One– and Two–Particle Excitations in Doped Hubbard Models

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We present a selfconsistent strong coupling scheme to evaluate the single particle Green's function for the two dimensional Hubbard model in the doped spin density wave state. For small doping we analyze the quasiparticle properties and the optical conductivity, emphasizing the role of multi spin–wave processes.

1. AF-POLARONS IN THE SDW STATE

The two dimensional Hubbard model is well established as a promising candidate to describe the electronic properties of the cuprate perovskites. Numerous investigations of this model have focused on the interplay of charge and spin degrees of freedom in the *t-J* limit. Early studies [1] starting from the itinerant regime for intermediate correlations have only recently been extended to incorporate strong coupling effects [2]. Here we report new results of this spin–polaron approach to the elementary excitations in the spin density wave (SDW) state of the Hubbard model.

The SDW representation of the 2D Hubbard Hamiltonian is [1, 2]

$$H = \sum_{\mathbf{k}\sigma,l=\pm 1}' iE_{\mathbf{k}} a^{l\dagger}_{\mathbf{k}\sigma} a^{l}_{\mathbf{k}\sigma} + H_U \qquad (1)$$

Here, $a^{l\dagger}_{\mathbf{k}\sigma}$ creates SDW quasiparticles in the conduction ($l = +1$) or valence band ($l = -1$), H_U is the residual Hubbard interaction, and $E_{\mathbf{k}} = [\epsilon^2_{\mathbf{k}} + \Delta^2]^{1/2}$ where $\epsilon_{\mathbf{k}}$ is the 2D square–lattice tight binding dispersion and Δ is the magnetic gap. Primed summations are restricted to the magnetic Brillouin zone. The broken spin rotational invariance of the SDW state implies gapless spin wave excitations. The central issue is to incorporate the renormalization of SDW quasiparticles due to *multi* spin wave shake–off. This is done by summing *all* noncrossing (NC) spin-wave exchange diagrams to the self–energy $\Sigma^{ll'}$ of the Greens function $G^{ll'}$. To this end we evaluate the transverse dynamical spin susceptibility $\chi^{\sigma-\sigma}(\mathbf{q},\mathbf{q}',z)$ within the RPA. Using a strong coupling expansion $U/t \gg 1$ we obtain [1, 2]

$$\chi^{\sigma-\sigma}(\mathbf{q},\mathbf{q},z) = \frac{-2J(\epsilon_{\mathbf{q}}/(4t)+1)}{z^2-\omega^2_{\mathbf{q}}} \quad . \qquad (2)$$

for $\mathbf{q} = \mathbf{q}'$ and $\chi^{\sigma-\sigma}(\mathbf{q}+\mathbf{Q},\mathbf{q},z) = -\chi^{\sigma-\sigma}(\mathbf{q},\mathbf{q},z)\sigma\omega/[2J(\epsilon_{\mathbf{q}}/(4t)+1)]$ for $\mathbf{q}-\mathbf{q}' = \mathbf{Q} = (\pi,\pi)$. The pole positions determine the spin–wave dispersion with $\omega_{\mathbf{q}} = 2J[1-(\epsilon_{\mathbf{q}}/4t)^2]^{1/2}$. Inserting this into the strong coupling limit of the NC Dyson–equation for the case of a single–hole a self–consistent integral equation for the valence band self–energy results

$$\Sigma^{-1\,-1}_{\sigma}(\mathbf{k},z) = U^2 \sum_{\mathbf{q}\neq 0}' \Big\{ (1+\frac{2J}{\omega_{\mathbf{q}}})\int_0^{\infty} d\omega \frac{A^{-1\,-1}_{\bar\sigma}(\mathbf{k}-\mathbf{q},\omega)}{\omega_{\mathbf{q}}+\omega+z} + (1-\frac{2J}{\omega_{\mathbf{q}}})\int_{-\infty}^{0} d\omega \frac{A^{-1\,-1}_{\bar\sigma}(\mathbf{k}-\mathbf{q},\omega)}{\omega_{\mathbf{q}}-\omega-z}\Big\} \qquad (3)$$

Here $A^{-1\,-1}_{\sigma}(\mathbf{k},\omega) = -Im[G^{-1\,-1}_{\sigma}(\mathbf{k},\omega+i\eta)]/\pi$ is the spectral function. Fig. 1 shows a typical valence band spectrum obtained by numerical solution of (3). It displays an *incoherent spin wave shake-off structure*, both, below the quasihole peak, similar to the *t-J* limit, and in the upper SDW band. The quasihole weight $Z_{\mathbf{k}}$ and the band width W are considerably reduced with respect to their bare SDW values. The suppression of $Z_{\mathbf{k}}$ is strongest at the zone center with, e.g., $Z_{\mathbf{k}=0} \approx 0.51$ for $U/t = 4$, in which case $W/W_{SDW} = 0.66$. Recent results [3] indicate a maximum of the quasihole energy at a wave vector $(\pi/2,\pi/2)$ in agreement with the *t-J* limit.

2. OPTICAL CONDUCTIVITY

In the following we consider the charge dynamics of the spin–fluctuation dressed quasiparticles for which we evaluate the regular part of

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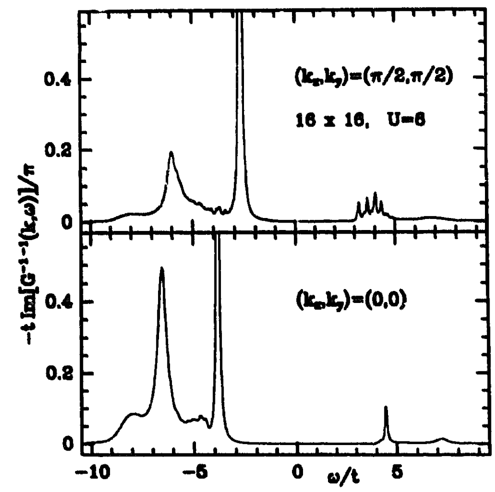

Fig. 1. Single hole spectral function

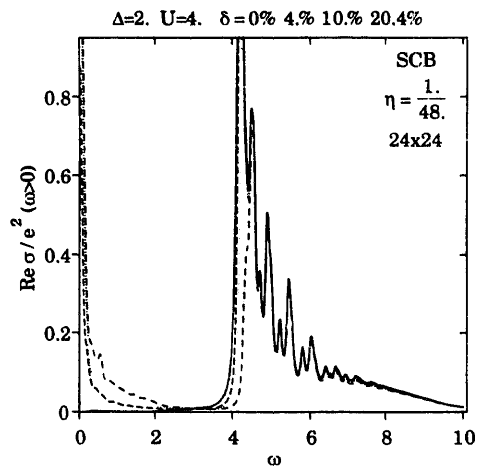

Fig. 2. Regular part σ_{reg} of the optical conductivity.

the complex, frequency dependent conductivity $\sigma_{reg}(\omega) = Re\sigma(\omega > 0)$. Standard linear response theory relates the conductivity to the retarded current–current correlation function

$$C^r_{xx}(z) = \frac{i}{N}\int_0^\infty e^{izt}\,dt \left\langle \left[J^P_x(t), J^P_x(0)\right]_- \right\rangle, \quad (4)$$

for the paramagnetic current operator $J^p_x = iet\sum_{i\sigma}(c^+_{i+x,\sigma}c_{i,\sigma} - c^+_{i,\sigma}c_{i+x,\sigma})$.

We use the polaron scheme for the Green's functions of the holes to calculate the required current-current correlation function C_{xx} as written in the form

$$C_{xx}(\omega) = i\frac{1}{N}\sum_{\mathbf{k}\sigma}\int\frac{d\nu}{2\pi}\Gamma_c(\mathbf{k},\omega,\nu)\Big[\Big\{G^{11}_\sigma(\mathbf{k},\nu) G^{11}_\sigma(\mathbf{k},\omega+\nu) + G^{-1-1}_\sigma(\mathbf{k},\nu)G^{-1-1}_\sigma(\mathbf{k},\omega+\nu)\Big\} n^2(\mathbf{k},\mathbf{k}) + \big\{G^{11}_\sigma(\mathbf{k},\nu)G^{-1-1}_\sigma(\mathbf{k},\omega+\nu) + G^{-1-1}_\sigma(\mathbf{k},\nu)G^{11}_\sigma(\mathbf{k},\omega+\nu)\big\}\, m^2(\mathbf{k},\mathbf{k})\Big]\gamma(\mathbf{k}). \quad (5)$$

Neglecting vertex corrections we use $\Gamma_c(\mathbf{k},\omega,\omega') = \gamma(\mathbf{k}) = \partial\epsilon(\mathbf{k})\partial k_x$. $m(\mathbf{k},\mathbf{k}')$ and $n(\mathbf{k},\mathbf{k}')$ are coherence factors[1]. In Eq. 5 we have omitted already those terms involving the interband Green's functions $G^{-1\,1}$ and $G^{1\,-1}$. They are absent in the large U/t limit for which the Green's function matrix $G^{ll'}$ is diagonal. Assuming that the SDW order is approximately preserved for a small but finite hole density we introduce a finite chemical potential into the Green's functions G^{ll} which contain the full incoherent background contributions from the spin–fluctuation dressing.

The results of this calculation are shown in Fig. 2 at different hole doping concentrations δ. For $\delta = 0$, only the optical excitations across the renormalized SDW energy gap contribute. For finite δ oscillator strength appears inside the gap. The corresponding spectral weight is removed from the high-energy interband excitations and shifted to low frequencies. The sharpness of the peak near $\omega = 0$ in Fig. 2 results from the flat quasiparticle dispersion along the magnetic Brillouin zone boundary.

The optical absorption at low frequencies is entirely due to the spin-fluctuation dressing of the quasiparticles, i.e. the incoherent part of the propagator. We may therefore directly identify the low frequency optical conductivity with the spin fluctuations accompanying the doped holes. This provides a possible explanation for the origin of the so-called mid-infrared band observed in lightly doped cuprate superconductors[4].

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