Conserving approximation for the three-band Hubbard model: flat quasiparticle dispersion

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Abstract

It is shown that the low-energy single-particle excitation-spectrum of the three-band Hubbard model at hole-dopings away from half-filling agrees remarkably well with Quantum Monte Carlo data and spectroscopic experiments within the framework of a conserving approximation that includes self-consistently the interaction with charge, spin, and two-particle fluctuations. The dispersion of the quasiparticle-peak obtained from the spectral-weight function is flat around the $(\pi, 0)$ and $(0, \pi)$ points as has been observed in recent angle-resolved photoemission measurement. The significant reduction of the quasiparticle-dispersion near the Fermi-energy is due to spin-fluctuations, rather than being induced by band effects.

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The nature of quasiparticle excitations in the high-$T_c$ superconductors (HTSC) is of central interest in order to characterize the normal-state of these materials. Angle-resolved photoemission spectroscopy (ARPES) \cite{1-4} shows on the one hand, the existence of a Fermi-surface in the normal-state in accordance with Luttinger’s theorem supporting the conventional Fermi-liquid concept. On the other hand, these experiments find a very flat dispersion of the quasiparticle excitations near the $X=(\pi,0)$ and $Y=(0,\pi)$ points. This extended saddle-point behavior cannot be derived from single-particle calculations (Hartree-Fock, LDA \cite{5}) which find, in contrast, a van Hove bandstructure singularity. The importance of many-body correlation effects for such a flat quasiparticle dispersion was revealed in recent Quantum Monte Carlo (QMC) simulations of both the three-band \cite{6} and the one-band Hubbard model \cite{7}. Related interpretations were also advanced recently on the basis of QMC simulations of the t-J model \cite{8}. However, in spite of the success of the numerical techniques in dealing with strongly correlated systems, the physical interpretation of purely numerical QMC results is often difficult without reference to more transparent theoretical approaches.

In this letter one-particle spectra for realistic parameters \cite{6,9,10} of the three-band Hubbard model are presented based on a conserving approximation \cite{11,12}. The obtained spectral distribution of the quasiparticle peak agrees remarkably well with QMC- and ARPES results. The main features of the experimental bandstructure, such as the flat dispersion near the Fermi-energy, bandwidth, and Fermi-velocities are reproduced by our theoretical approach. Furthermore, in contrast to the QMC simulations, we are able to distinguish the influence of different many-body scattering channels. We can clearly show that magnetic fluctuations are responsible for the drastic reduction of characteristic energy-scales in the quasiparticle excitation spectrum compared to their mean-field values. Thus, the flatness has a many-body origin, rather than being induced by band effects, a result which may have important implications particularly for mechanisms of superconductivity based on spin fluctuations \cite{13,14}. The results presented here were obtained at much lower temperatures than in numerical simulations such that a direct comparison with experiments is possible.

Our analysis is based on the two-dimensional three-band Hubbard model \cite{14,17} with
the Hamiltonian $H - \mu N = H_0 - \mu N + H_U$, where

$$H_0 - \mu N = \sum_{i,\sigma}(\varepsilon_d - \mu)n_{d_i\sigma} + \sum_{j,\sigma}(\varepsilon_p - \mu)n_{p_j\sigma} + \sum_{<i,j>,\sigma} t_{ij}(d_{i\sigma}^\dagger p_{j\sigma} + h.c.),$$

and

$$H_U = U_d \sum_i n_{d_i\uparrow} n_{d_i\downarrow}.$$  (1)

Here $d_{i\sigma}^\dagger$ and $p_{j\sigma}^\dagger$ denote the electron creation operators for Cu-3d$_{x^2-y^2}$ and O-2p orbitals at sites $i$ and $j$, respectively with spin $\sigma$, and $n_{d_i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$. The one-electron part $H_0 - \mu N$ is determined by the local orbital levels $\varepsilon_d$ (Cu) and $\varepsilon_p$ (O) with charge-transfer energy $\Delta = \varepsilon_p - \varepsilon_d$, and a Cu-O hopping $t_{ij} = \pm t$ between nearest-neighbor Cu-O sites $<i,j>$, where the sign takes into account the phase factors for the 2p and 3d$_{x^2-y^2}$ orbitals. $\mu$ is the chemical potential and the interaction part $H_U$ consists of the on-site Coulomb repulsion $U_d$ (Cu). The calculations were performed for the parameter set $U_d = 6, \Delta = 4$ in the hole representation (as everywhere, the energy-unit is $t = 1$). This choice follows from recent QMC studies [3][4][10], where it was shown that the above parameter set leads to a consistent description of several important features of the HTSC.

Bickers and Scalapino have developed a propagator-renormalized fluctuation-exchange (FLEX) approximation [11] for the one-band Hubbard model based on the conserving approximation (CA) of Baym and Kadanoff [18] which has resulted in significantly improved agreement with QMC results [12]. Properties of the superconducting state in the same model were also studied recently by that method [13]. The starting-point of this self-consistent field solution is the non-interacting Hamiltonian $H_0$ in Eq. [1]. Diagonalization of $H_0$ leads to the eigenvalues $E_n^0(k)$ $(n=1,2,3)$ which build up the unperturbed bandstructure. The single-particle propagator of the non-interacting system $G^0$ can now be expressed in terms of these energies $E_n^0(k)$ and the corresponding eigenvectors $c_{n\nu}(k)$:

$$[G^0(k,\omega_m)]_{\nu,\nu'} = \sum_n \frac{c_{n\nu}(k)c_{n\nu'}^*(k)}{i\omega_m - E_n^0(k) + \mu},$$  (2)

which becomes a matrix labeled by the orbital indices ($\nu = d, p_x, p_y$) of the three-band Hubbard model. We employ the Matsubara ($T \neq 0$) formalism where the discrete fermionic
frequencies are given by \( \omega_m = (2m + 1)\pi T \), \( m = \{-2, -1, 0, 1, 2, \ldots\} \). The Coulomb interaction \( H_U \) is accounted for within the field-theoretical FLEX approximation by a power series for the self-energy. This series includes diagrams (symmetric in particle-hole and particle-particle channels) taking into account the interaction of electrons with density (d), spin (s), and particle-particle (p) fluctuations. For the present three-orbital Hubbard model the single-particle self-energy is as follows:

\[
\left[ \Sigma(k) \right]_{dd} = \frac{T}{N} \sum_q \left\{ G(k - q)_{dd} \left( V^{(2)}(q) + V^{(d)}(q) + V^{(s)}(q) \right) + G(-k + q)_{dd} V^{(p)}(q) \right\},
\]

(3)

where

\[
\begin{align*}
V^{(2)}(q) &= U^2_d \cdot \chi_{ph}(q), \\
V^{(d)}(q) &= \frac{1}{2} U^2_d \chi_{ph}(q) \left( \frac{1}{1 + U_d \chi_{ph}(q)} - 1 \right), \\
V^{(s)}(q) &= \frac{3}{2} U^2_d \chi_{ph}(q) \left( \frac{1}{1 - U_d \chi_{ph}(q)} - 1 \right), \\
V^{(p)}(q) &= -U^2_d \chi_{pp}(q) \left( \frac{1}{1 + U_d \chi_{pp}(q)} - 1 \right).
\end{align*}
\]

(4)

\( k \) stands for the fermionic momenta and Matsubara frequencies \( (k, \omega_m) \), and \( q \) for the bosonic \( (q, \nu_n) \) ones. \( \chi_{ph} \) and \( \chi_{pp} \) are the propagators of non-interacting particle-hole and particle-particle fluctuations:

\[
\begin{align*}
\chi_{ph}(q) &= -\frac{T}{N} \sum_k \left[ G(k + q) \right]_{dd} \left[ G(k) \right]_{dd}, \\
\chi_{pp}(q) &= \frac{T}{N} \sum_k \left[ G(k + q) \right]_{dd} \left[ G(-k) \right]_{dd}.
\end{align*}
\]

(5)

Inserting this self-energy into Dyson’s equation the single-particle propagator has to be computed self-consistently:

\[
\left[ G(k, \omega_m) \right]^{-1} = \left[ G^0(k, \omega_m) \right]^{-1} - \left[ \Sigma[G, U](k, \omega_m) \right],
\]

(6)

with \( G^0 \) standing for the single-particle propagator of the non-interacting system.
The single-particle excitations are determined by the peaks of the spectral-weight function

\[ A(k, \omega) = -\frac{1}{\pi} \sum_{\nu} \text{Im} \left[ G(k, \omega) \right]_{\nu, \nu}. \]  

(7)

For the analytic continuation of the Green’s function \( G \) to real frequencies \( \omega \) we employ a simple Padé algorithm [20]. All results were obtained on \( k \)-space lattices of \( 16 \times 16 \) points in the first Brillouin zone (BZ).

In Fig. 1, we plot the dispersion of the quasiparticle peak in \( A(k, \omega) \), which is located closest to the chemical potential \( \mu \) along the symmetry lines in the BZ. The hole doping (\( \delta = 0.25 \) away from half-filling) and the relatively high temperature (\( T = 0.1t \)) were chosen to compare our FLEX approximation to our best converged QMC simulations which were performed on a \( 8 \times 8 \) lattice (192 sites) with periodic boundary conditions. The FLEX dispersion for the single-particle excitations is in good agreement with the QMC data, in particular, for the peaks in \( A(k, \omega) \) crossing the chemical potential \( \omega = 0 \) in Fig. 1.

In order to test the influence of the temperature on the spectrum, we have also performed both FLEX calculations and QMC simulations for the even higher \( T = 0.5t \) for various dopings. Like in similar investigations for the single-band Hubbard model at the electronic filling \( \langle n \rangle = 0.83 \) at the same temperature [21], we find the \( \omega = 0 \) crossing in \( A(k, \omega) \) slightly above the flat band region at \( X = (\pi, 0) \), whereas this crossing occurs below this region at \( T = 0.1t \). This indicates a strong dependence of the \( \omega = 0 \) crossing on \( T \) at least in the high-temperature regime.

For the much lower temperature \( T = 0.01t \approx 150K \), Fig. 2 displays the spectral weight \( A(k, \omega) \) for energies near the chemical potential \( \mu \) and the three \( k \)-space lines as in Fig. 1. The hole doping was set to \( \delta = 0.15 \) away from half-filling in order to compare with spectroscopic measurements in the metallic phase of the HTSC. The pairs of numbers on the right side of each panel have to be multiplied by \( \pi/8 \) to give the corresponding \( k \)-vectors in the two-dimensional BZ. These curves can be directly compared with experimental data obtained from angle-resolved photoemission spectroscopy (ARPES) [2,3]. Good agreement
is found for the quasiparticle excitation spectra calculated by the FLEX approximation and the spectroscopic measurements. The main features of the experimental data are reproduced by our theoretical approach: Along the $\Gamma - M$ high symmetry direction we find a dispersing quasiparticle peak which crosses through the Fermi-energy near $k = (\pi/2, \pi/2)$. The two other symmetry lines in Fig. 2 clearly show the existence of the flat band dispersion near $X = (\pi, 0)$, the most striking result of the ARPES experiments. The quasiparticle peak of $A(k, \omega)$ is broadened for excitation energies away from $\mu$ due to strong correlation effects. In fact, it can be seen that not only the position of the maxima in $A(k, \omega)$ (dispersion) but also the overall shape of the spectra agrees with the experimental results.

The single-particle bandstructure obtained from the low-lying peak in $A(k, \omega)$ is depicted in Fig. 3 in comparison to results of ARPES experiments in Bi2212. In order to discern the influence of different many-body scattering channels, we present the data of three approximative stages: In the Hartree-Fock (HF) or band-theory approximation (dashed line in Fig. 3) the HF bandwidth, Fermi-velocities, and the characteristic energy-dispersion at $(\pi, 0)$ are far away from agreement with the experiment. Charge fluctuations given by $V^{(d)}(q)$ in Eqs. 3 and 4 tend to reduce these differences (dotted line in Fig. 3), but only the inclusion of both longitudinal and transverse magnetic fluctuations $[22] V^{(s)}(q)$ leads to a flat quasiparticle band near the Fermi-energy. The particle-particle channel $V^{(p)}(q)$ contributes only in a minor way to the full FLEX calculations (full line in Fig. 3) for the given parameter set. Therefore, Fig. 3 demonstrates that spin-fluctuations are responsible for the reduced energy-scales compared to mean-field calculations, especially for the flat dispersion near $\mu$ and the reduced saddle-point energy at $(\pi, 0)$. The most dominant contributions stem from magnetic modes with a wave-vector $q$ near to the antiferromagnetic point $(\pi, \pi)$.

Finally, Fig. 4 shows a strong correlation between the energy difference $\Delta \equiv E(X) - \mu$ and the energy $\omega_{\text{spin}}$ of the maximum in $\text{Im}\chi_{\text{spin}}(q, \omega)$ at the incommensurate wavevector, where $\text{Im}\chi_{\text{spin}}$ reaches its largest value in the BZ. This suggests that for dopings $\delta \lesssim 0.25$, the energy difference $\Delta$ is locked-in to the magnetic excitations close to the AF-point [23]. Moreover, we observe in our FLEX-calculations a linear $\omega$-dependence of $\text{Im}\Sigma$ down to
approximately the same energy-scale. Below this energy-scale, \(\text{Im } \Sigma \sim \omega^2\) as expected for a Fermi-liquid. Details of these features will be given elsewhere [24].

In summary, we presented the single-particle excitation spectrum of the three-band Hubbard model within the framework of a conserving approximation. This many-body approach is based on a self-consistent evaluation of Dyson’s equation including fluctuation-exchange (particle-hole and particle-particle) self-energy contributions. The results are in remarkable agreement with Quantum Monte Carlo data and spectroscopic experiments for low-lying single-particle excitation energies. The low-energy physics of this FLEX calculation is controlled by many-body fluctuations in the magnetic scattering channel leading to a significant reduction of characteristic bandstructure energy-scales from their mean-field values.

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REFERENCES

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[1] C. G. Olson et al., Phys. Rev. B 42, 381 (1990).

[2] G. Mante et al., Z. Phys. B 80, 181 (1990).

[3] D. S. Dessau et al., Phys. Rev. Lett. 71, 2781 (1993). Z.-X. Shen and D. S. Dessau, Phys. Reports, to be published.

Care has to be taken for the nomination of the high-symmetry points: The X-point of our two-dimensional cubic lattice corresponds to the M-point for the Bi 2212 compound and the M-point of our calculations corresponds to the X-point in Bi 2212.

[4] A. A. Abrikosov, J. C. Campuzano and K. Gofron, Physica C 214, 73 (1993).

[5] S. Massidda, J. Yu, and A. J. Freeman, Physica C 52, 251 (1988); H. Krakauer and W. E. Pickett, Phys. Rev. Lett. 60, 1665 (1988).

[6] G. Dopf, J. Wagner, P. Dieterich, A. Muramatsu, W. Hanke, Phys. Rev. Lett. 68, 2082 (1992).

[7] N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. 72, 705 (1994).

[8] E. Dagotto, A. Nazarenko, and M. Boninsegni, Phys. Rev. Lett. 73, 728 (1994).

[9] G. Dopf, A. Muramatsu, W. Hanke, Phys. Rev. Lett. 68, 353 (1992).

[10] G. Dopf, A. Muramatsu, and W. Hanke, Europhys. Lett. 17, 559 (1992).

[11] N. E. Bickers and D. J. Scalapino, Annals of Physics 193, 207 (1989).

[12] N. E. Bickers and S. R. White, Phys. Rev. B 43, 8044 (1991).
[13] D. J. Scalapino, E. Loh, and J. E. Hirsch, Phys. Rev. B 34, 8190 (1986); N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. 62, 961 (1989).

[14] T. Moriya, Y. Takahashi, and K. Ueda, J. Phys. Soc. Jpn. 59, 2905 (1990).

[15] P. Monthoux, A. V. Balatsky, and D. Pines, Phys. Rev. Lett. 67, 3448 (1991); P. Monthoux and D. Pines, Phys. Rev. Lett. 69, 961 (1992).

[16] C. M. Varma, et al., Solid State Comm. 62, 681 (1987).

[17] V. J. Emery, Phys. Rev. Lett. 58, 2794 (1987).

[18] G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961); G. Baym, Phys. Rev. 127, 1391 (1962).

[19] P. Monthoux and D. J. Scalapino, Phys. Rev. Lett. 72, 1874 (1994).

[20] H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. 29, 179 (1977).

[21] N. Bulut, D. J. Scalapino and S. R. White, Preprint UCSBTH–94–05.

[22] D. M. Frenkel and W. Hanke, Phys. Rev. B 42, 6711 (1990).

[23] It should be noted that the temperature $T=0.01t \approx 150K$ is still above the temperature where experimentally the onset of a spin-gap has been observed.

[24] R. Putz, W. Hanke, A. Muramatsu, to be published.
FIGURES

FIG. 1. Quasiparticle dispersion along three cuts through the Brillouin zone with the high-symmetry points $\Gamma=(0,0)$, $X=(\pi,0)$, $M=(\pi,\pi)$. The FLEX result for hole-doping $\delta=0.25$ and temperature $T=0,1t$ is compared with QMC data.

FIG. 2. Spectral-weight function $A(k,\omega)$ for excitation energies near the chemical potential and $k$-vectors along high-symmetry lines in the BZ.

FIG. 3. Quasiparticle dispersion along high-symmetry lines in the BZ. Hartree-Fock (HF) results (dashed line) and FLEX calculations which include only the charge scattering channel (dotted line) and all symmetrically chosen particle-hole and particle-particle channels (full line) are compared to ARPES experiments (open circles: Ref. [2], full circles: Ref. [3]).

FIG. 4. Energy-difference $E(X) - \mu$ and energy of magnetic excitations $\omega_{\text{spin}}$ close to the AF-point as a function of doping.
$U_d = 6$
\[\Delta = 4\]
\[\delta = 0.25\]
\[\beta = 10\]
Energy relative to the chemical potential \( \mu \)

Spectral function \( A(k, \omega) \)

\[ \Gamma \rightarrow X \quad X \rightarrow M \quad \Gamma \rightarrow M \]
$U_d = 6$
$\Delta = 4$
$\delta = 0.15$
$\beta = 100$
$U_d = 6$
$\Delta = 4$
$\beta = 100$

Energy scale / $t$

$E(X) - \mu$

$\omega_{\text{spin}}$