Analysis of the elementary excitations in high-$T_c$ cuprates: explanation of the new energy scale observed by ARPES

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Using the Hubbard Hamiltonian we analyze the energy- and momentum-dependence of the elementary excitations in high-$T_c$ superconductors resulting from the coupling to spin fluctuations. As a result of the energy dependence of the self-energy $\Sigma(k, \omega)$, characteristic features occur in the spectral density explaining the 'kink' in recent ARPES experiments. We present results for the spectral density $A(k, \omega)$ resulting from the crossover from $\text{Im} \Sigma(k, \omega) \propto \omega$ to $\text{Im} \Sigma(k, \omega) \propto \omega^2$, for the feedback of superconductivity on the excitations, and for the superconducting order parameter $\Delta(k, \omega)$. These results relate also to inelastic neutron scattering and tunneling experiments and shed important light on the essential ingredients a theory of the elementary excitations in the cuprates must contain.

For understanding the high-$T_c$ cuprates their elementary excitations are of central significance. Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool for studying the elementary excitations in high-$T_c$ superconductors because the spectral density contains all information about self-energy effects. Due to an improved angular resolution (momentum distribution curve (MDC) and energy distribution curve (EDC)), data became available which provide new insight on the momentum and frequency dependence of the self-energy $\Sigma(k, \omega)$. In particular, a 'kink' feature at $\hbar \omega \sim 50 \pm 15$ meV has been observed in hole-doped cuprates like Bi$_2$Sr$_2$CaCu$_2$O$_8$, Pb-doped Bi$_2$Sr$_2$CuO$_6$, and La$_{2-x}$Sr$_x$CuO$_4$. Experiments by Shen et al., observe the kink feature in all directions in the first Brillouin Zone (BZ). It exists in both the normal and superconducting states. On the other hand, Kaminski et al., discuss the break only along the $(0,0) \rightarrow (\pi, \pi)$ direction occuring when one goes from the normal to the superconducting state. Therefore, they did not analyze the feature observed by the other group. However, it is quite interesting that a close analysis of data of Kaminski et al., in the normal state reveals the same changes of the Fermi velocity, $v_F$, as noted by Shen et al.

Thus, there seems to exist a 'new' energy scale in hole-doped cuprates. Remarkably, the electron-doped counterparts (e.g. Nd$_{2-x}$Ce$_x$CuO$_4$) do not show a 'kink'. So far, interpretations are given in terms of the presence of a strong electron-phonon interaction, stripe formation, or coupling to a resonating mode. It is interesting that the experiments also observe a change in the dispersion of the elementary excitations going from the normal to the superconducting state. We will show that this results from the feedback effect of superconductivity on the elementary excitations.

In this letter we present a study of the spectral density $A(k, \omega)$ of the elementary excitations using an electronic theory based on Cooper-pairing due to an exchange of antiferromagnetic spin fluctuations. In particular, we show that the 'kink' in the spectral density can be naturally explained from the interaction of the quasiparticles (holes) with spin fluctuations. In agreement with recent experiments we will demonstrate that the 'kink' feature is present in both the normal and superconducting state. Thus, we are able to explain recent ARPES experiments which study in detail the spectral density and in particular the energy dispersion $\omega(k) = \epsilon(k) + \Sigma(k, \omega)$. It is significant that the self-energy $\Sigma(k, \omega)$ resulting from the scattering of the quasiparticles on spin fluctuations can explain the main features observed. We argue that our results for the elementary excitations suggest a crossover from Fermi liquid...
hopping integral. The imaginary part of the self-energy
self-consistently using the 2D one-band Hubbard Hamil-
tons. Here, \( \epsilon_k \) is a tight-binding energy dispersion on a square
lattice and \( \Sigma(k, \omega) \) and \( \Sigma'(k, \omega) \) are the real and imag-
inary part of the self-energy, respectively. We perform
our calculations for the elementary excitations
\begin{equation}
\omega(k, T) = \epsilon(k) + \Sigma(k, \omega, T)
\end{equation}
The superconducting gap function \( \phi(k, \omega) \) is calculated self-consistently using the 2D one-band Hubbard Hamiltonian for a CuO\(_2\)-plane, which reads on a square lattice
\begin{equation}
H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i \sigma}^+ c_{j \sigma} + c_{j \sigma}^+ c_{i \sigma}) + U \sum_i n_{i \uparrow} n_{i \downarrow}
\end{equation}
where \( \text{Im} \chi(q, \omega) \) is the imaginary part of the spin
suscetibility within the random phase approximation.
We determine the coupling of the quasi-particles to the
spin fluctuations using an effective perturbation theory
(FLEX) [12–14] which we calculate directly on the real \( \omega \)-axis.

These equations are standard, however it is important
to realize that due to the combined effects of Fermi sur-
face topology and \( \chi(q = Q, \omega) \) at the antiferromagnetic
wave-vector \( Q_{AF} = (\pi, \pi) \), the \( k \) and \( \omega \) dependence of
\( \Sigma(k, \omega) \) become very pronounced and change the disper-
sion \( \omega(k) \). It is known that the strong scattering of quasi-
particles on antiferromagnetic spin fluctuations results
in a non-Fermi liquid behavior of the quasiparticle self-
energy for low-lying energy excitations, in particular, in
\( \text{Im} \Sigma \sim \omega \) [13–14]. Clearly, it follows already from the
Eq. (4) that the expected doping and momentum depen-
dence resulting from the crossover from \( \Sigma \propto \omega^2 \) to \( \Sigma \propto \omega \),
i.e. to a non-Fermi liquid behavior, can be reflected in
\( \omega(k) \) and \( A(k, \omega) \). Simply speaking, the change in the
\( \omega \)-dependence of the self-energy \( \Sigma(k, \omega) \) changes the ve-
locity of the elementary excitations. Thus, for a given
\( k \)-vector, the MDC curve shows a 'kink' at some char-
acteristic frequency controlled by \( \omega_{sf} \) (\( \omega_{sf} = \text{spin fluctua-
tion energy} \)).

Regarding the superconducting state the \( k \)-
and \( \omega \)-dependence of the order parameter \( \Delta(k, \omega) \) is
important and yields the feedback of the superconducting
state on the elementary excitations.

This quite new structure in \( \omega(k, T) \) which is present
in both the normal and superconducting state is shown
in the figures exemplarily for optimal doping and results
from our calculations obtained by solving the above equa-
tions self-consistently within a conserving approximation
[13]. The full momentum and frequency dependence of
the quantities is kept and no further parameter is intro-
duced.

In Fig. 4 we present results for the frequency and mo-
mentum dependence of the spectral density in the normal
state exemplarily along the \( (0, 0) \rightarrow (\pi, 0) \) direction cal-
culated using the canonical parameters \( U = 4t \) and \( t = 250 \) meV
[17]. The changes in the \( k \)-dependence of the peak in \( A(k, \omega) \) reflect the characteristic features in the self-energy \( \Sigma(k, \omega) \) or in the velocity \( v_k \) of the quasiparticles.

The kink occurs at energies about \( \hbar \omega \approx 65 \pm 15 \) meV for optimal doping (\( x = 0.15 \)) and \( T_c \approx 65 \) K. We also find that the ‘kink’ feature is present in all directions
in the BZ (\( \omega \approx \omega_{sf} + v_F(\phi) k \), \( k \rightarrow (k, \phi) \)) and, in
particular, along the diagonal \( (0, 0) \rightarrow (\pi, \pi) \) as shown in the inset of Fig. 1. We get that the kink is
similar pronounced in both directions. Moreover, we see
from our calculations that this feature has only a weak
temperature dependence over a wide temperature range.
It changes only at very small temperatures which we will
describe later.

In Fig. 2 we show the positions of the peaks along
\( (0, 0) \rightarrow (\pi, 0) \) shown in Fig. 1 as a function of \( (k - k_F) \)
for different temperatures. We obtain only small changes due to superconductivity which almost coincide with the ‘kink’ position. Remarkably, the deviation at $k - k_F \approx 0.05 \ A^{-1}$ is due to the frequency dependence of the self-energy and reflects the transition from Fermi-liquid to a non-Fermi liquid behavior $(\Sigma \propto \omega)$ for low-energy frequencies as a function of temperature. We show in the inset the behavior of $\Sigma(k, \omega)$ calculated at very low temperatures $T = 0.003t \approx 0.9K$ (dashed line).

In order to investigate the effect of the self-energy $\Sigma(k, \omega)$ on the dispersion $\omega(k, T)$ we show in Fig. 3 results of our calculations for $\text{Im } \Sigma(k, \omega)$ at the wave vector along the node line of the superconducting order parameter in the first BZ. The transition from $\Sigma(k, \omega) \propto \omega^2$ to $\Sigma(k, \omega) \propto \omega$ for low-lying frequencies is shown for various temperatures. Note, the deviation from Landau’s theory (see solid curve in Fig. 3), $\text{Im } \Sigma \propto \omega$, results in our picture from the strong scattering of the quasi-particles on the spin fluctuations and is expected to disappear at temperatures $T \to 0$, see inset of Fig. 3. In particular, the changes in the velocity of quasiparticles are determined in EDC as $v^* = v_F / (1 + \Sigma''(\omega)/\omega)$ versus frequency. At the frequencies around 65 meV the $\text{Re } \Sigma(k, \omega)$ shows a flattening as can be seen via a Kramers-Kronig analysis of $\text{Im } \Sigma$.

Therefore, at this frequency the effect of the scattering on spin fluctuations almost disappears. Thus, we find a Fermi liquid behavior. Our results also agree with previous ones obtained within the spin-fermion model [5]. In our microscopic theory we also recover Fermi liquid behavior for $T \sim \omega < \omega_{sf}$. Here, $\omega_{sf}$ is the characteristic spin fluctuation energy measured in INS (roughly the peak position of $\text{Im } \chi(Q, \omega)$ [13]) and is typically around 25meV for hole-doped superconductors [24]. Previously we have shown that our $\omega_{sf}$ gives a good description of INS data [4]. On the other hand, for $T < T_c$ the scattering is also strongly reduced not only due to $\omega < \omega_{sf}$, but also due to a feedback effect of superconductivity which will be discussed in connection with Fig. 4.

There is a wide discussion whether or not layered cuprate superconductors behave like conventional Fermi liquids. Earlier experiments (for a review, see Ref. [21]) reveal non-Fermi liquid properties, in particular a linear resistivity $\rho(T)$ for optimal doping, non well-defined quasiparticle peaks above the superconducting transition temperature $T_c$ seen in ARPES [22], and a strong temperature dependence of the uniform spin susceptibility observed by nuclear magnetic resonance (NMR) [23]. The phenomenological concepts of a Marginal Fermi liquid (MFL) and a Nested Fermi liquid (NFL) have been introduced in order to explain the deviations in the normal state from Fermi liquid theory [15, 16]. Our results shed more light on this question. In agreement with the picture of Ruvalds and co-workers we obtain the $\omega$- and $T$-dependence of the self-energy mainly due to scattering of the quasiparticles on spin fluctuations which is strongest for a nested Fermi topology. This also provides a microscopic justification for the MFL approach.
Thus, for optimal doping ($x = 0.15$), the microscopic FLEX approximation includes the phenomenological concepts of both NFL and MFL. It would be interesting to extend our studies to the underdoped regime, however, the origin of the pseudogap is still unknown.

In Fig. 4 we demonstrate the feedback of superconductivity on $\Sigma(k,\omega)$. We expect that it is the strongest for $k \approx (\pi, 0.1 \pi)$ where the gap $\Delta(\omega)$ is maximal. One sees that mainly the superconducting properties in $\Delta(k,\omega)$ and in particular in $\text{Im} \Delta(k,\omega)$ induce changes in the self-energy. For the comparison with the experiment we also present our results for the superconducting gap. Note, this behavior of $\Sigma(k,\omega)$ and $\Delta(k,\omega)$ is related also to INS and optical conductivity experiments. In particular, the peak position of $\text{Im} \Sigma(k_n,\omega)$ is approximately at $3\Delta_0 - \omega_{sf} \approx \omega_{res} + \Delta_0$ ($\omega_{res}$ denotes the resonant frequency observed in INS) according to our previous analysis. This is in a good agreement with results obtained within the frame of the spin-fermion model.

It is remarkable that for electron-doped superconductors with a different dispersion $\epsilon_k$ in particular with a flat band lying 300meV below $\epsilon_F$ at $(\pi, 0)$, we get no 'kink' feature up to frequencies about 100meV. This is also in agreement with experiment. The reason behind this is that $\text{Im} \chi(q,\omega)$ has a peak at larger frequencies and which is much less pronounced than for hole-doped cuprates.

In summary, calculating the pronounced momentum and frequency dependence of the quasiparticle self-energy $\Sigma$ in hole-doped high-$T_c$ cuprates we find that this results in a 'kink' structure in the dispersion $\omega(k)$ which agrees well with recent ARPES experiments. For describing the physics in the cuprates it is important that the origin of the pseudogap is the coupling of the quasiparticles to the spin fluctuations. The reason for the kink structure is a change in the $\omega$-dependence of the self-energy $\Sigma$ from non-Fermi liquid to a Fermi liquid behavior. Due to a different spectrum $\text{Im} \chi(q,\omega)$ of the spin fluctuations in electron-doped cuprates we do not find a 'kink' in the corresponding spectral density. Furthermore, the feedback effects due to superconductivity on the elementary excitations clearly reflect the symmetry of the superconducting order parameter. The calculated density of states $N(\omega) \equiv A(\omega) = 1/N \sum_k A(k\omega)$ compares well with SIN tunneling data. However, due to spatial averaging such experiments do not exhibit a kink structure.

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