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Single particle excitations in itinerant antiferromagnets at small doping

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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 including the dispersion and the quasiparticle weight. Novel incoherent contributions to the spectral function resulting from multi spin wave processes are discussed.

1. INTRODUCTION

Experimental and theoretical evidence on the cuprate perovskites has converged towards the two dimensional Hubbard model as a promising candidate to describe these systems which exhibit high temperature superconductivity [1] in the vicinity of a metal to antiferromagnetic (AF) insulator transition. Many investigations of the Hubbard model have focused on the interplay between charge and spin degrees of freedom close to half filling starting from the localized limit. Efforts to study the elementary excitations in the itinerant regime for intermediate correlations are less exhaustive [2]. In this contribution we report results of a strong coupling theory for spin fluctuation induced single particle renormalization in the spin density wave (SDW) state of the Hubbard model.

2. AF-POLARONS IN THE SDW STATE

The starting point is the SDW representation of the 2D Hubbard model

$$H_{HUB} = \frac{1}{2} \sum_{\mathbf{k},\sigma,l=\pm1} l \cdot E_{\mathbf{k}} a^{l\,\dagger}_{\mathbf{k}\,\sigma} a^{l}_{\mathbf{k}\,\sigma} + H_{RES} \quad (1)$$

Here $a^{l\,(\dagger)}_{\mathbf{k}\,\sigma}$ are conduction/valence band SDW particles for l=±1, respectively, and H_{RES} is the residual Hubbard interaction H_U. The mean field kinetic energy $E_{\mathbf{k}}$ is given by $E_{\mathbf{k}} = (\epsilon^2_{\mathbf{k}} + \Delta^2)^{1/2}$ where $\epsilon_{\mathbf{k}}$ is the 2D tight binding energy and Δ is the selfconsistent magnetic gap. Within the magnetic Brillouin zone (MBZ) the operators $a^{l\,(\dagger)}_{\mathbf{k}\,\sigma}$ are given in terms of the original fermions $c^{\dagger}_{\mathbf{k}\,\sigma}$ by

$$\begin{aligned} a^{l\,\dagger}_{\mathbf{k}\,\sigma} &= v_{l\,\mathbf{k}} c^{\dagger}_{\mathbf{k}\,\sigma} + l\sigma v_{l\,\mathbf{k}+\mathbf{Q}} c^{\dagger}_{\mathbf{k}+\mathbf{Q}\,\sigma} \\ v_{l\,\mathbf{k}} &= v_{-l\,\mathbf{k}+\mathbf{Q}} = [(1 + l\epsilon_{\mathbf{k}}/E_{\mathbf{k}})/2]^{1/2} \end{aligned} \quad (2)$$

$\mathbf{Q}$ is the square lattice nesting vector and $a^{l\,\dagger}_{\mathbf{k}\,\sigma}$ is extended to the 1st Brillouin zone (BZ) by $a^{l\,\dagger}_{\mathbf{k}\,\sigma} = l\sigma a^{l\,\dagger}_{\mathbf{k}-\mathbf{Q}\,\sigma}$. The resulting algebra is given by $\{a^{l}_{\mathbf{k}\,\sigma}, a^{l'\,\dagger}_{\mathbf{k}'\,\sigma'}\} = \delta_{\sigma\sigma'}\delta_{ll'}(\delta_{\mathbf{k}\mathbf{k}'} + l\sigma\delta_{\mathbf{k}\mathbf{k}'+\mathbf{Q}})$. The bare fermions are expressed via $c^{\dagger}_{\mathbf{k}\,\sigma} = \sum_{l=\pm1} v_{l\,\mathbf{k}} a^{l\,\dagger}_{\mathbf{k}\,\sigma}$ for *all* $\mathbf{k} \in$ 1st BZ.

To describe AF spin waves only the retarded transverse spin susceptibility $\chi^{+-}(\mathbf{q},\mathbf{q}',t) = i\Theta(t)\langle[\sigma^{+}_{-\mathbf{q}}(t), \sigma^{-}_{\mathbf{q}'}]\rangle$ is needed, where $\sigma^{+}_{\mathbf{q}} = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}+\mathbf{q}\,\uparrow} c_{\mathbf{k}\,\downarrow}$. To evaluate this susceptibility we employ the RPA approximation. We have extended the analysis of ref. [2] to include the possibility of Landau damping [3] at finite doping. We found the spin waves to be *stable against relaxation due to intra band scattering.* Therefore we resort to a strong coupling expansion of the RPA susceptibility at zero doping. Extracting the spin wave poles in the large U–limit we find a 2x2 matrix representation in $\mathbf{q}$ space

$$\begin{aligned} \chi^{+-}(\mathbf{q},\mathbf{q},z) &= \frac{-2J(\epsilon_{\mathbf{k}}/(4t) + 1)}{z^2 - \omega^2_{\mathbf{q}}} \\ \chi^{+-}(\mathbf{q}+\mathbf{Q},\mathbf{q},z) &= \frac{z}{z^2 - \omega^2_{\mathbf{q}}} \end{aligned} \quad (3)$$

where $\chi^{+-}(\mathbf{q},\mathbf{q},z) \equiv \chi^{+-}(\mathbf{q}+\mathbf{Q},\mathbf{q}+\mathbf{Q},z)$ and $\chi^{+-}(\mathbf{q}+\mathbf{Q},\mathbf{q},z) \equiv \chi^{+-}(\mathbf{q},\mathbf{q}+\mathbf{Q},z)$. J is

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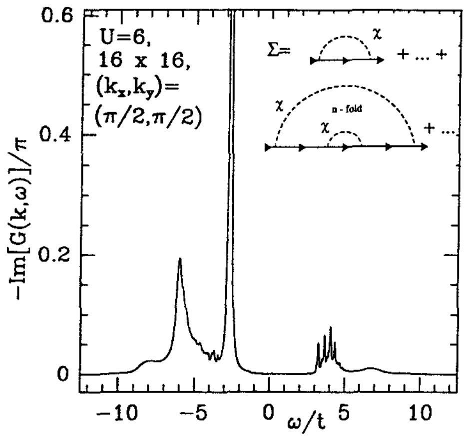

Figure 1. Spectral function.

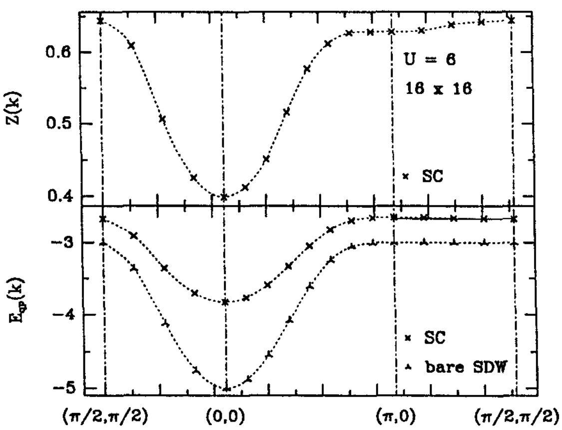

Figure 2. Quasi particle properties

the AF exchange coupling given by $4t^2/U$ where t is the bare hopping integral and $\omega_{\mathbf{q}} = 2J[1 - \epsilon_{\mathbf{k}}^2/(16t^2)]^{1/2}$ is the spin wave dispersion. $z = \omega + i\eta$ is a complex frequency.

We now formulate a Dyson equation for the Green's function $G_\sigma^{l\,m}(\mathbf{k},\tau) = -\langle T_\tau a^l_{\mathbf{k}\,\sigma}(\tau) a^{m\,\dagger}_{\mathbf{k}\,\sigma}\rangle$ of the SDW particles. *Strong coupling* to the spin degrees of freedom is approximated by including *multiple spin wave scattering* in the self energy $\Sigma_\sigma^{l\,m}(\mathbf{k},\tau)$ as sketched in the inset of Fig. 1. In the large U limit we find $G_\sigma^{1\,-1}(\mathbf{k},\tau) = G_\sigma^{-1\,1}(\mathbf{k},\tau) \equiv 0$. At small doping we focus on the Green's function of a *single hole.* In that case particle hole symmetry leaves only the retarded valence band self energy to be determined

$$\Sigma_\sigma^{-1\,-1}(\mathbf{k},z) = U^2 \sum_{\mathbf{q}\neq\mathbf{0}}{}' \{ (1+\frac{2J}{\omega_{\mathbf{q}}}) \int_0^\infty d\omega \frac{A_\sigma^{-1\,-1}(\mathbf{k}-\mathbf{q},\omega)}{\omega_{\mathbf{q}}+\omega+z} + (1-\frac{2J}{\omega_{\mathbf{q}}}) \int_{-\infty}^0 d\omega \frac{A_\sigma^{-1\,-1}(\mathbf{k}-\mathbf{q},\omega)}{\omega_{\mathbf{q}}-\omega-z}\} \quad (4)$$

Here $A_\sigma^{-1\,-1}(\mathbf{k},\omega) = -Im[G_\sigma^{-1\,-1}(\mathbf{k},\omega+i\eta)]/\pi$ is the spectral function of the retarded propagator. The primed $\mathbf{q}$–summation is restricted to the MBZ.

3. RESULTS AND DISCUSSION

We have solved Eqn.(4) by iteration on finite lattices. In Fig. 1 a characteristic spectrum of the valence band propagator is shown on the MBZ boundary for U/t=6 on a 16x16 lattice. Besides a renormalized quasiparticle peak the spectral density displays considerable incoherent weight due to spin wave shake off, *both*, above the magnetic gap *and* below the quasiparticle pole. Earlier investigations [4] have missed the latter effect due to a lack of selfconsistency. The valence band incoherent weight is reminiscent of similar findings on t–J type models. Fig. 2 depicts quasiparticle properties along the irreducible wedge of the MBZ for parameters identical to those of Fig. 1. The Z–factor is smallest at the valence band bottom where the spin wave shake off is strongest. A pronounced band narrowing of $E_{qp}(\mathbf{k})$ is evident. Moreover we find a non linear dependence of the effective gap on U. For all values of U investigated we observed $E_{qp}(\mathbf{k})$ to have pockets at $(\pi/2,\pi/2)$ at the *1-loop* level, *however*, they are shifted to $(\pi,0)$ for an infinite number of loops.

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