the Fermi momentum is simply given by

$$k_F = (2 - l)\,\pi/4\,. \tag{8}$$

In (7) $\varphi_{k\alpha i}$ denotes the i-th component of the α-th eigenvector (ordered with increasing eigenvalue) of the 4×4 matrix in (4) with fixed k. The number of k-values between 0 and $\pi/4$ which occur in the sum (7) is equal to $L/4$.

Equations (4) and (7) constitute a self-consistent set of equations which has been solved numerically. In the undoped system $l = 1$ the Fermi momentum (8) lies at the magnetic zone boundary. Therefore, at this point antiferromagnetism is favorable at every nonzero U in one dimension. For finite doping and in higher dimensions one finds a finite m only above a critical value U_c of U.

3. Ferromagnetic Case

Let us discuss the ferromagnetic case. Now the magnetization m is homogeneous,

$$m = \langle d_{j\uparrow}^{+} d_{j\uparrow} \rangle - \langle d_{j\downarrow}^{+} d_{j\downarrow} \rangle \tag{9}$$

in contrast to (2). Then the Hartree-Fock decoupling of (1) gives a one-particle Hamiltonian like in (3) for every spin direction σ with the effective potential

$$\bar{\varepsilon}_D + v_{j\sigma}\,, \qquad v_{j\sigma} = \sigma v\,. \tag{10}$$

After Fourier transformation we obtain

$$H_0 = \sum_{k=-\pi/2}^{\pi/2} \sum_{\sigma} (d_{k\sigma}^{+} c_{k\sigma}^{+}) \begin{pmatrix} \bar{\varepsilon}_\sigma & v_k \\ v_k & 0 \end{pmatrix} \begin{pmatrix} d_{k\sigma} \\ c_{k\sigma} \end{pmatrix} \tag{11}$$

with

$$\bar{\varepsilon}_\sigma = \varepsilon_D + \frac{U}{2}(n + \sigma m).$$

Please note that now, in contrast to (4), the k-values range from $-\pi/2$ to $\pi/2$. The matrix in (11) can be diagonalized very easily. That gives two eigenvalues

$$\varepsilon_\sigma^{\pm}(k) = \frac{\bar{\varepsilon}_\sigma}{2} \pm \sqrt{\frac{\bar{\varepsilon}_\sigma^2}{4} + v_k^2} \tag{12}$$

for every value of k and σ. The occupation of spin up $n_\uparrow = (n + m)/2$ and spin down $n_\downarrow = (n - m)/2$ can be calculated by minimizing the energy in analogy to (5). That gives

$$n_\sigma = \frac{1}{2L} \sum_{k=-k_{F\sigma}}^{k_{F\sigma}} \left(1 - \frac{\frac{\bar{\varepsilon}_\sigma}{2}}{\sqrt{\frac{\bar{\varepsilon}_\sigma^2}{4} + v_k^2}} \right), \tag{13}$$

where the Fermi momenta $k_{F\sigma}$ are determined by the two conditions

$$\varepsilon_\uparrow^-(k_{F\uparrow}) = \varepsilon_\downarrow^+(k_{F\downarrow}) \qquad \text{and} \qquad k_{F\uparrow} + k_{F\downarrow} = l\pi/2 . \tag{14}$$

The numerical, self-consistent solution of (11) and (13) gives a ferromagnetic solution if the correlation exceeds a critical value U_c which is nonzero for every parameter value, different from the antiferromagnetic case. In the case of two magnetic solutions we must decide which of them is more stable. This can be done by comparing the ground state energies, which gives the phase diagram presented in Fig. 1.

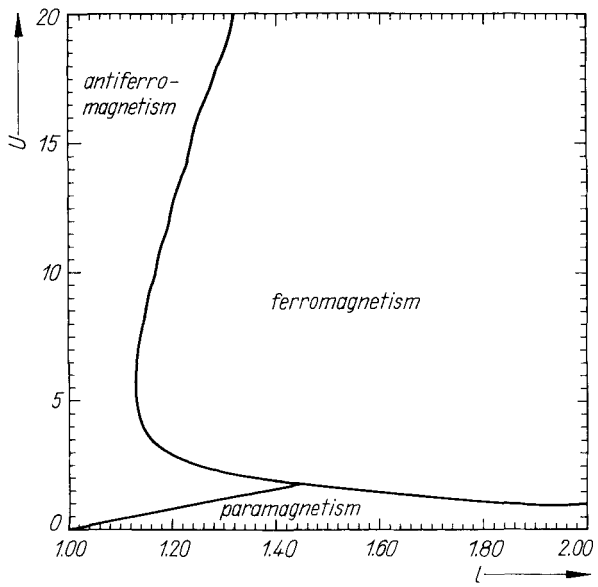

Fig. 1. The magnetic phase diagram of the Emery model for $t = 1$ and $\varepsilon_D = -3$

4. Discussion of the Phase Diagram

The most important features of the phase diagram are the following: With increasing hole doping the antiferromagnetic state becomes unstable. In addition to the already known transition to the paramagnetic state [5] we find also the transition to the ferromagnetic state for larger U. It is interesting to note that paramagnetism occurs in the rather small region $U < 1.5t$. The width of the antiferromagnetic region has a minimum at $U \approx 5t$. That resembles the results of [9] which have been used to explain the much larger region of antiferromagnetism in electron doped superconductors in comparison with hole doped ones [10]. It is also interesting that the width of the antiferromagnetic state increases with increasing U in Fig. 1. But one should expect a newly decrease for still larger U.

The occurrence of the ferromagnetic state can be understood not only from the analogy to the one-band Hubbard problem, but also from a Schrieffer-Wolff transformation in the charge fluctuation region $U \gg t, |\varepsilon_D| \gtrapprox t$ [11] or in the spin fluctuation region $U \gg t, |\varepsilon_D| \gg t$ [12]. Since the results agree qualitatively, we discuss in the following the charge fluctuation region [11]. The Schrieffer-Wolff transformation gives an antiferromagnetic exchange of fourth order between neighbouring Cu spins $\boldsymbol{S}_i$,

$$2 \frac{t^4}{U(U + \varepsilon_D)^2} \boldsymbol{S}_i \boldsymbol{S}_j , \tag{15}$$

which is responsible for the antiferromagnetism. But there exists also an antiferromagnetic exchange of second order between neighbouring copper $\boldsymbol{S}_i$ and oxygen spins $\boldsymbol{s}_m$,

$$2 \frac{t^2}{(U + \varepsilon_D)} \boldsymbol{S}_i \boldsymbol{s}_m . \tag{16}$$

This term can work only if some oxygen states are filled, i.e. it becomes important with increasing doping and gives rise to a ferromagnetic coupling between neighbouring copper spins.

The applicability of the HFA can be discussed using the analogy to the Hubbard model where a lot of work has already be done. According to this analogy one expects improved methods to give a reduced critical concentration and a reduced region of ferromagnetism. A first reduction is achieved already by the Gutzwiller approximation [9] which is also a mean field method but deals much better with the charge degrees of freedom. The next step could be the inclusion of local magnetic moments by the cluster Bethe lattice method [8, 9]. Further it would be interesting to test the unrestricted HF [13, 14] which has a great amount of possible solutions. All these methods show a reduced region of ferromagnetism especially for large doping. Instead of the ferromagnetic solution one finds paramagnetic states with difficult short-range order. For a better comparison with the experiments it would be interesting to apply these methods also to the more realistic Emery model.

In conclusion we have shown that the phase diagram of the Emery model has a large region of ferromagnetism within the Hartree-Fock approximation. Due to the known imperfections of the HFA it is an open question if this ferromagnetic long-range order survives in an exact phase diagram or if we found only some hints for a possible short-range ferromagnetic correlation.

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