Properties of the $t$-$J$ Model in the Dynamical Mean Field Theory: One-Particle Properties in the Antiferromagnetic Phase

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Abstract

We study the one-particle properties of the $t$-$J$ model within the framework of Vollhardt’s dynamical mean field theory. By introducing an $AB$ - sublattice structure we explicitly allow for a broken symmetry for the spin degrees of freedom and are thus able to calculate the one-particle spectral function in the antiferromagnetic phase. We observe surprisingly rich structures in the one-particle density of states for $T < T_N$ at finite doping up to 15%. These structures can be related to the well known results for one single hole in the Néel background. We are thus able to establish the relevance of this at a first sight academic limit to physical properties of the $t$-$J$ model with a finite density of holes in the thermodynamical limit.

Keywords: $t$-$J$ model, dynamical mean field theory, antiferromagnetism
1 Introduction and Model

From the very beginning of the investigation on the properties of the high-temperature superconductors [1] it was obvious that strong local correlations together with long-ranged antiferromagnetic (AF) exchange play an important role for the understanding of the anomalous normal state properties of these materials [2]. Several models of strongly correlated electrons have been proposed since then to describe the essential physics of the cuprates [3]. The most common ones are the one- and three-band Hubbard model [4, 5] and the $t$-$J$ model [6]. The latter is the most basic one taking into account explicitly both the strong local correlations and the magnetic interactions among itinerant electrons. It can be viewed as as an effective model describing essentially the low energy physics of the more general Hubbard models in the strong coupling limit [7, 8, 6].

Using standard notation, the Hamiltonian of the $t$-$J$ model reads

$$H_{t-J} = -t \sum_{<ij>\sigma} \tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j), \tag{1}$$

where $<ij>$ denotes the sum over nearest neighbours only and $\tilde{c}^\dagger_{i\sigma} = (1 - n_{i,-\sigma})c^\dagger_{i\sigma}$ creates an electron at site $i$ with spin $\sigma$ if and only if this site is unoccupied. Due to the constraint of no double occupancy imposed by the projected single-particle operators the hopping term is already nontrivial and contains strong correlation effects. The second term describes the AF exchange coupling of spins at nearest neighbour sites, denoted by the operators $\vec{S}_i$ and $\vec{S}_j$ respectively. The $n_i n_j$-term appears in the strong coupling expansion of the Hubbard model. We will drop it because it does not directly affect the magnetic properties we are interested in.

There is a large amount of knowledge about this model for the very special case of only one hole moving in an AF background (see e.g. [9, 10, 11, 12, 3] and references therein.) This limiting case proved to be of special interest since it could be solved exactly for $d = \infty$ [13]. The most important physical aspect is that the moving hole feels a binding potential growing linearly with the distance from its starting point due to the disturbance of the AF background during its motion [3]. This linear potential leads to a sequence of discrete poles as spectrum for the one particle excitations with a distinct dependence on $J/t$ [10, 13]. This rather simple picture appears to remain valid even for finite-dimensional systems [3].
when transverse spin fluctuations are important. In order to compare with experiments it is equally important to study the case of quasiparticle motion away from half filling at finite temperatures. To our knowledge so far no results are available for this case in the thermodynamic limit.

Here we want to study this situation in the framework of a dynamical mean field theory (DMFT), which is known to become exact in the limit of infinite spatial dimensions. This approach provides an extension of the work of Strack and Vollhardt [13] for one hole to the more general situation described above. We find a multi-peak structure in the spectral functions that can be related straight forwardly to the discrete spectrum of the one hole case.

The paper is organized as follows. We give a short review of our method and notation in the next section. In Sec.3 the possible evaluation of a magnetic phase diagram is considered. Sec.4 shows resulting spectral functions and the first part of their interpretation. A brief review on the physics of one hole in the fully polarized AF state together with an interpretation of the results from section 4 in connection with this picture is then given in Sec.5, before the concluding remarks of Sec.6 summarize the paper.

2 Method

The ideas of the DMFT for correlated electrons on a lattice are based on the substantial simplifications found in the limit of infinite dimensions [14]. The most striking consequence of the $d=\infty$-limit concerns the irreducible one-particle selfenergy $\Sigma_{\sigma}(k, z)$, which is due to the Coulomb interaction in Hubbard-like models. This quantity becomes purely local, i.e. it looses all $k$ dependence in the limit $d=\infty$ [15, 16]. Nevertheless it keeps a highly nontrivial behaviour as a function of frequency.

In order to perform the limit $d \to \infty$ systematically the hopping matrix element $t$ has to be rescaled by

$$t = \frac{t^*}{2\sqrt{d}},$$

with a constant $t^*$ [14]. We will chose $t^* = 1$ as the unit of energy. For a simple hypercubic lattice with nearest-neighbour hopping only the bare density of states is then found to be a
Gaussian:
\[ \rho_0(\varepsilon) = \frac{1}{\sqrt{\pi}} e^{-\varepsilon^2}. \] (3)

Besides \( t \), also the next neighbour exchange interaction \( J \) (which is proportional to \( t^2/U \)) has to be rescaled according to
\[ J = \frac{J^*}{2d}. \] (4)

It is well known that this type of interaction becomes trivial for \( d \to \infty \) in the sense that the Hartree approximation becomes exact [17, 16]. In our case this means that the spin-interaction has to be treated at the mean field level:
\[ J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \to J \sum_{<ij>} (<\vec{S}_i \cdot \vec{S}_j> + <\vec{S}_i \cdot \vec{S}_j> + <\vec{S}_i \cdot \vec{S}_j>) \] (5)
\[ \to 2J \sum_{<i,j>} S^z_i < S^z_j >, \] (6)
for a polarization in \( z \)-direction. Here \( 2 < S^z_j > = < n^\uparrow_j - n^\downarrow_j > \) [18]. Obviously \( < S^z_j > \) vanishes in the paramagnetic phase and in this case the \( t-J \) model for \( d=\infty \) is equivalent to the \( U=\infty \) Hubbard model.

Here we are interested mainly in the one-particle properties of the \( t-J \) model (1) in the antiferromagnetic state, i.e. when \( < S^z_j > \neq 0 \). To allow for such a solution we must provide a small symmetry-breaking field and in addition formulate all quantities on an A-B lattice [19]. Note that the use of two sublattices does not affect the locality of the self energies! Hence, the one-particle Green’s function may be represented as a matrix on the sublattices of the form
\[ G_\sigma(k, z) = \left( \begin{array}{cc} \zeta^A_\sigma & -\varepsilon_k \\ -\varepsilon_k & \zeta^B_\sigma \end{array} \right)^{-1}. \] (7)

For simplicity we introduced the abbreviation \( \zeta^{A/B}_\sigma = z + \mu - \Sigma^{A/B}_\sigma(z) + h^{A/B}_\sigma \) with the local selfenergies \( \Sigma^{A/B}_\sigma(z) \) and the staggered magnetic field \( h^{A/B}_\sigma = \frac{1}{2}J^*\sigma(< n^B_A - n^B_A >) \), which results from the exchange interaction (3) on a hypercubic lattice.

The local Green’s function is obtained by summing over \( k \) with the result
\[ G^{A/B}_\sigma(z) = \int d\varepsilon \frac{\zeta^{B/A}_\sigma}{\zeta^{A/B}_\sigma - \varepsilon^2} \rho_0(\varepsilon). \] (8)
Due to the additional symmetry \[ \text{(9)} \]

\[
G^A_{\sigma}(z) = G^B_{\sigma}(z)
\]
it is sufficient to perform the calculations for the A-sublattice only and to use the spin index for the bookkeeping.

The actual calculation is a straightforward extension of the method used for the paramagnetic phase \[ \text{(20), (21), (22)} \]. Due to the local nature of the selfenergies it is possible to reduce the solution of the lattice problem to that of a single site impurity problem with local energy \( \varepsilon_{\sigma} - \mu \) = \( - (\mu + h_{\sigma}) \) in contact with an effective medium described by a Green’s function \( G_{\sigma}(z) \). The latter contains all contributions from the local correlations except for those at the impurity site, i.e.

\[
G_{\sigma}^{-1}(z) = G_{ii,\sigma}^{-1}(z) + \Sigma_{\sigma}(z).
\]

This equation relates the Green’s function of the effective medium to the local Green’s function \( G_{ii,\sigma}(z) \) defined by \((8)\). The remaining atomic problem is solved by using the resolvent method \[ \text{(23), (24)} \] and the so-called Non Crossing Approximation (NCA) \[ \text{(24), (21)} \], from which we obtain the self energies of the effective impurity problem. Numerically exact methods like e.g. Quantum Monte Carlo are not available for this particular problem due to the fact that we actually have to solve an impurity Anderson model with \( U = \infty \) \[ \text{(25)} \]. Thus, taking the impurity self energy as new approximation for the local self energies of the lattice problem \( \text{(8)} \), we are able to determine \( \Sigma_{\sigma}(z) \) selfconsistently by iteration. For details of this procedure see e.g. \[ \text{(21)} \].

3 Phase diagram

In the following we are interested in solutions in the AF state. Therefore we choose slightly different starting conditions for up and down spins in our iteration procedure and look for solutions with a finite order parameter \( < S^z > \), which is nonvanishing only in the AF phase. There are of course other methods for obtaining the phase boundary, such as calculating the free energies for the para- and AF-solutions or the susceptibility of the \( t-J \) model. A detailed discussion of the static magnetic properties following from the susceptibility will be presented in a forthcoming publication \[ \text{(26)} \].
As it turns out, the task to calculate the complete magnetic phase diagram of the $t$-$J$ model as function of temperature, doping, and $J/t$ using the method outlined in the previous section cannot be performed for the following reasons. First, the self-consistency cycle for the order parameter $< S^z >$ converges extremely slow close to the phase boundary. Second, we could not set a reasonable boundary for $< S^z >$ below which one may safely assume that one is indeed in the paramagnetic phase and not in the AF but with only a very small staggered magnetization. The latter uncertainty for example leads to a comparatively large error in the exact position of the phase boundary. We thus rest content with comparing a few points of the phase diagram obtained with the present calculations to the more accurate results obtained from the staggered susceptibility [26]. This is done in Fig. 1, where we show results for the critical $J$ as function of $T$ at fixed $n$. Evidently both methods lead within the error bars to the same values of $J_c$, as was to be expected.

Figure 1: Phase diagram $J_c(T, \delta)$ as function of $T$ for $n = 0.98$. The full line represents a fit to the results from a calculation of the staggered susceptibility [26]. These are compared with our data points, which are marked by triangles if $|n_{\uparrow} - n_{\downarrow}| > 0.0001$ and by stars otherwise.
4 Spectral functions

We now concentrate on the behaviour of the spectral function

\[ A_{\sigma}(\omega) = -\frac{1}{\pi} \text{Im} G_{\sigma}(\omega + i\delta) \]  

close to the transition from the paramagnetic to the AF state. Fig. 2 shows the typical behaviour as the coupling constant \( J^* \) is increased for fixed temperature \( T = t^*/8 \) and filling \( n = n_\uparrow + n_\downarrow = 0.98 \). For \( J^* = 0.25 \) the system is in the paramagnetic state, in which case the

![Figure 2: Single-particle DOS for the t-J model at \( \beta = 8/t^* \) and \( n = 0.98 \) for different values of \( J^* \). The full curves represent the DOS for the majority spin and the dashed curves the one for the minority spin on a given site. Note that with increasing polarisation \( \Delta n = |n_\uparrow - n_\downarrow| \) the DOS develops pronounced structures below the Fermi energy.](image)

model is equivalent to a \( U=\infty \) Hubbard model. The structure near the chemical potential was earlier already related to some kind of single-band Kondo effect \cite{21, 27}. With increasing \( J^* \) one eventually enters into the AF regime, where the spectral functions of up and down spins (full and dotted lines, respectively) become inequivalent and show a pronounced multi-peak structure. The latter will be discussed in the next section. A similar series of pictures
would be obtained, if the filling or the temperature were varied with the other parameters fixed.

In order to show that the structures in both spin directions have the same origin, we shift the energy scales about the staggered magnetic field $h_\sigma$ that enters the local energy $\varepsilon_\sigma$. Fig.3 shows that indeed the peak positions coincide.

Note that in the following figures we will use energy scales for the different spectral functions, therefore, that are shifted in the same way. The spectral function of the minority spins (we will refer to it as $A_\downarrow(\omega)$ in the following) will sometimes also be rescaled in height by a suitable factor in order to be easier compared with $A_\uparrow(\omega)$. Note also, that the total spectral weight for the two spin directions may be different since we are looking only on the lower Hubbard band for which no sumrule applies.

![Figure 3](image_url)

Figure 3: (a) Single-particle DOS for $\beta = 8/t^*$, $J^* = 0.4t^*$ and $< n >= 0.98$ with $\Delta n = 0.81$. (b) DOS for the same parameters as in (a) but with the zero of energy chosen according to the individual $\mu_\sigma$. Also, the minority DOS was rescaled by a factor of 7 to show the structures more clearly.

An interesting problem concerns the question what happens to the Kondo-like peak,
observable in the paramagnetic state (Fig. 2) near the Fermi energy in the case of a fi-

\[ \omega - \mu \]

\[ A(\omega) \]

\[ \omega - \mu + h_\sigma \]

Figure 4: (a) DOS for \( J^* = 0, \beta = 8/t^* \) and \( <n> = 0.98 \). Note the structure at \( \omega = \mu \) in \( A(\omega) \). (b) DOS for \( J^* = 0.4t^* \), other parameters as in (a). The resonance at the Fermi level observed in (a) appears again at the same position in both spectral functions. Since those were shifted by an amount \( h_\uparrow - h_\downarrow \) with respect to each other, this structure is split in comparison to the case \( J = 0 \).

nite sublattice magnetization. In fact, for low temperatures and small doping the spectral function shows an additional shoulder at the Fermi energy if the spectra are shifted by the molecular field \( h_\sigma \) (Fig. 3). This can be seen clearly in Fig. 4, where we compare the spectrum in the antiferromagnetic state with the corresponding spectrum in the absence of the exchange interaction. It is tempting to identify this feature with a Kondo resonance in the antiferromagnetic state. However, due to the restricted parameter and temperature range it is not possible to answer this question definitely and to exclude artefacts of the non-crossing approximation.
5 Comparison to one hole in the Néel state

We now want to discuss in detail the multi-peak structure in the spectral function, which in our opinion can be related to bound states of a hole in a linear potential. This becomes clear if we compare our results with the theory of Strack and Vollhardt [13]. There it is shown that the problem of one hole in the Néel background can be solved exactly in the limit $d = \infty$. In addition, a particularly comprehensive deduction of the one-particle Green’s function is given.

Before we start to present their results we should mention, that the definition of the Green’s function and the choice of the energy scale in [13] are slightly different from ours: The zero of energy is the energy of the Néel state with one hole $|iN > = c_i|N >$ and the hole’s Green’s function is defined by

$$G_{ii}^h(\omega) = \frac{1}{\omega - H} |iN > .$$

(12)

From this definition it can easily be seen that the sign of energy is changed and the energy scale is shifted about the chemical potential and the exchange field. Note also that a different way of scaling for the hopping energy in [13] was used, namely $t = \hat{t}/\sqrt{2d}$. According to this we have to transform the results of [13] in a proper way before comparing them to our thermodynamic Green’s functions.

Following the notation of [13] the hole’s Green’s function reads

$$G_{ii}^h(\omega) = \frac{1}{\omega - \hat{t}^2 - \frac{J^*}{2} - \frac{J^*}{2} \hat{t}^2 - \frac{J^*}{2} \hat{t}^2 \cdots} .$$

(13)

It has poles at frequencies

$$\omega_n = -2\hat{t} - \frac{J^*}{2} - a_n t^* \left[ \frac{J^*}{2t} \right]^2 ,$$

(14)

where $a_n$ are the zeros of the Airy function $Ai(4\hat{t}/J^*)$. $G_{ii}^h(\omega)$ has been calculated using the retraceable path approximation of Brinkman and Rice (BR) [9], which becomes exact in the limit of high dimensions [28]. The poles correspond to bound states of a particle in a linear
or string potential $\tilde{V}_m = mJ^*/2$. It is generated if the hole moves away from the initial site by $m$ steps, destroying pairs of antiferromagnetic bonds along its path, thus enhancing the energy roughly by $m \times (2E_{bond}) = mJ^*/2$ (cf. Fig.5). Note, however, that even in $d=\infty$ the

![Diagram of hole moving in antiferromagnetic background]

Figure 5: Illustration of the origin of the linear potential for a single hole moving in an antiferromagnetic background. The shaded symbols mark destroyed bonds along the hole’s path.

potential $\tilde{V}_m$ is only exact and well defined for the described situation of one hole moving in the AF background. Therefore, the most important question that arises obviously is to what extent these bound states will survive and how the spectrum will be modified, as one turns to low but finite doping and to finite temperatures.

Let us now return to our results for the one particle spectrum of the $t$-$J$ model in the AF phase. In Fig.3 a set of distinct peaks can be seen, which we believe are directly related to the bound states of one hole. Of course, temperature and finite doping will lead to the observed broadening. The more interesting question thus is to what extent the positions of the peaks in Fig. 3 are related to those in equation (14).

In Fig. 6 we present a direct comparison for the following examples:

a) $J = 0.7, n \approx 0.95, \Delta n \approx 0.64, \beta = 4.0$  
c) $J = 0.5, n = 0.98, \Delta n \approx 0.86, \beta = 7.0$
b) $J = 0.4$, $n = 0.95$, $\Delta n \approx 0.68$, $\beta = 8.0$  
d) $J = 0.4$, $n = 0.98$, $\Delta n \approx 0.81$, $\beta = 8.0$.

Figure 6: Some examples for the fit of the peak positions by the modified one-hole picture. Parameters are given in the text.

The vertical lines represent the poles of the one-hole Green’s function (13). As mentioned before, the energy scale for the poles has to be inverted and shifted to allow a direct comparison with our data. As we cannot calculate accurately the chemical potential of the N-particle Néel state, the shift is chosen to yield a reasonable fit to the peak positions of $A_\sigma(\omega)$. In the four examples we find quite good agreement with the distance of the peak positions, particularly when the system is very close to half filling like in the cases b) and c). This also holds for other parameters we examined.

One can try to simulate the effect of finite doping in the theory of Strack and Vollhardt by assuming isolated holes, which move in a partially polarized background. The analytic form of the Green’s function of this hole remains the same as in (13), with the only difference
that $J^*$ is replaced by an effective exchange interaction

$$J^\text{eff} = |n^\uparrow - n^\downarrow|J^*$$ (15)

which is reduced by means of the polarization of the actual system. This procedure leads to a better correspondence for the cases a) and d) but not for the other cases.

6 Conclusion

In this paper we presented results for the dynamics of the $t-J$ model in the antiferromagnetic state. These were obtained in the framework of the dynamical mean field theory which becomes exact in the limit of infinite dimensions (systems with many next neighbours). The spectral function of single-particle excitations for finite doping and finite temperature has features (a sequence of peaks) which are similar to those found for a single hole in an antiferromagnetic groundstate and which can be understood by the motion of a hole in a string potential. Our results show that this special case is relevant also for finite hole concentrations and finite temperatures, at least for $d \to \infty$. In this limit we were able to neglect spin-fluctuations in the antiferromagnetic state, which become more important in low dimensions. Then also the concept of a string potential breaks down. Due to this effect we expect a further broadening of the peak structure in the spectral function. Therefore it is not clear wether these structures will also be present in $d = 2$ and $d = 3$ for finite doping. However, for one hole exact diagonalisation studies for one hole in $d = 2$ show structures which can be related to the $d=\infty$ spectrum.

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