Effects of spin fluctuations in the \( t-J \) model

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Recent experiments on the Fermi surface and the electronic structure of the cuprate superconductors showed the importance of short range antiferromagnetic correlations for the physics in these systems. Theoretically, features like shadow bands were predicted and calculated mainly for the Hubbard model. In our approach we calculate an approximate selfenergy of the \( t-J \) model. Solving the \( U = \infty \) Hubbard model in the Dynamical Mean Field Theory (DMFT) yields a selfenergy that contains most of the local correlations as a starting point. Effects of the nearest neighbor spin interaction \( J \) are then included in a heuristical manner. Formally like in \( J \)-perturbation theory all ring diagrams, with the single bubble assumed to be purely local, are summed to get a correction to the DMFT-selfenergy. This procedure causes new bands and can furnish strong deformation of quasiparticle bands.

The obvious importance of antiferromagnetic (AF) correlations for the physics of cuprate superconductors found an impressing confirmation through ARUPS-experiments performed by Aebi et al. [1]. There, in a Fermi surface (FS) mapping of \( \text{Bi}_{2}\text{Sr}_{2}\text{CaCu}_{2}\text{O}_{8}(001) \) shadows of the FS were observed. The interpretation as an effect of short range antiferromagnetic correlations led to an intensive discussion of so called shadow features, which have been predicted by Kampf and Schrieffer [2] in a semi-phenomenological theory for the Hubbard model.

In the paper we present an approximate evaluation of the self energy for the \( t-J \) model \( H_{tJ} \) consisting of two parts: The hopping term

\[
H_{t} = -\frac{t}{2\sqrt{2}} \sum_{\langle ij \rangle \sigma} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma}
\]

acting only in the space of no double occupancy \((\tilde{c}_{i\sigma}^{\dagger} = (1 - n_{i,-\sigma}) c_{i\sigma}^{\dagger})\) is equivalent to the \( U = \infty \) Hubbard model. The spin interaction is described explicitly by

\[
H_{J} = J \sum_{\langle ij \rangle} (\vec{S}_{i} \cdot \vec{S}_{j} - \frac{1}{4} n_{i} n_{j}).
\]

The main idea of our approach is to take into account both, the spin fluctuations due to \( H_{J} \) and the strong local correlations in \( H_{t} \). For the latter the dynamical mean field theory (DMFT) [3, 4, 5], which becomes exact in the limit of infinite spatial dimensions, proved to be quite a good tool. It yields a strictly local selfenergy, which reflects the metal-insulator transition for increasing \( U \) as well as a Kondo-like resonance around the Fermi energy. Even as an approximation for a two-dimensional system the DMFT-results seem to be reliable when being compared to e.g. Quantum Monte Carlo calculations [6, 7, 8]. We perform the DMFT using the so called Non Crossing Approximation (NCA) [9, 10] to solve the related local problem. For details of this procedure see ref. [5].

The quantities obtained with this method are first the local selfenergy for calculating the approximate one-paricle Green’s function of the twodimensional \( U = \infty \) Hubbard model

\[
G_{t}(\mathbf{k}, z) = \frac{1}{z + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{\text{loc}}(z)}
\]

and second the full local magnetic susceptibility \( \chi_{\text{loc}}(\omega) \). The dispersion is given by the Fourier transform of the next neighbor hopping \( \varepsilon_{\mathbf{k}} = -t^{*}/\sqrt{2} (\cos k_{x}a + \cos k_{y}a) \).

In addition to the correlation effects already contained in \( G_{t}(\mathbf{k}, z) \), spin fluctuations are now included by a formal perturbation expansion in \( H_{J} \), taking \( H_{t} \) as the unperturbed part of the Hamiltonian and \( G_{t}(\mathbf{k}, z) \) as the unperturbed GF (\( J = 0 \)).

As a first step all ring diagrams are summed resulting in a RPA-like structure for the effective interaction. In contrast to the standard RPA, however, the intermediate polarization diagram...
is the full susceptibility of the $U = \infty$ Hubbard model. Since the latter depends only very weakly on $q$, we further replace the latter quantity by $\chi_{\text{loc}}(z)$, which can be easily calculated from the effective local problem.

This procedure results in an effective interaction

$$\tilde{V}(q) = \frac{3}{2} \frac{J(q)}{1 + J(q)\chi_{\text{loc}}(i\nu_m)} - \frac{1}{2} \frac{J(q)}{1 + J(q)\chi_{\text{loc}}(i\nu_m)},$$

from which we obtain a selfenergy contribution

$$\Sigma_{\text{fluct}}(k) = -\sum_q G_t(k - q)\tilde{V}(q). \quad (5)$$

Here we use the notation $k = (k, i\omega_n)$ and an implicit sum over bosonic Matsubara frequencies is contained in equations (4) and (5). $\Sigma_{\text{fluct}}$ is calculated on the real frequency axis. The $q$-sum in eq. (5) is performed via Fast Fourier Transform on a 32x32 lattice and the sum over Matsubara frequencies by contour integration.

The complete selfenergy is then given by

$$\Sigma(k, z) = \Sigma_{\text{loc}}(z) + \Sigma_{\text{fluct}}(k, z) + \Sigma_{\text{Hartree}}, \quad (6)$$

where $\Sigma_{\text{Hartree}}$ is a real number and here determined by the occupation number of the DMFT-result. This scheme is iterated with the resulting Green’s function replacing $G_t$ in equation (5) until selfconsistency was reached.

Fig. 1 shows the resulting spectral functions $A(k, \omega)$ (full lines) at the $\Gamma$- and the $M$-point. The solid upper curve ($\Gamma$-point) shows an additional peak, exactly at the position of the quasiparticle peak at the $M$-point. The parameters are doping $\delta = 0.15$, coupling constant $J = 0.144t^*$, inverse temperature $\beta = 10.0t^*$.

In conclusion an extension of the dynamical mean field theory was presented including nonlocal spin-fluctuations in the $t$-$J$ model. With this approximation we are able to obtain shadow features in the spectral functions. So far our numerical calculations yield shadow bands only above the Fermi surface. In the experiment shadow bands cross the Fermi surface. We hope to reproduce this effect by including a next-nearest neighbor hopping $t'$ in our tight-binding bandstructure.

This work was supported by grant number Pr 298/3-1 from the Deutsche Forschungsgemeinschaft.
Figure 2: Bandstructure for the system with (crosses) and without (triangles) spin fluctuations. Around the Γ-point a new branch is visible, which shows the symmetry of a reduced Brillouin zone, although the system is paramagnetic. The parameters are the same as in Fig. 1.

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