

Spectral Function of Superconducting Cuprates near Optimal Doping

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We argue that the unusual peak-dip-hump features observed in photoemission experiments on Bi2212 at $T \ll T_c$ can be explained by the interaction of the fermionic quasiparticles with overdamped spin fluctuations. We show that the strong spin-fermion interaction combined with the feedback effect on the spin damping due to superconductivity yields the fermionic spectral function $A(\mathbf{k}_F, \omega)$ which simultaneously displays a quasiparticle peak at $\omega = \Delta$ and a broad maximum (hump) at $\omega \gg \Delta$. In between the two regimes, the spectral function has a dip at $\omega \sim 2\Delta$. We argue that our theory also explains the tunneling data. [S0031-9007(98)07732-1]

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In recent years, the bulk of studies of cuprate superconductors was focused on their unusual normal state properties. Less attention was paid to the behavior of cuprates in the superconducting state. It was generally believed that the superconducting behavior, even in underdoped cuprates, is rather conventional in the sense that most experiments can be explained in the framework of the BCS-type theory for a d -wave superconductor. Recently, however, this belief has been challenged by photoemission experiments on Bi2212 materials [1,2]. These experiments demonstrated that even in slightly overdoped cuprates and at $T \ll T_c$, the spectral function $A(\mathbf{k}, \omega)$ near $(0, \pi)$ is qualitatively different from the one expected for a conventional superconductor. Specifically, in a conventional case, $A(\mathbf{k}, \omega)$ possesses a single sharp peak at $\omega = \sqrt{\Delta_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}}^2}$ where $\Delta_{\mathbf{k}}$ is the superconducting gap and $\epsilon_{\mathbf{k}}$ is the fermionic dispersion. The photoemission data for Bi2212 do show a sharp quasiparticle peak near the Fermi surface, but they also reveal two extra features in $A(\mathbf{k}, \omega)$: a dip at frequencies right above the peak and a broad maximum (hump) at somewhat larger frequencies. Moreover, as one moves away from the Fermi surface, the sharp peak loses its intensity but does not disperse, while the position of the hump varies with \mathbf{k} and gradually recovers the normal state dispersion.

Several phenomenological theories [1,3] identified the sharp peak observed in photoemission below T_c as a dispersionless collective mode of yet unknown origin. In the present Letter, we present an alternative explanation of the photoemission data. We argue that the unusual superconducting properties of cuprates can be explained by a strong interaction between electrons and overdamped spin fluctuations peaked at some momentum Q near (π, π) [4]. Similar arguments were earlier displayed by Grabowski *et al.* [5] who found peak-dip-hump features in their numerical study of the Hubbard model within the fluctuation exchange approximation. Our results qualitatively agree with theirs; however, we consider the problem analytically and present a physical explanation of the effect. Specifi-

cally, we show that the peak/dip/hump features in the spectral function emerge as a combination of two effects: (i) an almost complete destruction of the Fermi-liquid behavior in the normal state, which eliminates the quasiparticle peak and gives rise to a hump in the spectral function at higher frequencies, and (ii) a reduction of the spin damping at small frequencies in the superconducting state which, as a feedback effect, restores Fermi-liquid behavior of the spectral function in the frequency range $\omega < 2\Delta$. As a result, the spectral function near the Fermi surface possesses a quasiparticle peak at $\omega \sim \Delta$, a dip at $\omega \approx 2\Delta$ where the spectral function experiences a crossover to a non-Fermi liquid behavior, and a hump at a higher frequency. As \mathbf{k} moves away from the Fermi surface, the hump disperses with \mathbf{k} while the quasiparticle peak loses only its intensity as it cannot move farther in frequency than 2Δ . This behavior fully agrees with the photoemission results [1,2].

The point of departure in our calculations is the spin-fermion model for cuprates [6,7] in which low-energy fermions interact with their low-energy collective spin degrees of freedom. The input parameters for the model are the spin correlation length ξ , Fermi velocity v_F , and the spin-fermion coupling g . Perturbation theory holds in powers of the dimensional ratio $\bar{g} \propto g/(v_F \xi^{1/2})$ which obviously increases with decreasing doping. It was argued on the basis of a comparison with NMR data [6,7] that $\bar{g} \geq 1$ already in slightly overdoped cuprates, i.e., for comparison with experiments one needs to solve the spin-fermion model in the strong coupling limit.

One can show quite generally that due to the particular Fermi-surface (FS) geometry in cuprates, which allows for hot spots (i.e., points on the FS connected by Q), the full dynamical spin susceptibility possesses a dynamical exponent $z = 2$ [8]. For $\bar{g} \geq 1$, the $z = 2$ behavior extends above typical energies $v_F \xi^{-1/2}$ which dominate perturbation series. In this situation, the fermionic self-energy near hot spots, $\Sigma_f(\epsilon_{\mathbf{k}}, \omega)$, turns out to be independent of the quasiparticle energy [7], and is related via an integral equation over frequency with the dynamical part of the bosonic

self-energy $\Sigma_b(\Omega)$ at \mathbf{Q} . In the same regime, vertex corrections become irrelevant [9]. Furthermore, since \mathbf{Q} is the distance between hot spots, $\Sigma_b(\Omega)$ in turn is dominated by momentum integration near hot spots, i.e., it can be expressed as a frequency integral of $\Sigma_f(\omega)$. As a result, the problem generally reduces to a solution of two coupled integral equations for $\Sigma_f(\omega)$ and $\Sigma_b(\Omega)$.

For the normal state, the actual situation is simpler since in the absence of symmetry breaking, the fermionic self-energy, which depends only on frequency, does not affect the polarization bubble [10]. As a consequence, the exact $\Sigma_b(\Omega)$ is unaffected by Σ_f and is the same as for free fermions. Expanding the fermionic dispersion to linear order in $k - k_f$, one obtains [7] $\Sigma_b \xi^2 = i\Omega/\omega_{sf}$ where $\omega_{sf} = (3/16)v_F/(\bar{g}^2\xi)$. Accordingly, $\Sigma_f(\omega)$ is obtained by a straightforward integration over frequency and has the form [7] $\Sigma_f(\omega) = 2\omega/(1 + \sqrt{1 - i|\omega|/\omega_{sf}})$. For the normal state Green's function we then find $G_n(\mathbf{k}, \omega) \approx Z/[\Sigma_f(\omega) - \bar{\epsilon}_k]$ where $Z = \bar{g}^{-2}$ and $\bar{\epsilon}_k = Z\epsilon_k$. At small frequencies, $\omega < \omega_{sf}$, $\Sigma_f(\omega) \approx \omega + i\omega|\omega|/(4\omega_{sf})$, i.e., the Fermi-liquid behavior is preserved, and the spectral function $A(\mathbf{k}, \omega)$ has a conventional Fermi-liquid peak at $\omega = \bar{\epsilon}_k$ though with a reduced residue Z . For $\omega > \omega_{sf}$, however, the system crosses over to a region which is in the basin of attraction of the quantum critical point, $\xi = \infty$. In this region, $\bar{g}^2\Sigma_f(\omega) \approx e^{i\pi/4}|A\omega|^{1/2}\text{sgn}(\omega)$ where $A = 4\bar{g}^4\omega_{sf}$ is independent of ξ . As a result, instead of a sharp quasiparticle peak, the spectral function possesses only a broad maximum at $\omega = \bar{\epsilon}_k^2/(4\omega_{sf}) = \epsilon_k^2/A$. Experimentally, $\omega_{sf} \sim 10\text{--}20$ meV at optimal doping [6], which is comparable to the resolution of the photoemission experiments. In this situation, the photoemission experiments probe $\omega > \omega_{sf}$ where $A(\mathbf{k}, \omega)$ displays only a broad maximum (see Fig. 1a).

Consider now the situation at $T \ll T_c$. We argue that there are two key effects associated with superconductivity. First, the quasiparticle Green's function is modified due to the fermionic pairing. Second, there is a feedback effect on the bosonic self-energy $\Sigma_b(\mathbf{Q}, \omega)$ due to the opening of the superconducting gap which in turn influences the fermionic self-energy. Physically, this feedback effect is related to the fact that the opening of the superconducting gap near $(0, \pi)$ reduces the spin damping at low frequencies and hence increases ω_{sf} in the same frequency range. In other words, ω_{sf} in a superconductor acquires a frequency dependence. The full self-consistent treatment of the superconducting state is rather involved as not only Σ_f and Σ_b , but also the pairing susceptibility are self-consistently connected to each other. In our analysis below we assume that (i) the spectral weight of the pairing susceptibility at $T \ll T_c$ is mostly contained in the δ -functional peak, and (ii) that the feedback effect from superconductivity on the fermionic self-energy can be absorbed into the frequency dependence of ω_{sf} . The first assumption is valid as long as superconducting fluctuations are weak, which is likely to be the case outside the pseudogap regime. It implies that the BCS approximation is valid, i.e., that

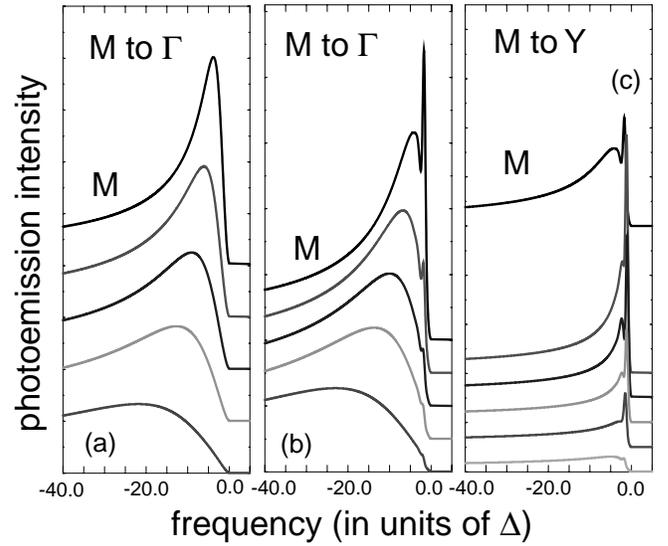


FIG. 1. The calculated quasiparticle spectral function in the normal state (a) and in the superconducting state along $M - \Gamma$ $[(0, \pi) - (0, 0)]$ (b) and $M - Y$ $[(0, \pi) - (\pi, \pi)]$ (c). The results are presented for $b = 5$. For the M point, we used $\bar{\epsilon} = \bar{\Delta}$. The theoretical data are convoluted with the Gaussian resolution function with the half width 0.25Δ .

$G_{sc}^{-1}(\mathbf{k}, \omega) = G_n^{-1}(\mathbf{k}, \omega) + \Delta_{\mathbf{k}}^2 G_n(-\mathbf{k}, -\omega)$ where $\Delta_{\mathbf{k}}^2$ is the strength of the d -wave pairing susceptibility. At this stage, we again reduce the problem to a set of two integral equations for Σ_f and Σ_b . The second assumption in essence eliminates the integral equation for Σ_f as it implies that $\Sigma_f(\omega) \approx 2\omega/[1 + \sqrt{1 - i|\omega|/\omega_{sf}(\omega)}]$. This assumption is physically motivated as the reduction of the spin damping at low frequencies is the key feedback effect due to superconductivity. Nevertheless, its application requires care as in a superconductor, Σ_b contains both imaginary and real parts (the latter gradually vanishes at $\omega \gg \Delta$). In a Fermi gas, both parts of Σ_b are *nonanalytic* functions of frequency at $\omega = 2\bar{\Delta}$ [$\text{Im} \Sigma_b \propto \Theta(\omega - 2\bar{\Delta})$] while $\text{Re} \Sigma_b \propto \ln|\omega - 2\bar{\Delta}|$, and $\text{Re} \Sigma_b$ has to be kept to preserve the analyticity of the retarded spin susceptibility at $T = 0$. In our case, the fermionic self-energy reduces the jump in $\text{Im} \Sigma_b$, but as long as $\text{Im} \Sigma_b$ is nonanalytic, $\text{Re} \Sigma_f$ still has to be kept at $T = 0$. On the other hand, the singularity in the real part of Σ_b is rather weak (logarithmical) even in a Fermi gas, and we expect that it is washed out by thermal fluctuations already at temperatures $T \sim T_{cl}$ which are much smaller than $\bar{\Delta}$. In the calculations below, we assume that $T_{cl} \ll T \ll \bar{\Delta}$, in which case the neglect of $\text{Re} \Sigma_f(\omega)$ does not yield unphysical results, and at the same time, one can neglect terms $\sim T/\Delta$, i.e., evaluate the polarization bubble at $T = 0$.

We now present our calculations. Substituting $G_n(\mathbf{k}, \omega)$ into the equation for $G_{sc}(\mathbf{k}, \omega)$, we obtain

$$G_{sc}(\mathbf{k}, \omega) = Z \frac{\Sigma_f(\omega) + \bar{\epsilon}_k}{\Sigma^2(\omega) - (\bar{\Delta}_{\mathbf{k}}^2 + \bar{\epsilon}_k^2)}, \quad (1)$$

where $\bar{\Delta}(\mathbf{k}) = Z\Delta(\mathbf{k})$. As in the normal state, the possibility to observe a sharp quasiparticle peak in the spectral

function depends on the ratio $\omega/\omega_{\text{sf}}(\omega)$: for $\omega < \omega_{\text{sf}}(\omega)$, $A(\mathbf{k}, \omega)$ possesses a conventional quasiparticle peak at $\omega = (\bar{\Delta}_{\mathbf{k}}^2 + \bar{\epsilon}_{\mathbf{k}}^2)^{1/2}$, while for $\omega > \omega_{\text{sf}}(\omega)$, it possesses only a broad maximum at $\omega = (\bar{\Delta}_{\mathbf{k}}^2 + \bar{\epsilon}_{\mathbf{k}}^2)/4\omega_{\text{sf}}(\omega)$.

Our next goal is to obtain $\omega_{\text{sf}}(\omega)$. For this we need to evaluate the polarization bubbles made of *full* normal and anomalous Green's functions. Near $(0, \pi)$, where $\bar{\Delta}(\mathbf{k})$ is close to its maximum value $\bar{\Delta}$, it is convenient to measure $\omega_{\text{sf}}(\omega)$ in units of $\bar{\Delta}$, i.e., introduce $b_\omega = \bar{\Delta}/\omega_{\text{sf}}(\omega)$ and $b = b_\infty = \bar{\Delta}/\omega_{\text{sf}}(\infty)$ where $\omega_{\text{sf}}(\infty)$ is the normal state value of ω_{sf} . In these variables, we obtained after momentum integration in the polarization bubbles

$$b_\omega = \frac{b}{\omega} \times \text{Re} \int_0^\infty d\Omega \frac{\bar{\Delta}^2 - \Sigma(\Omega_+)\Sigma(\Omega_-) + D(\Omega_+)D(\Omega_-)}{D(\Omega_+)D(\Omega_-)}, \quad (2)$$

where $\Omega_\pm = \Omega \pm \omega/2$, and $D(\Omega) = \sqrt{\Sigma^2(\Omega) - \bar{\Delta}^2}$. Unlike the normal state, this integral equation cannot be reduced to an algebraic one because the superconducting Green's function *cannot* be written as the normal state Fermi-gas result plus a momentum-independent self-energy. In other words, the condition for the non-renormalizability of Σ_b is lost in a superconductor.

The functional form of b_ω depends on the value of b which varies with doping. In overdoped cuprates, $\omega_{\text{sf}}(\infty) \gg \Delta$, i.e., $b \ll 1$. In this limit, the damping of the fermions in the polarization bubble is negligible [i.e., $\Sigma_f(\Omega_\pm) \approx \Omega_\pm$], the integral equation reduces to an algebraic one, and b_ω has the same functional form as the spin damping in the superconducting Fermi gas: it is zero for $\omega < 2\bar{\Delta}$, jumps to $b_\omega = b\pi/2$ at $\omega \geq 2\bar{\Delta}$, and gradually approaches b with increasing frequency [11]. In this situation, at frequencies comparable to Δ , $\omega/\omega_{\text{sf}} \ll 1$, i.e., the spectral function at $k = k_F$ indeed possesses a quasiparticle peak at $\omega = \bar{\Delta}$. It does not, however, possess a broad maximum at larger frequencies since at small b , ω becomes larger than $\omega_{\text{sf}}(\omega)$ only at $\omega \gg \bar{\Delta}^2/4\omega_{\text{sf}}(\omega)$.

Near optimal doping, however $\Delta \sim 30\text{--}40$ meV while $\omega_{\text{sf}} \sim 10\text{--}20$ meV, i.e., $b > 1$, and it further increases with decreasing doping. This is also corroborated by earlier calculations of Δ which yielded [7] $b \propto \xi$. Naively, one might expect that in this situation, b_ω becomes smooth, and the condition $\omega < \omega_{\text{sf}}(\omega)$ is satisfied only at frequencies much smaller than Δ . If this were the case, then one would not be able to observe the sharp quasiparticle peak below T_c . Solving Eq. (2) numerically (see Fig. 2), we found, however, that while the high frequency part of b_ω evolves with increasing b from a frequency independent to an almost linear in frequency form, a sharp drop in b_ω survives even for moderately large b . These results can also be obtained analytically. Analyzing the results, we found that for moderately large b , one still has $\omega < \omega_{\text{sf}}(\omega)$ at $\omega < 2\Delta$, however at $\omega > 2\Delta$, $\omega > \omega_{\text{sf}}(\omega)$.

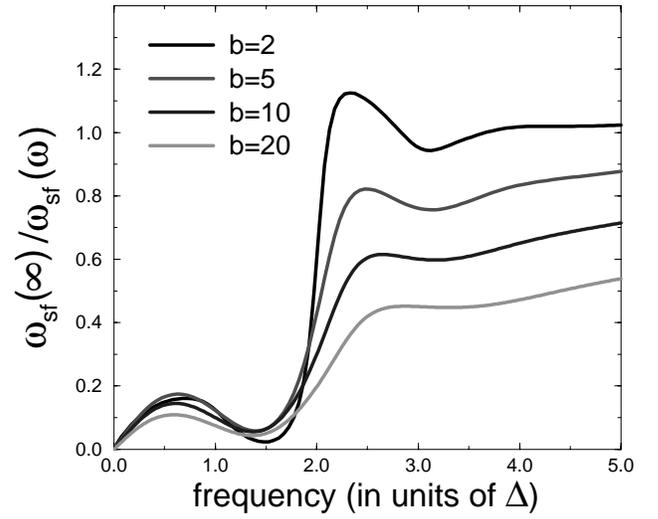


FIG. 2. The solution of the integral equation for the frequency-dependent spin-fluctuation frequency $\omega_{\text{sf}}(\omega)$ in the superconducting state. In the normal state, $\omega_{\text{sf}} = \omega_{\text{sf}}(\infty)$. For all $b = \bar{\Delta}/\omega_{\text{sf}}(\infty)$, $\omega_{\text{sf}}^{-1}(\omega)$ sharply drops at around $2\bar{\Delta}$. At very low frequencies, this result is valid only at finite T , while at $T = 0$, ω_{sf}^{-1} should be zero below some critical frequency [12]—its finite value here is an artifact of restricting with only the imaginary part of the bosonic self-energy.

This implies that the system is in the Fermi-liquid regime at $\omega < 2\bar{\Delta}$ (and, hence, still possesses a sharp quasiparticle peak at $\omega = \bar{\Delta}$), but it crosses over to the strong coupling regime at $\omega > 2\Delta$. Furthermore, for $b \gg 1$, the conditions $\omega > 2\bar{\Delta}$ and $\omega = \bar{\Delta}^2/4\omega_{\text{sf}}(\omega) \sim \bar{\Delta}b \gg \bar{\Delta}$ can be satisfied simultaneously. This implies that in addition to a peak at $\omega = \bar{\Delta}$, the spectral function at $k = k_F$ also possesses a broad maximum at $\omega \sim b\bar{\Delta} \gg \bar{\Delta}$. In between the two regimes, i.e., at $\omega \approx 2\bar{\Delta}$, the spectral function has a dip. This form of the spectral function, which we plotted in Fig. 1, is fully consistent with the photoemission data [1,2]. Furthermore, we find that the quasiparticle peak does virtually not disperse with \mathbf{k} as the region of Fermi liquid behavior does not extend farther than $2\bar{\Delta}$ away from the Fermi surface. Instead, the peak gradually decreases in amplitude as one moves away from \mathbf{k}_F . This is clearly seen in Figs. 1b,c. In contrast, the position of the hump follows $\omega \propto (\bar{\Delta}_{\mathbf{k}}^2 + \bar{\epsilon}_{\mathbf{k}}^2)$. Near $(0, \pi)$, where $\bar{\epsilon}_{\mathbf{k}}$ is small, the dispersion is weak, whereas farther away from the Fermi surface it disperses with \mathbf{k} and gradually recovers the normal state dispersion. In Fig. 3, we plotted the frequency position of the quasiparticle peak and hump in the superconducting state versus the normal state position of the hump. This dependence on momentum is also fully consistent with the photoemission data [1]. For even larger b , we found that though b_ω drops below $2\bar{\Delta}$, still $\bar{\Delta}/\omega_{\text{sf}}(\bar{\Delta}) > 1$, i.e., the system does not recover the quasiparticle peak below T_c . We attribute this behavior to heavily underdoped cuprates.

We also compute the density of states $N(\omega)$ in the superconducting state assuming that the dominant contribution to $N(\omega)$ comes from momenta near $(0, \pi)$. Integrating

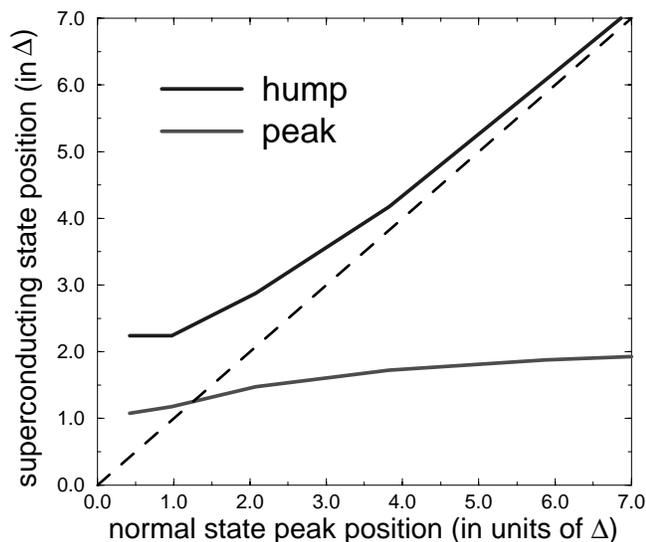


FIG. 3. The frequency position of the quasiparticle peak and the hump in the superconducting state versus position of the hump in the normal state obtained from Fig. 1.

$A(\mathbf{k}, \omega)$ over $\bar{\epsilon}_{\mathbf{k}}$, we obtain

$$N(\omega) \propto \text{Re} \frac{\Sigma_f(\omega)}{\sqrt{\Sigma^2(\omega) - \bar{\Delta}^2}}. \quad (3)$$

The plots of $N(\omega)$ for various b are presented in Fig. 4. We see that for all values of b , $N(\omega)$ possesses a peak at $\omega = a\bar{\Delta}$ where $a \approx 1$ for small b and gradually increases with increasing b . For larger b , $N(\omega)$ displays a dip at frequencies slightly larger than $2\bar{\Delta}$; the amplitude of the dip increases with b . Above the dip, $N(\omega)$ increases as $\sqrt{\omega}$ and eventually saturates. These results are in full agreement with the tunneling data in Ref. [13] except for the observed anisotropy between $N(\omega > 0)$ and $N(\omega < 0)$ for which we do not have an explanation.

Finally, we discuss the value of the gap and its variation with doping. Our theory predicts that at some distance away from the Fermi surface, the quasiparticle peak in $A(\mathbf{k}, \omega)$ should be located at $\omega \approx 2\bar{\Delta}$. Applying this result to nearly optimally doped Bi2212 materials studied in Refs. [1,2], we obtain $\bar{\Delta} \sim 25\text{--}30$ meV. Almost the same result is obtained by extracting $2\bar{\Delta}$ from the onset of the dip in the measured $N(\omega)$ [13]. The gap obtained formally as half distance between the peaks in $N(\omega)$ is larger, but Fig. 4 shows that this distance becomes progressively larger than $\bar{\Delta}$ with increasing b . We performed the same analysis of the tunneling data for the $T_c = 83$ K underdoped material, and obtained almost the same value of $\bar{\Delta}$ as at optimal doping. We therefore argue that $\bar{\Delta}$ almost saturates around optimal doping, and the observed increase of the peak frequency in $N(\omega)$ with decreasing doping is mostly due to strong coupling effects which shift the peaks towards higher frequencies.

To summarize, in this paper we present the explanation of the unusual peak/dip/hump features observed in photoemission experiments on Bi2212 at $T \ll T_c$. We show

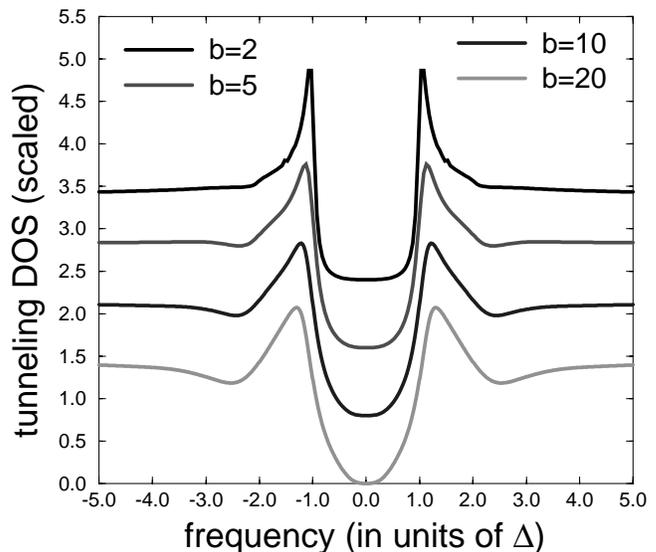


FIG. 4. The tunneling density of states in the superconducting state. Observe the development of a dip with increasing b .

that these features emerge due to a strong spin-fermion interaction combined with the feedback effect on the spin damping due to fermionic pairing. We argue that our theory also explains the tunneling data for the superconducting density of states. We predict that the superconducting gap saturates around optimal doping, and that the observed increase of the peak frequency in the tunneling density of states with decreasing doping is chiefly due to strong coupling effects.

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