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Angaben zur Veröffentlichung / Publication details:

Brenig, Wolfram, and Arno P. Kampf. 1994. "Single particle excitations in itinerant antiferromagnets." *Journal of Low Temperature Physics* 95 (1-2): 329–34. https://doi.org/10.1007/bf00754948.

Single Particle Excitations in Itinerant Antiferromagnets

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We present a self-consistent strong coupling scheme to evaluate the single-particle Green's function for the two dimensional Hubbard model in the spin-density-wave state. We analyse the single quasihole properties including its dispersion and its spectral weight factor. Significant incoherent contributions to the spectral function are found resulting from multi spin wave processes in accordance with similar results for the $t-J$ model and small Hubbard clusters.

PACS numbers: 75.10L, 75.30F, 75.30D.

1. INTRODUCTION

The vicinity of antiferromagnetism and superconductivity in the layered high temperature superconductors has stimulated research to understand the properties of carriers doped into an antiferromagnetic (AF) insulating state in two dimensions. In strong coupling approaches the competition between AF ordering of localized spin degrees of freedom and the delocalisation of doped holes is the key issue. For the $t-J$ model exact diagonalization,[1] cumulant,[2] and spin-polaron methods[3] corroborate a Fermi-liquid picture of the single hole states at half filling. The quasihole bandwidth, however, is strongly renormalized by a factor approximately proportional to J/t for $J \lesssim t$. Moreover, the quasihole spectral weight $Z \sim \alpha(J/t)^{\beta}$, with $\alpha, \beta \sim 1$, is significantly reduced from unity. This corresponds to a large redistribution of spectral intensity into the incoherent part of the single particle propagator. Similar results are found for the Hubbard model in the intermediate to strong coupling regime.[5,4]

Less extensively studied are the *spectral properties* of the elementary excitations in the weak coupling limit of the Hubbard model. In this case the spin-density-wave (SDW) state is an appropriate starting point to explore the single particle dynamics. Similar to the $t-J$ model, holes which are doped into the SDW state give rise to frustration effects on a length scale of the order of the magnetic coherence length ξ_{SDW}.[6-8] In this paper we focus on the *dynamical* properties of a single hole doped into the SDW state. In this case the hole motion is accompanied by multi spin wave excitation processes which reduce the quasihole's spectral weight and renormalize the bandwidth and the single particle gap.

2. SDW SPIN DYNAMICS

The starting point of our analysis is the SDW representation of the Hubbard model on a square lattice at half filling[6]

$$H = \sum_{\mathbf{k}\sigma,l=\pm 1}' l E_{\mathbf{k}} a^{l\dagger}_{\mathbf{k}\sigma} a^{l}_{\mathbf{k}\sigma} + H_U \quad . \tag{1}$$

Here, $a^{l\dagger}_{\mathbf{k}\sigma}$ creates a SDW quasiparticle in the conduction or valence band for $l = +1$ or -1, respectively, and H_U is the residual Hubbard interaction. The mean field dispersion for the upper and lower SDW band is given by $E_{\mathbf{k}} = \pm[\epsilon^2_{\mathbf{k}} + \Delta^2]^{1/2}$ in terms of the tight binding energy $\epsilon_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y a))$ and the magnetic SDW energy gap Δ. The primed summation is restricted to the MBZ. The magnitude of Δ follows from the gap equation $1/U = \frac{1}{N}\sum'_{\mathbf{k}} 1/E_{\mathbf{k}}$ which is the Hartree-Fock (HF) self-consistency condition for the staggered magnetization $\langle S_z(\mathbf{Q})\rangle$ in the broken symmetry state. $\mathbf{Q} = (\pi, \pi)$ is the square lattice nesting wave vector. Due to the doubling of the unit cell the SDW quasiparticles are restricted to the MBZ, i.e. to momenta where $\epsilon_{\mathbf{k}} < 0$. They are related to the bare fermion operators $c^{l\dagger}_{\mathbf{k}\sigma}$ of the original Hubbard model by the linear transformation $a^{l\dagger}_{\mathbf{k}\sigma} = v^l_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} + l\sigma v^{-l}_{\mathbf{k}} c^\dagger_{\mathbf{k}+\mathbf{Q}\sigma}$ with $v^l_{\mathbf{k}} = [(1 + l\epsilon_{\mathbf{k}}/E_{\mathbf{k}})/2]^{1/2}$.

The broken spin rotational invariance of the SDW state implies the existence of gapless collective spin excitations. In order to calculate these Goldstone modes we consider the transverse dynamical spin susceptibility $\chi^{\sigma-\sigma}(\mathbf{q}, \mathbf{q}', t) = i\langle T S^\sigma_{\mathbf{q}}(t) S^{-\sigma}_{\mathbf{q}'}(0)\rangle$ including RPA fluctuations around the HF groundstate. Here $\sigma = \pm 1$ and $\chi^{\sigma-\sigma}(\mathbf{q}, \mathbf{q}', t)$ is a symmetric 2×2 matrix with respect to the momentum indices which is finite only if $\mathbf{q} = \mathbf{q}'$ or $\mathbf{q} = \mathbf{q}' \pm \mathbf{Q}$. Summing the RPA bubble series leads to

$$\chi^{\sigma-\sigma}_{RPA}(\mathbf{q}, \mathbf{q}', \omega) = \sum_{\tilde{\mathbf{q}}} \chi^{\sigma-\sigma}_0(\mathbf{q}, \tilde{\mathbf{q}}, \omega)\left[1 - U\chi^{\sigma-\sigma}_0(\tilde{\mathbf{q}}, \mathbf{q}', \omega)\right]^{-1} \quad , \tag{2}$$

where $[1 - U\chi^{\sigma-\sigma}_0(\tilde{\mathbf{q}}, \mathbf{q}', \omega)]^{-1}$ is a matrix inverse in momentum space. The bare particle-hole susceptibility $\chi^{\sigma-\sigma}_0$ is calculated with the HF c-electron propagators.

To extract the collective spin dynamics we resort to a strong coupling expansion assuming $U \gg t$. This procedure has previously been shown[6,7] to reproduce the results of linear spin wave theory for the 2D AF Heisenberg model of localized spins with an exchange constant $J = 4t^2/U$. In this limit the transverse susceptibility $\chi^{\sigma-\sigma}_S \equiv \chi^{\sigma-\sigma}_{RPA}|_{U/t\gg 1}$ is found to display undamped propagating spin wave excitations:

$$\begin{bmatrix} \chi^{\sigma-\sigma}_S(\mathbf{q}, \mathbf{q}, \omega) \\ \chi^{\sigma-\sigma}_S(\mathbf{q}+\mathbf{Q}, \mathbf{q}, \omega) \end{bmatrix} = \frac{1}{\omega^2 - \omega^2_{\mathbf{q}} + i\eta} \begin{bmatrix} -2J(1 + \epsilon_{\mathbf{q}}/4t) \\ \sigma\omega \end{bmatrix} \tag{3}$$

with the spin wave dispersion $\omega_{\mathbf{q}} = 2J[1 - (\epsilon_{\mathbf{q}}/4t)^2]^{1/2}$. The coupling to these low energy spin wave modes is assumed to be the dominant source for the renormalization of the single particle properties. We will go beyond previously applied

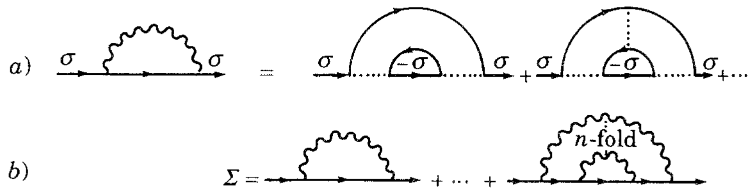

Fig. 1. a) One–loop self–energy correction from the coupling to transverse spin fluctuations in the RPA ladder series. b) NC scheme for the self–energy. The wiggly line represents the RPA ladder series of a).

lowest order one loop calculations[7,9,10] and evaluate the electronic self–energy in a self–consistent non–crossing (NC) scheme.

3. AF–POLARONS IN THE SDW STATE

The SDW quasiparticles couple strongly to the spin wave excitations. Therefore, we focus on the renormalization due to *multi* spin wave shake–off which is described by the NC diagrams of Fig. 1 for the self–energy. Accounting for all possible Umklapp contractions in the c–electron representation, or equivalently all inter– and intra–band processes in the a–electron picture the NC approximation consists of four coupled integral equations. To reduce this complexity we consider the formal limit of $U \gg t$. Using the transverse spin susceptibility of (3) and working in the a–electron representation with the transformation coefficients $v^l_{\mathbf{k}}$ replaced by their large U value, i.e. $1/\sqrt{2}$, the strong coupling version of the NC equations reads

$$
\begin{aligned}
\Sigma^{l\,l}_{\sigma}(\mathbf{k}, i\epsilon_\mu) &= -T\,U^2 \sum_{\mathbf{q},\omega_\nu}{}' \left[\chi_S^{-\sigma\,\sigma}(\mathbf{q},\mathbf{q},i\omega_\nu) + \chi_S^{-\sigma\,\sigma}(\mathbf{q}+\mathbf{Q},\mathbf{q}+\mathbf{Q},i\omega_\nu) + \right. \\
&\qquad \left. l\sigma\, 2\,\chi_S^{-\sigma\,\sigma}(\mathbf{q}+\mathbf{Q},\mathbf{q},i\omega_\nu)\right] G^{-l\,-l}_{-\sigma}(\mathbf{k}-\mathbf{q}, i\epsilon_\mu - i\omega_\nu) \qquad (4) \\
\Sigma^{-l\,l}_{\sigma}(\mathbf{k}, i\epsilon_\mu) &= -T\,U^2 \sum_{\mathbf{q},\omega_\nu}{}' \left[\chi_S^{-\sigma\,\sigma}(\mathbf{q},\mathbf{q},i\omega_\nu) - \right. \\
&\qquad \left. \chi_S^{-\sigma\,\sigma}(\mathbf{q}+\mathbf{Q},\mathbf{q}+\mathbf{Q},i\omega_\nu)\right] G^{l\,-l}_{-\sigma}(\mathbf{k}-\mathbf{q}, i\epsilon_\mu - i\omega_\nu) \quad . \qquad (5)
\end{aligned}
$$

Here $\omega_\nu = 2\nu\pi T$ and $\epsilon_\mu = (2\mu+1)\pi T$ are Matsubara frequencies. $\Sigma^{l\,l'}_{\sigma}(\mathbf{k}, i\epsilon_\mu)$ and $G^{l\,l'}_{\sigma}(\mathbf{k}, i\epsilon_\mu)$ are the momentum diagonal components of the a–fermion self–energy and the *dressed* a–Green's function, respectively, for band indices $l, l' = \pm 1$. Starting from the HF propagator the iterative solution of (5) leads to a vanishing *interband* Green's functions. This leaves only (4) for the *intraband* Green's function. Since both, the kernel of this integral equation and the bare SDW Green's functions are spin independent one may replace $G^{l\,l}_{-\sigma}$ by $G^{l\,l}_{\sigma}$ on the r.h.s. of (4). Finally, in the limit of a single hole particle–hole symmetry leads to the relation[9] $A^{-1\,-1}_{\sigma}(\mathbf{k},\omega) = A^{1\,1}_{\sigma}(\mathbf{k},-\omega)$ for the spectral functions $A^{l\,l}_{\sigma}(\mathbf{k},\omega) = -Im[G^{l\,l}_{\sigma}(\mathbf{k},\omega+i\eta)]/\pi$. Therefore, we are left with only a single integral equation e.g. for the valence band propagator. We perform the required frequency summations and proceed via an

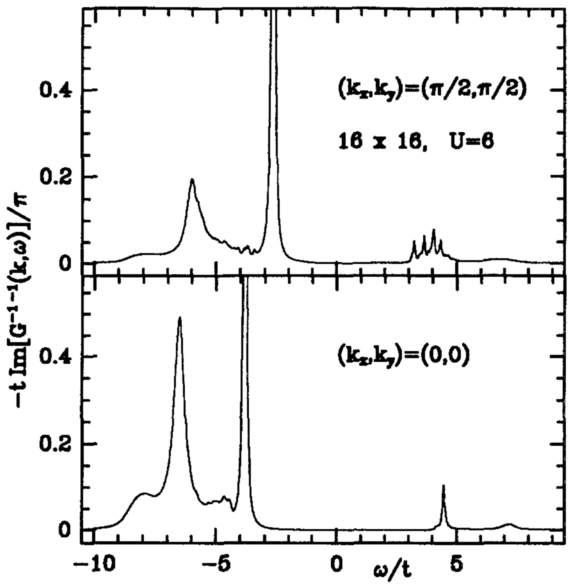

Fig. 2. Single–hole spectral function for $U = 6$ and for the two momenta $\mathbf{k} = (0,0)$ and $\mathbf{k} = (\pi/2, \pi/2)$ on a 16×16 lattice. Energies are given in units of t.

analytic continuation to the retarded quantities. In the zero temperature limit we obtain

$$\Sigma_{\sigma}^{-1\ -1}(\mathbf{k}, z) = U^2 \sum_{\mathbf{q}\neq 0}{}' \left\{ (1 + \frac{2J}{\omega_{\mathbf{q}}}) \int_0^{\infty} d\omega' \frac{A_{\sigma}^{-1\ -1}(\mathbf{k}-\mathbf{q}, \omega')}{\omega_{\mathbf{q}} + \omega' + z} + (1 - \frac{2J}{\omega_{\mathbf{q}}}) \int_{-\infty}^{0} d\omega' \frac{A_{\bar{\sigma}}^{-1\ -1}(\mathbf{k}-\mathbf{q}, \omega')}{\omega_{\mathbf{q}} - \omega' - z} \right\} , \qquad (6)$$

where $z = \omega + i\eta$. This expression represents the central equation for our self–consistent treatment of a spin polaron in the SDW state.

4. RESULTS AND DISCUSSION

Results for the single hole spectral function obtained from an iterative solution of (6) are shown in Fig. 2 on a 16×16 sites lattice. A moderate value of U has been chosen which, however, still justifies the use of the strong coupling limit in the self-consistent NC polaron scheme. Besides the renormalization of the quasihole peak the figure display a considerable shift of spectral weight into a spin wave shake-off structure below the quasihole energy and into the upper SDW band. Similar incoherent spectral weight is found in the one hole spectrum of the $t - J$ model only on the low energy side of the quasihole peak since the upper Hubbard band is removed by the strict exclusion of doubly occupied sites. This is the result of both,

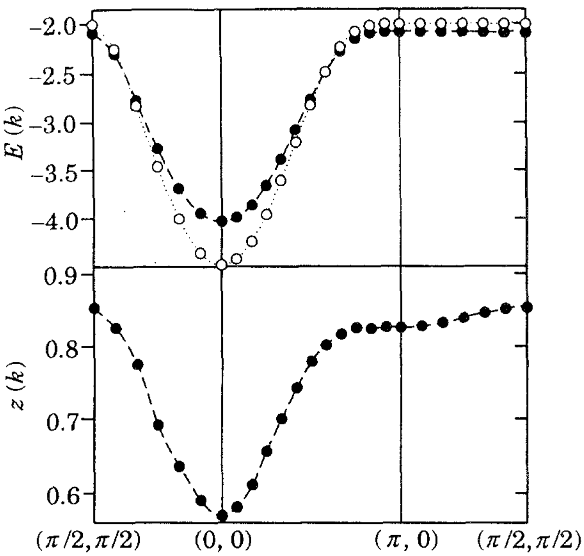

Fig. 3. Quasiparticle properties for $U = 4t$ on a 24×24 lattice along a closed triangular path in the MBZ. The upper panel shows the NC quasiparticle dispersion (•) as compared to the SDW dispersion (∘) $E(\mathbf{k})$ for $2\Delta = U$. The lower panel shows the corresponding quasiparticle weight factor.

exact diagonalization studies[1] and approximate NC calculations.[3] On the other hand the incoherent low energy continuum is missing in earlier calculations which have been performed in the SDW state using a one-loop approximation only.[9] This approach lacks the relevant transfer of spectral weight resulting from the multiple spin wave excitations. In this sense our self-consistent polaron scheme interpolates between these two limits. But the physical situation in both cases is quite different: In the $t-J$ limit of the Hubbard model a spin wave emission leads to mobility of a hole inserted into the AF ordered background while in the SDW case spin waves cause a mass enhancement of the SDW quasiparticles.

The loss of spectral weight into the incoherent part is strongest at the MBZ center. This is evident from Fig. 3 which shows the quasihole spectral weight factor $z(\mathbf{k})$ and the dispersion along the irreducible wedge of the MBZ for $U = 4t$ on a 24×24 lattice. A comparison to the HF SDW dispersion demonstrates a significant band narrowing of the polaron band. Most striking is the result that the degeneracy of the HF bands along the MBZ boundary is barely lifted. Although not clearly visible in the figure, the energy maximum of the quasiparticle band occurs at $\mathbf{k} = (\pi, 0)$. This is a result which arises only on the multi-loop level since for the one-loop calculation the maximum does appear at $\mathbf{k}_p = (\pi/2, \pi/2)$.[9] While it seems generally accepted for the $t-J$ model that the maximum is at $\mathbf{k}_p = (\pi/2, \pi/2)$ this issue is much more subtle for the Hubbard model. Quantum Monte Carlo calculations on small clusters with finite hole concentrations have found no evidence for hole pockets near $\mathbf{k}_p$ and a Fermi surface whose shape is hardly changed when compared to the Fermi surface of the noninteracting tight binding band.[11] Lanczos diagonalization studies on a 4×4 Hubbard cluster have found near degeneracy between $\mathbf{k}_p$ and $(\pi, 0)$ but in slight favor for the maximum to occur at $(\pi, 0)$[5] in agreement with the self-consistent NC calculation.

Finite size analysis for the linear lattice sizes $N = \{8, 12, 16, 20, 24\}$ indicates linear scaling in $1/N$ for $z(\mathbf{k})$ and the renormalization of the bandwidth W. Quantitatively, e.g. for $U = 4t$, the bandwidth extrapolates to $W = 1.85t$ for $N \to \infty$ as compared to the SDW bandwidth $W_{SDW} = 2.81t$ and the spectral weight factors extrapolate to $z((\pi/2, \pi/2)) = 0.8$ and $z((0, 0)) = 0.51$ in the infinite lattice limit.

In conclusion we have analysed the single–particle properties in the SDW state using a noncrossing scheme. Extensions including the weak coupling limit and an analysis of the renormalization of the spin wave excitations are currently in progress.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge helpful discussions with Prof. K.W. Becker, Prof. P. Fulde, and Prof. E. Müller–Hartmann. This work has been performed within the program of the Sonderforschungsbereich 341 supported by the Deutsche Forschungsgemeinschaft.

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