

Analysis of the resonance peak and magnetic coherence seen in inelastic neutron scattering of cuprate superconductors: A consistent picture with tunneling and conductivity data

D. Manske,¹ I. Eremin,^{1,2} and K. H. Bennemann¹¹*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*²*Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany*

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Assuming the exchange of antiferromagnetic spin fluctuations as the Cooper pairing mechanism we calculate the doping dependence of the resonance peak seen in inelastic neutron scattering and the magnetic coherence effect. Most importantly, we find that the resonance peak in the magnetic susceptibility, $\text{Im } \chi(\mathbf{q}, \omega)$, appears *only* in the superconducting state, that it scales with T_c , and that magnetic coherence is a result of a d -wave order parameter. We further analyze the structure of $\text{Im } \chi$ below T_c , the position of the peak at ω_{res} and the consequences for photoemission, tunneling spectroscopy, and the optical conductivity.

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For analyzing the pairing mechanism in high- T_c superconductors it is important to understand the spin-excitation spectrum as observed by inelastic neutron scattering (INS).^{1,2} In particular the doping and temperature dependence of the spin susceptibility $\text{Im } \chi(\mathbf{q}, \omega)$ and its relationship to the superconducting transition temperature T_c are important. INS experiments show the appearance of a resonance peak at ω_{res} only below T_c (Ref. 1) and find a constant ratio of $\omega_{res}/T_c \approx 5.4$ for underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) and overdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO).²⁻⁵ Recent INS data on $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) reveal strong momentum- and frequency-dependent changes of $\text{Im } \chi(\mathbf{q}, \omega)$ in the superconducting state, which the authors called magnetic coherence effect.⁶ In particular, $\text{Im } \chi(\mathbf{Q}_i)$ with $\mathbf{Q}_i = (1 \pm \delta, 1 \pm \delta)\pi$ is strongly suppressed compared to its normal-state value below $\omega \lesssim 8$ meV, while it increases above this frequency. Furthermore, the incommensurate peaks become sharper in the superconducting state.⁶ Several theoretical approaches have been considered for the resonance peak,⁷⁻¹¹ its relation to the spectral function seen in angle-resolved photoemission spectroscopy (ARPES) and tunneling data,^{12,13} and for the magnetic coherence,¹⁴ but no unified theory has been presented. Here, using an electronic theory, we perform calculations to demonstrate the significance of the feedback of superconductivity on $\text{Im } \chi$. This permits us to derive for underdoped and overdoped cuprates the relationship between different measurements like optical conductivity and tunneling. So far the resonance peak and magnetic coherence have been treated separately and in both cases without taking into account this important feedback of superconductivity on $\text{Im } \chi$.

In this paper we use an electronic theory for the spin susceptibility and for the Cooper pairing via exchange of antiferromagnetic spin fluctuations to analyze the consequences of the superconducting feedback on magnetic coherence and the resonance peak, and on the relationship between INS, tunneling, and optical conductivity. The investigation of the effect of superconductivity on $\text{Im } \chi$ is an extension of our previous work.^{10,15} Using random-phase approximation (RPA) and self-consistent FLEX (Ref. 16) calculations for $\text{Im } \chi(\mathbf{q}, \omega)$, we present results for the kinematic gap (or spin gap) ω_0 , ω_{res} , ω_{res}/T_c , and the gap function $\Delta(\omega)$ in rea-

sonable agreement with experiments. Most importantly, we find that our electronic theory can explain consistently within the same picture inelastic neutron scattering, optical conductivity, and SIN tunneling data. Furthermore, the same physical picture gives results for underdoped and overdoped cuprates.^{17,18}

In order to analyze the kinematic gap and the position of the resonance peak it is instructive to start with the bare Lindhard BCS susceptibility⁷ at $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$

$$\text{Im } \chi_0(\mathbf{Q}, \omega) = \frac{1}{2} \sum_k \{ [1 - 2f(E_k)] \delta(\omega + 2E_k) + [2f(E_k) - 1] \delta(\omega - 2E_k) \}, \quad (1)$$

where $f(E_k)$ is the Fermi function and $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ is the dispersion of the Cooper pairs in the superconducting state. We use a gap function with d -wave symmetry, $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y)/2$, which can be calculated self-consistently within our FLEX approach. For the normal-state dispersion, we employ a tight-binding band

$$\epsilon_{\mathbf{k}} = -2t[\cos k_x + \cos k_y - 2t' \cos k_x \cos k_y - \mu/2]. \quad (2)$$

Here, t is the nearest-neighbor hopping energy, t' denotes the ratio of next-nearest-neighbor to nearest-neighbor hopping energy, and μ is the chemical potential. We use t' as a fitting parameter in order to describe the Fermi surface topology of both materials YBCO and LSCO. In Eq. (1) we take $t' = 0$ and, for simplicity, we do not consider a bilayer coupling via a hopping integral t_{\perp} .^{19,20} $\text{Im } \chi_0(\mathbf{Q}, \omega)$ involves two characteristic frequencies. The first, ω_{DOS} , arises from the density of states of the Bogolubov quasiparticles (i.e., the Cooper pairs) which have a gap in their spectrum due to superconductivity, $\omega_{DOS} \approx 2\Delta(x, T)$. Here, x is the doping concentration. The second, ω_0 , at which $\text{Im } \chi_0(\mathbf{Q}, \omega)$ starts to increase, represents the existence of a d -wave superconducting order parameter and is the so-called kinematic gap.^{7,20} We point out that for $t' > 0.3$ the kinematic gap is washed out.

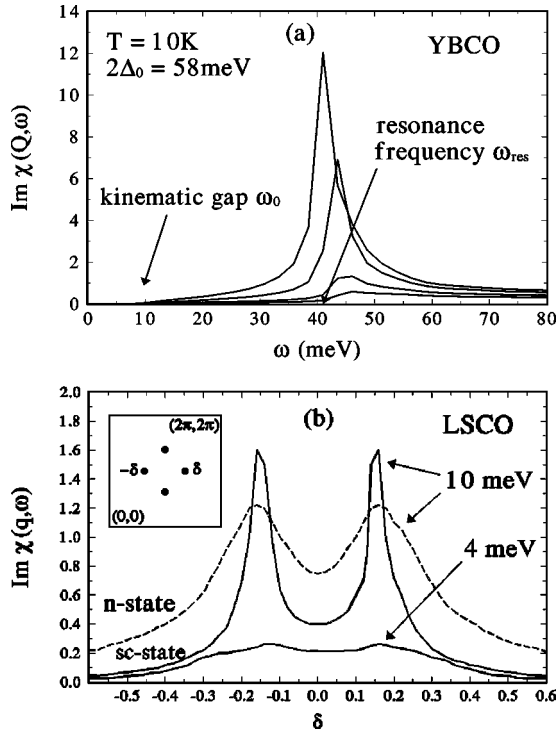


FIG. 1. Numerical results for the resonance peak and magnetic coherence in the weak-coupling limit. (a) Imaginary part of the RPA spin susceptibility (in units of states/eV) versus ω in the superconducting state at wave vector $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$ for $U/t = 1, 2, 3$, and 4 (from bottom to top). As in Ref. 1 we find $\omega_{res} = 41$ meV. Below the kinematic gap ω_0 , $\text{Im} \chi(\mathbf{Q}, \omega)$ is zero. (b) Calculated magnetic coherence: the solid curves correspond to the superconducting state whereas the dotted curve is calculated in the normal state. The observed four peaks occur at $\mathbf{Q}_i = (1 \pm \delta, 1 \pm \delta)\pi$ and in the figure we show only the peaks at $\mathbf{Q}_i = (1, 1 \pm \delta)\pi$. In our calculations we find $\delta \approx 0.18$. These results are in fair agreement with experiments, see Ref. 6.

In Fig. 1(a), results for the spin susceptibility

$$\text{Im} \chi(\mathbf{Q}, \omega) = \frac{\text{Im} \chi_0(\mathbf{Q}, \omega)}{[1 - U \text{Re} \chi_0(\mathbf{Q}, \omega)]^2 + U^2 [\text{Im} \chi_0(\mathbf{Q}, \omega)]^2} \quad (3)$$

are shown. Here, U stands for an effective Hubbard interaction. We choose $t' = 0.2$ in order to describe the Fermi surface topology of both YBCO and LSCO. Generally, one finds that the structure of $\text{Im} \chi$ is determined by $\text{Im} \chi_0$ if $(U \text{Re} \chi_0) \neq 1$ and by $(U \text{Re} \chi_0) = 1$ if this can be fulfilled. We again find the two characteristic frequencies ω_0 and $\omega_{res} \approx \omega_{DOS}$ at which $\text{Im} \chi$ is peaked. Furthermore, one clearly sees that for increasing U the peak in $\text{Im} \chi$ shifts to lower energies, and most importantly, becomes resonant for $U = U_{cr}$, which satisfies the condition

$$\frac{1}{U_{cr}} = \text{Re} \chi_0(\mathbf{q} = \mathbf{Q}, \omega = \omega_{res}), \quad (4)$$

which signals the occurrence of a spin-density-wave collective mode. The real part is given (at $T = 0$) by

$$\begin{aligned} \text{Re} \chi_0(\mathbf{Q}, \omega_{res}) &= \sum_{\mathbf{k}} \frac{E_{\mathbf{k}} E_{\mathbf{k}+\mathbf{Q}} - \epsilon_{\mathbf{k}} \epsilon_{\mathbf{k}+\mathbf{Q}} - \Delta_{\mathbf{k}} \Delta_{\mathbf{k}+\mathbf{Q}}}{(E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{Q}})^2 - \omega^2} \frac{E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{Q}}}{2E_{\mathbf{k}} E_{\mathbf{k}+\mathbf{Q}}}. \end{aligned} \quad (5)$$

$\text{Re} \chi_0(\mathbf{Q}, \omega_{res})$ has been investigated in detail in Ref. 10, where it was found that the spin-density-wave collective mode that satisfies Eq. (4) can explain the dip and hump feature observed in the photoemission spectra on BSCCO.²¹ In particular, it was shown that the broad humps are at the same position for both the normal and superconducting state.

We find from Eq. (3) that in the normal state where no resonance appears, the spin-wave spectrum is mainly determined by the spin-fluctuation frequency ω_{sf} (roughly the peak position) and

$$\text{Im} \chi(\mathbf{Q}, \omega) = \frac{\omega \omega_{sf}}{\omega^2 + \omega_{sf}^2}. \quad (6)$$

In the superconducting state one finds that $\text{Im} \chi$ peaks resonantly at ω_{res} where $\omega_{res} \approx 2\Delta$ as it can be already seen from Eq. (1). More precisely, we find for *optimal doping*, where Eq. (4) determines the structure of $\text{Im} \chi$, the important relation $\omega_{res}(T) = 2\Delta_0(T) - \omega_{sf}(T)$. Physically speaking, the resonance peak appearing in INS only below T_c is mainly determined by the maximum of the superconducting gap, but renormalized by normal-state spin excitations. This provides a simple explanation for the observed 41 meV resonance peak in optimally doped YBCO,¹ because Raman data suggest $2\Delta = 58$ meV (Ref. 22) and $\omega_{sf}^{\text{NS}} \approx 17$ meV (at 100 K) as extracted from NMR experiments.²³

In Fig. 1(b) we show results for the \mathbf{q} dependence of $\text{Im} \chi(\mathbf{q}, \omega)$. We perform our calculations for $U = 2t$ and a superconducting gap of $2\Delta = 10$ meV as measured in Raman scattering in optimally doped $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.²⁴ For $\omega = 10$ meV we get two peaks at $\mathbf{q} = \mathbf{Q}_i$. In the superconducting state we find a sharpening of the peaks due to the occurrence of a gap. This simply means that the lifetime of the quasiparticles is enhanced due to a reduced scattering rate. At 4 meV these peaks are strongly suppressed as seen in the experiment.⁶ Furthermore, we find no signal for $\omega < 4$ meV. This is due to the kinematic gap seen in Fig. 1(a) which is independent of \mathbf{q} . Note, the situation would be totally different if LSCO would have an isotropic gap where all states for $0 < \omega < 2\Delta_0 \approx 20$ meV would be forbidden. In this case no kinematic gap (or spin gap) would be observed. Thus, we can conclude from Fig. 1 that, already in the weak-coupling limit where no lifetime of the Cooper pairs (i.e., Δ independent of ω) is considered, we are able to explain the resonance peak and the magnetic coherence effect.

In order to consider the important feedback effect of Δ on the spin excitation spectrum, we now discuss our results obtained in the strong-coupling limit (i.e., ω dependent) solving self-consistently the generalized Eliashberg equations within the FLEX approximation.^{15,16} Note that only U/t and the tight-binding dispersion relation $\epsilon(\mathbf{k})$ (with its band filling μ) enter the theory as free parameters.

In Fig. 2(a) we present results for $\text{Im} \chi(\mathbf{Q}, \omega)$ calculated for $U = 4t$ and for an optimum doping concentration x

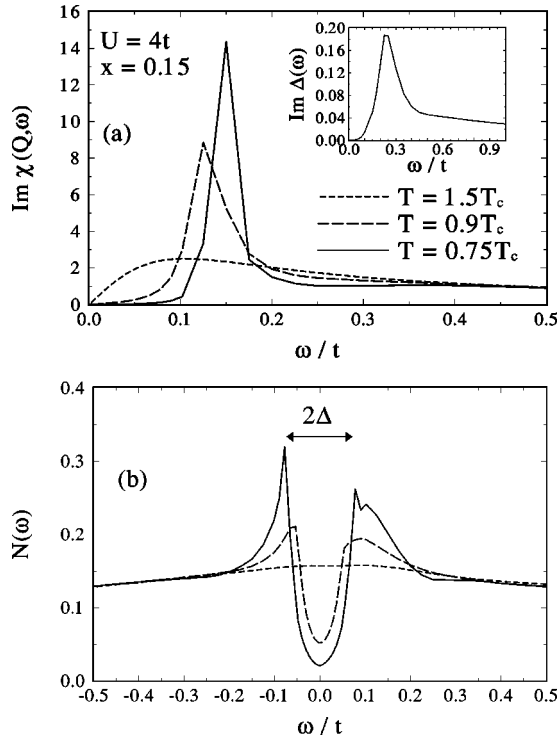


FIG. 2. Consistent picture of INS and tunneling data. (a) Imaginary part of the RPA spin susceptibility at $\mathbf{q}=\mathbf{Q}=(\pi, \pi)$ calculated within the FLEX approximation. For the normal state (dotted) we get $\omega_{sf}=0.1t$ and in the superconducting state we obtain $\omega_{res}=0.15t$. Assuming $t=250$ meV we find that $0.16t=40$ meV. Inset: Imaginary part of the gap function at $T=0.075T_c$ for wave vector $\mathbf{q}=(\pi, 0)$. (b) Calculated density of states for the same parameters and temperatures as in (a).

$=0.15$ ($\mu=1.65$). In the normal state (dotted curve) we find $\omega_{sf}=0.1t$, whereas for $T<T_c$ the resonance peak (solid curve) appears at $\omega_{res}=0.15t$. The dashed curve corresponds to $T=0.9T_c$ where the superconducting gap starts to open. Thus, the peak position reveals information on the temperature dependence of the superconducting gap. For temperatures $T<0.75T_c$ the resonance peak remains at $\omega_{res}=0.15t$ and only the peak height increases further. We find that the height of the peak is of the order of the quasiparticle lifetime $1/\Gamma(\omega_{res})$, where $\Gamma(\mathbf{k}, \omega)=\omega \text{Im} Z(\mathbf{k}, \omega)/\text{Re} Z(\mathbf{k}, \omega)$. Z denotes the mass renormalization within the Eliashberg theory. Thus we can conclude that the resonance peak becomes observable because the scattering rate decreases drastically below T_c .¹⁰

In Fig. 2(b) we show the corresponding calculated density of states $N(\omega)$. Below $T<0.75T_c$ we find that the value of 2Δ determined from peak to peak stays approximately constant and is very close to the value ω_{res} seen in INS, i.e., 41 meV, as shown in Fig. 2(a). This is in good agreement with measured SIN tunneling data in Ref. 25. However, in SIN tunneling a renormalized value of 2Δ is observed. Note, a direct measurement of $\Delta(\omega)$ (e.g., SIS tunneling) would lead to higher values. For example, we show in the inset of Fig. 2(a) the imaginary part of the gap function at wave vector $\mathbf{q}=(\pi, 0)$ where the gap has its maximum. It is peaked at $\omega=0.25t$.

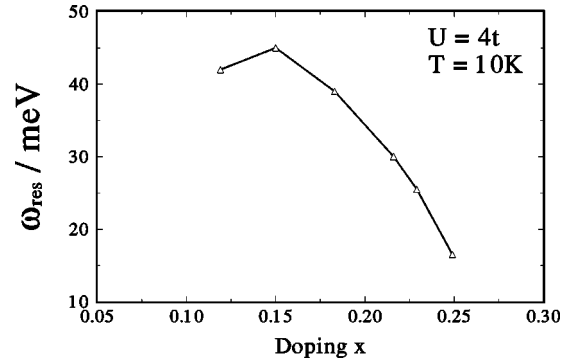


FIG. 3. Calculated FLEX results ω_{res} versus doping. In the overdoped regime, with $T_c \propto \Delta_0$ (Ref. 18), we find a constant ratio of $\omega_{res}/T_c \approx 8$.

In Fig. 3 we show results for ω_{res} as a function of the doping concentration. We find that for a fixed U Eq. (4) cannot be fulfilled in the overdoped case.²⁶ Thus we find that in this regime the resonance peak is mainly determined by $\text{Im} \chi_0(\mathbf{Q}, \omega)$ and thus by $2\Delta_0$. On general grounds one expects $T_c \propto \Delta_0$ in the overdoped regime, where the system behaves mean-field- (BCS) like. Recently, this has been confirmed within the FLEX approach.¹⁸ Thus, we conclude that ω_{res}/T_c should be a constant ratio. We find $\omega_{res}/T_c \approx 8$, which is larger than the observed value in BSCCO.² This is due to an underestimation of T_c within FLEX.

In contrast to the overdoped case we find in the underdoped regime, where $T_c \propto n_s$ (n_s denotes the superfluid density),¹⁸ that the resonance condition Eq. (4) yields $\omega_{res} \propto \omega_{sf}$, which is decreasing. Note that the superconducting gap guarantees that Eq. (4) is fulfilled. Thus we find a decreasing resonance frequency for decreasing doping in agreement with earlier calculations.^{11,27} To summarize our discussion we have the following result:

$$\omega_{res} \approx \begin{cases} \omega_{sf}, & \text{underdoped} \\ 2\Delta_0 - \omega_{sf}, & \text{optimal doping} \\ 2\Delta_0, & \text{overdoped,} \end{cases} \quad (7)$$

where the optimally doped case corresponds to $x_{opt}=0.15$ holes per copper site. This predicted doping dependence of the resonance peak position should be further tested experimentally.

In order to discuss the consequences of our analysis, in particular the feedback of superconductivity on $\text{Im} \chi$ for various superconducting properties, we derive²⁸

$$\text{Im} \Sigma(\omega) = -\frac{U^2}{4} \int_{-\infty}^{\infty} d\omega' \left[\coth\left(\frac{\omega'}{2T}\right) - \tanh\left(\frac{\omega' - \omega}{2T}\right) \right] \\ \times \text{Im} \chi(\mathbf{Q}, \omega') \sum_{\mathbf{k}} \delta(|\omega - \omega'| - E_{\mathbf{k}}), \quad (8)$$

where $N(\omega) = \sum_{\mathbf{k}} \delta(|\omega| - E_{\mathbf{k}})$ is the density of states. Equation (8) is valid in *both* the normal and superconducting state. It permits discussion of how much $\Sigma(\omega)$ reflects ω_{sf} and ω_{res} , for example. We see that the feedback of superconductivity on $\text{Im} \chi$ causes approximately a shift for the

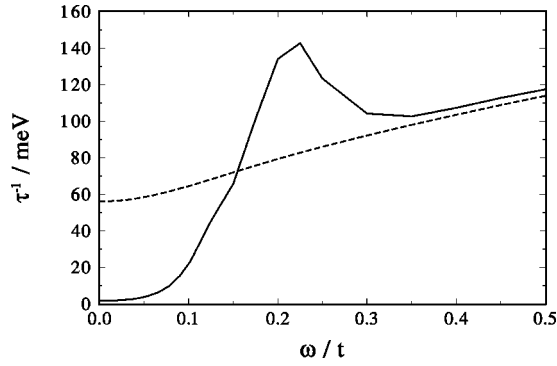


FIG. 4. Calculated scattering rate in the normal state for $T = 1.5T_c$ (dotted curve) using Eq. (8) and superconducting state $0.75T_c$ (solid curve) using Kubo formula and yielding a threshold ($2\Delta_0 + \omega_{res}$). The results are in fair agreement with Ref. 29.

elementary excitations $\omega \rightarrow \omega + \Delta_0$ for the superconducting state in the spectral density $U^2 \text{Im} \chi(\mathbf{Q}, \omega)/4$. Note using Eq. (6) for Eq. (8) would not take into account the important feedback of superconductivity on $\text{Im} \chi(\omega)$. Hence we use for the superconducting state the Kubo formula and calculate σ from (GG+FF). Equation (8) can be used to demonstrate the relationship between INS and optical conductivity measurements for the normal state. Using Drude theory we find that

the scattering rate $\tau^{-1}(\omega)$ agrees qualitatively with $-2 \text{Im} \Sigma(\omega)$ in the normal state. However, in order to get a quantitative agreement with experimental data one has to use $\tau^{-1}(\omega) = \Gamma(\mathbf{Q}, \omega)$. This is shown in Fig. 4, in good agreement with Ref. 29. From this analysis we can conclude that optical conductivity data and thus the lifetime of the quasiparticles, as well as the resonance peak and SIN tunneling data, can be understood within our electronic theory.

In summary, we are able to explain consistently all characteristic facts about the spin excitation spectrum and its doping dependence in high- T_c cuprates within an electronic theory. In particular we find that the resonance peak is a rearrangement of spectral weight of the normal state, which happens only below T_c . Furthermore we show that magnetic coherence is connected with the resonance peak and can be explained by a kinematic gap and by a d -wave symmetry of the superconducting order parameter. By taking into account the feedback of superconductivity on $\text{Im} \chi(\mathbf{q}, \omega)$ we argue that ARPES results, tunneling data, and measurements of the optical conductivity are consistent. This further strengthens spin-fluctuation exchange as the relevant mechanism for Cooper pairing in high- T_c cuprates.

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