Analysis of the Elementary Excitations in High-T_c Cuprates: Explanation of the New Energy Scale Observed by Angle-Resolved Photoemission Spectroscopy

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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 $\Sigma(\mathbf{k}, \omega)$, characteristic features occur in the spectral density explaining the "kink" in recent angle-resolved photoemission spectroscopy experiments. We present results for the spectral density $A(\mathbf{k}, \omega)$ for the feedback of superconductivity on the excitations, and for the superconducting order parameter $\Delta(\mathbf{k}, \omega)$. 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.

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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. Because of 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 $\Sigma(\mathbf{k}, \omega)$. In particular, a "kink" feature at $\hbar\omega \sim 50 \pm 15$ meV has been observed in hole-doped cuprates like $Bi_2Sr_2CaCu_2O_8$, Pb-doped $Bi_2Sr_2CuO_6$, and $La_{2-x}Sr_xCuO_4$ [1–5]. Experiments by Bogdanov *et al.* [4] and Lanzara *et al.* [5] 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.* [3] discuss the break only along the $(0,0) \rightarrow (\pi, \pi)$ direction occurring when one goes from the normal to the superconducting state. Therefore, they did not analyze the feature observed by the other group [4,5]. However, it is quite interesting that a close analysis of data of Kaminski *et al.* [3] in the normal state reveals the same changes of the Fermi velocity, v_F, as noted by Bogdanov *et al.* [4] and Lanzara *et al.* [5]. Thus, there seems to exist a "new" energy scale in hole-doped cuprates. Remarkably, the electron-doped counterparts (e.g., $Ne_{2-x}Ce_xCuO_4$) do not show a kink [6]. So far, interpretations are given in terms of the presence of a strong electron-phonon interaction [5,6], stripe formation [7], or coupling to a resonating mode [3,8]. 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 [1–3]. 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 $A(\mathbf{k}, \omega)$ 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 states [2,4–6]. Thus, we are able to explain recent ARPES experiments which study in detail the spectral density and in particular the energy dispersion $\omega(\mathbf{k}) = \epsilon(\mathbf{k}) + \Sigma(\mathbf{k}, \omega)$. It is significant that the self-energy $\Sigma(\mathbf{k}, \omega)$ 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 to a non-Fermi-liquid behavior. Furthermore, we obtain a picture consistent with inelastic neutron scattering (INS) and tunneling measurements [9].

The theoretical analysis is based on the spectral density for the elementary excitations [10] within Nambu space [11] which are given by, after continuation to the real ω axis,

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma''(\mathbf{k}, \omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + [\Sigma''(\mathbf{k}, \omega)]^2} . \tag{1}$$

Here $\epsilon_{\mathbf{k}}$ is a tight-binding energy dispersion on a square lattice, and $\Sigma'(\mathbf{k}, \omega)$ and $\Sigma''(\mathbf{k}, \omega)$ are the real and imaginary parts of the self-energy, respectively. We perform our calculations for the elementary excitations

$$\omega(\mathbf{k}, T) = \epsilon(\mathbf{k}) + \Sigma(\mathbf{k}, \omega(\mathbf{k}, T), T) . \tag{2}$$

The superconducting gap function $\phi(\mathbf{k}, \omega)$ is calculated self-consistently using the 2D one-band Hubbard Hamiltonian for a CuO_2 plane, which reads on a square lattice

$$H = -\sum_{\langle ij \rangle \sigma} t_{ij} (c^+_{i\sigma} c_{j\sigma} + c^+_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{3}$$

Here $c_{i\sigma}^{+}$ creates an electron with spin σ on site i, U denotes the on-site Coulomb interaction, and t_{ij} is the hopping integral. The imaginary part of the self-energy is given by [9]

$$\mathrm{Im}\Sigma(\mathbf{k},\omega) = -\frac{U^2}{4}\int d\omega'\left[\coth\left(\frac{\omega'}{2T}\right) - \tanh\left(\frac{\omega'-\omega}{2T}\right)\right]\sum_{\mathbf{k}'}\mathrm{Im}\chi(\mathbf{k}-\mathbf{k}',\omega')\delta(|\omega-\omega'|-\epsilon_{\mathbf{k}'}), \tag{4}$$

where $\mathrm{Im}\chi(\mathbf{q},\omega)$ is the imaginary part of the spin susceptibility within the random phase approximation. We determine the coupling of the quasiparticles to the spin fluctuations using an effective perturbation theory (FLEX) [12–14] which we calculate directly on the real ω axis.

These equations are standard; however, it is important to realize that due to the combined effects of Fermi surface topology and $\chi(\mathbf{q}=\mathbf{Q},\omega)$ at the antiferromagnetic wave vector $\mathbf{Q}_{\mathrm{AF}} = (\pi,\pi)$, the $\mathbf{k}$ and ω dependence of $\Sigma(\mathbf{k},\omega)$ become very pronounced and change the dispersion $\omega(\mathbf{k})$. It is known that the strong scattering of quasiparticles on antiferromagnetic spin fluctuations results in a non-Fermi liquid behavior of the quasiparticle self-energy for low-lying energy excitations, in particular, in $\mathrm{Im}\Sigma \sim \omega$ [15,16]. Clearly, it follows already from Eq. (2) that the expected doping and momentum dependence 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 $\omega(\mathbf{k})$ and $A(\mathbf{k},\omega)$. Simply speaking, the change in the ω dependence of the self-energy $\Sigma(\mathbf{k},\omega)$ changes the velocity of the elementary excitations. Thus, for a given $\mathbf{k}$ vector, the MDC curve shows a kink at some characteristic frequency controlled by ω_{sf} (ω_{sf} = spin fluctuation energy). Regarding the superconducting state the $\mathbf{k}$ and ω dependence of the order parameter $\Delta(\mathbf{k},\omega)$ is important and yields the feedback of the superconducting state on the elementary excitations.

This quite new structure in $\omega(\mathbf{k},T)$ 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 equations self-consistently within a conserving approximation [13]. The full momentum and frequency dependence of the quantities is kept, and no further parameter is introduced.

In Fig. 1 we present results for the frequency and momentum dependence of the spectral density in the normal state exemplarily along the $(0,0)\rightarrow(\pi,0)$ direction calculated using the canonical parameters $U = 4t$, and $t = 250$ meV [17]. The changes in the $\mathbf{k}$ dependence of the peak in $A(\mathbf{k},\omega)$ reflect the characteristic features in the self-energy $\Sigma(\mathbf{k},\omega)$ or in the velocity $v_{\mathbf{k}}$ 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 [$\omega \approx \omega_{\mathrm{sf}} + \mathbf{v}_F(\phi)\mathbf{k}$, $\mathbf{k} = \mathbf{k}(k,\phi)$] and, in particular, along the diagonal $(0,0)\rightarrow(\pi,\pi)$ direction as shown in the inset of Fig. 1. We get that the kink is similarly 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 $(\mathbf{k}-\mathbf{k}_F)$ for different temperatures. We obtain only small changes due to superconductivity which almost coincide with the kink position. Remarkably, the deviation at $\mathbf{k}-\mathbf{k}_F \approx 0.05$ Å^{-1} is due to the frequency dependence of the self-energy and reflects the transition from Fermi liquid to a non-Fermi liquid behavior along the route $(0,0)\rightarrow(\pi,0)$ in the Brillouin zone (BZ) for both normal and superconducting states. In the inset we show results for the difference in the peak positions for the normal and superconducting states along the $(0,0)\rightarrow(\pi,0)$ direction in order to see also the feedback of superconductivity. Note, this disappears for $\mathbf{k}-\mathbf{k}_F \approx 0.05$ Å^{-1} corresponding to approximately 65 meV. We get changes of about 10 meV while Kaminski *et al.* [3] observe along the $(0,0)\rightarrow(\pi,\pi)$ direction a larger difference of about 20 meV. By inspecting Eq. (4) this is expected, since the feedback effect of superconductivity on χ is larger for $\mathbf{Q} \approx (\pi,\pi)$.

In order to investigate the effect of the self-energy $\Sigma(\mathbf{k},\omega)$ on the dispersion $\omega(\mathbf{k},T)$, we show in Fig. 3 results of our calculations for $\mathrm{Im}\Sigma(\mathbf{k}_n,\omega)$ at the wave vector along the node line of the superconducting order parameter in the first BZ. The transition from $\Sigma(\mathbf{k},\omega)\propto\omega^2$ to $\Sigma(\mathbf{k},\omega)\propto\omega$ for low-lying frequencies is shown for

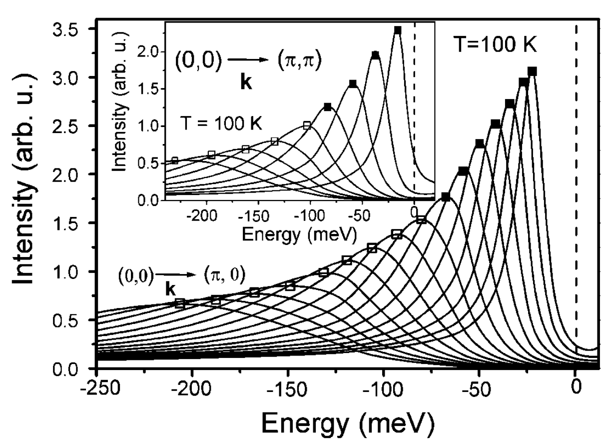

FIG. 1. Calculated self-energy effects in the spectral density of the quasiparticles in hole-doped superconductors in the normal state at $T = 100$ K and along the $(0,0)\rightarrow(\pi,0)$ direction. The dashed line at $\omega = 0$ denotes the unrenormalized chemical potential. In the inset the spectral density along the $(0,0)\rightarrow(\pi,\pi)$ direction is shown. In both cases at energies about $\hbar\omega \approx 65 \pm 15$ meV a "kink" occurs, since the velocity of the quasiparticles changes. The results are in good agreement with experiments (see, for example, Fig. 3 in Ref. [4] or Fig. 4b in Ref. [5]). Note the width of the spectral density peak is for $(0,0)\rightarrow(\pi,0)$ twice the one for $(0,0)\rightarrow(\pi,\pi)$.

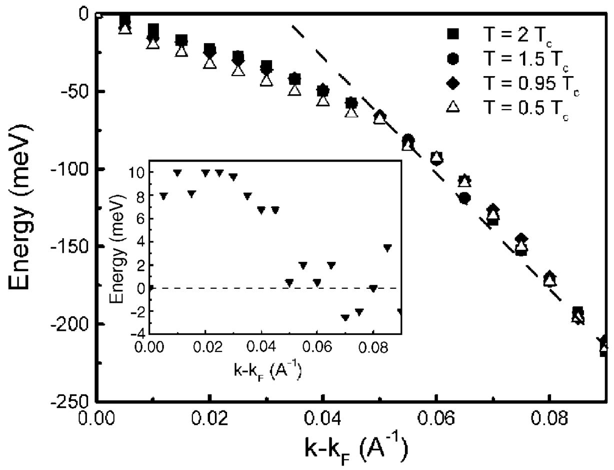

FIG. 2. Positions of the peaks in the spectral density $A(\mathbf{k}, \omega)$ versus $\mathbf{k} - \mathbf{k}_F$ (energy dispersion) along the $(0,0) \to (\pi, 0)$ direction of the BZ calculated within the FLEX approximation. This has to be compared with the position of the peaks derived from the momentum distribution curve (MDC) for a hole-doped superconductor as measured in experiment. The curves show a "kink" at energies about $\hbar\omega \approx 65 \pm 15$ meV. The dashed line is a guide to the eyes. We find small changes due to superconductivity which almost coincide with the kink position. Inset: Change in the peak position in $A(\mathbf{k}, \omega)$ in the superconducting state ($T = 0.5T_c$). The results are in fair agreement with ARPES data [3].

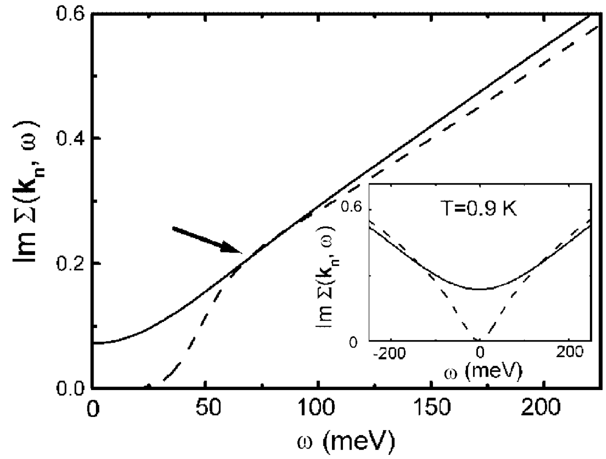

FIG. 3. Calculated frequency dependence of the quasiparticle self-energy at the node $\Sigma(\mathbf{k}_n, \omega)$, $\mathbf{k}_n = (0.4, 0.4)\pi$. The solid curves correspond to the normal state at $T = 2T_c$, whereas the dashed curves refer to the superconducting state at $T = 0.5T_c$. At $\mathbf{k} = \mathbf{k}_n$, where the superconducting gap vanishes, one clearly sees approximately at $\hbar\omega = 65$ meV a crossover from Fermi liquid behavior ($\Sigma \propto \omega^2$) 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 $\Sigma(\mathbf{k}_n, \omega)$ calculated at very low temperatures $T = 0.003t \simeq 0.9$ K (dashed line).

various temperatures. Note, the deviation from Landau's theory (see solid curve in Fig. 3), $\mathrm{Im}\Sigma \sim \omega$, results in our picture from the strong scattering of the quasiparticles 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 $v_F^* = v_F/(1 + \frac{d\Sigma_k'(\omega)}{d\omega})$ versus frequency. At the frequencies around 65 meV the $\mathrm{Re}\Sigma_k(\omega)$ shows a flattening as can be seen via a Kramers-Kronig analysis of $\mathrm{Im}\Sigma$. 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 [18]. In our microscopic theory we also recover Fermi liquid behavior for $T \sim \omega \ll \omega_{\mathrm{sf}}$. Here ω_{sf} is the characteristic spin fluctuation energy measured in INS [roughly the peak position of $\mathrm{Im}\chi(\mathbf{Q}, \omega)$ [19]] and is typically around 25 meV for hole-doped superconductors [20]. Previously, we have shown that our ω_{sf} gives a good description of INS data [9]. On the other hand, for $T < T_c$ the scattering is also strongly reduced not only due to $\omega < \omega_{\mathrm{sf}}$, 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 [16] we obtain the ω 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 [24]. Thus, for optimal doping ($x = 0.15$), the microscopic FLEX approximation includes the phenomenological concepts of both NFL and MFL [25]. It would be interesting to extend our studies to the underdoped regime; however, the origin of the pseudogap is still unknown [26].

In Fig. 4 we demonstrate the feedback of superconductivity on $\Sigma(\mathbf{k}, \omega)$. We expect that it is the strongest for $\mathbf{k} \approx (\pi, 0.1\pi)$ where the gap $\Delta(\omega)$ is maximal. One sees that mainly the superconducting properties in $\Delta(\mathbf{k}, \omega)$ and in particular in $\mathrm{Im}\Delta(\mathbf{k}, \omega)$ 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 $\Sigma(\mathbf{k}, \omega)$ and $\Delta(\mathbf{k}, \omega)$ is related also to INS and optical conductivity experiments. In particular, the peak position of $\mathrm{Im}\Sigma(\mathbf{k}_a, \omega)$ is approximately at $3\Delta_0 - \omega_{\mathrm{sf}} \approx \omega_{\mathrm{res}} + \Delta_0$ (ω_{res} denotes the resonant frequency observed in INS) according to our previous analysis [9]. This is in a good agreement with results obtained within the frame of the spin-fermion model [18].

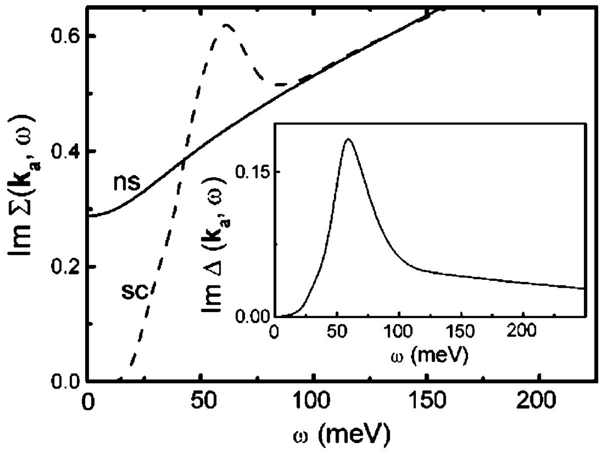

FIG. 4. Calculated frequency dependence of the quasiparticle self-energy $\Sigma(\mathbf{k}_a, \omega)$ at the wave vector $\mathbf{k} = \mathbf{k}_a \approx (1, 0.1)\pi$ (antinode). The solid curves correspond to the normal state at $T = 2T_c$, whereas the dashed curves refer to the superconducting state at $T = 0.5T_c$. For the wave vector $\mathbf{k}_a$ the feedback effect of superconductivity on the self-energy is shown. Inset: Superconducting gap function $\Delta(\omega)$ at wave vector $\mathbf{k} = \mathbf{k}_a$ versus frequency. Since the behavior of Δ and Σ is controlled by $\mathrm{Im}\chi(\mathbf{q}, \omega)$, we are able to connect these results to the resonance peak observed by INS in cuprates [9].

It is remarkable that for electron-doped superconductors with a different dispersion ϵ_k [27], in particular with a flat band lying 300 meV below ϵ_F at $(\pi, 0)$, we get no kink feature up to frequencies about 100 meV. This is also in agreement with experiment [6]. The reason behind this is that $\mathrm{Im}\chi(\mathbf{q}, \omega)$ has a peak at larger frequencies and is much less pronounced than for hole-doped cuprates [19].

In summary, calculating the pronounced momentum and frequency dependence of the quasiparticle self-energy Σ in hole-doped high-T_c cuprates we find that this results in a kink structure in the dispersion $\omega(\mathbf{k})$ which agrees well with recent ARPES experiments. For describing the physics in the cuprates it is important that the origin of this is the coupling of the quasiparticles to the spin fluctuations. The reason for the kink structure is a change in the ω dependence of the self-energy Σ from non-Fermi liquid to a Fermi liquid behavior. Because of a different spectrum $\mathrm{Im}\chi(\mathbf{q}, \omega)$ 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 $N(\omega) \equiv A(\omega) = 1/N \sum_{\mathbf{k}} A(\mathbf{k}\,\omega)$ compares well with SIN tunneling data [9]. However, due to spatial averaging such experiments do not exhibit a kink structure. In the following analysis we will also include effects due to electron-phonon interaction.

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