Magnetic fluctuations and resonant peak in cuprates: Towards a microscopic theory

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Magnetic fluctuations and evolution of the resonant peak with doping in superconducting cuprates are studied within the planar t-J model. The analysis is based on the equations of motion for spins and the memory-function approach to dynamics of magnetic response where the main damping of the low-energy spin collective mode comes from the decay into fermionic degrees of freedom. In general the normal-state damping is large, leading to a overdamped collective mode. At an intermediate doping in the superconducting phase, a d-wave gap leads to a sharp resonant peak with reduced intensity and downward dispersion. At low doping the damping function is closely related to the c-axis optical conductivity, and the resonant-peak behavior is determined by two energy scales: the pseudogap and the coherent superconducting gap.

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I. INTRODUCTION

Since its discovery in inelastic neutron-scattering experiments in superconducting (SC) $YBa_2Cu_3O_7$,[1] the magnetic resonance peak has been the subject of numerous experimental investigations as well as theoretical analyses and interpretations. The magnetic peak has been systematically followed in $YBa_2Cu_3O_{6+x}$ (YBCO) into the underdoped regime,[2–4] where the resonant frequency ω_r decreases while the peak intensity is increasing. Its pronounced appearance is still related to the onset of SC, although it could start appearing even at $T>T_c$. More recent results confirm similar behavior in Bi2212 and Tl2201 cuprates.[5]

Several theoretical hypotheses have been considered for the origin of the resonant peak that it is (a) a bound state in the electron-hole excitation spectrum,[6] (b) a consequence of a novel symmetry between antiferromagnetism (AFM) and SC,[7] and (c) that it represents a collective spin-wave-like mode induced by strong AFM correlations.[8,9] There is also an ongoing debate whether the resonant peak is intimately related to the mechanism of SC and regarding whether it can account for anomalies in single-electron properties.

We are here following the scenario of the resonant mode (as well as the low-frequency mode in the normal state) being a soft collective mode, a precursor of magnon modes in an undoped AFM. In a doped system the mode is gapped due to the loss of AFM long-range order. Such a scenario of a resonant magnetic mode seems to correspond well to experimental facts, in particular the qualitative development of the resonant mode with doping and its onset for $T<T_c$. However, the status of the theory of the resonant mode—and of the magnetic response in cuprates in general—is not satisfactory, both from the point of understanding and even more so of the appropriate analytical method. Relevant microscopic models, such as the Hubbard model and the t-J model, have been so far studied in the weak coupling or random-phase approximation (RPA),[6] neglecting strong correlations. The latter have been considered using the Hubbard-operator technique,[10,11] and more recently within the self-consistent slave-boson approach,[12] self-consistent spin-fluctuation method,[13] as well as within the phenomenological spin-fermion model.[8,9]

Our aim is to develop a theory of the dynamical spin susceptibility $\chi_{\mathbf{q}}(\omega)$ within the t-J model. We use the memory-function formalism of Mori,[14] which enables us to go beyond the previous approximations[6,10,12] in analyzing the collective excitations. In analogy to the previous study of spectral functions,[15] we employ the method of equations of motion (EQM) to generate spin dynamics and in particular to establish the effective decay of localized spins into fermionic degrees of freedom. This process predominantly contributes to the damping of the collective mode. We explicitly calculate this decay vertex and thus provide connection with more phenomenological approaches.[8,9] Since the memory-function formalism does not provide directly the static susceptibility, we rather enforce it via the fluctuation-dissipation sum rule relating it to static (equal-time) spin correlation functions, which are more robust and rather well known from numerical and analytical work.[16]

The paper is organized as follows. In Sec. II, we briefly outline the memory-function approach of Mori. In Sec. III, the equation of motion for the second time derivative of the spin variable $\mathbf{S}_j$ in site representation is presented and the relevance of different contributions to damping is assessed. It is based on a mean-field-type argument and on the experimental fact that the damping of spin excitations is large, since the magnetic response is strongly overdamped for $T>T_c$. In Sec. IV, the damping function is analyzed in terms of coherent vs incoherent dynamics. In Sec. V, we first discus the optimally doped regime introducing a BCS d-wave-like dispersion of quasiparticle excitations for $T\ll T_c$. In the low-doping regime, we believe that the incoherent response is more appropriate and the damping is proportional to the perpendicular, i.e., out-of-plane conductivity $\sigma_c(\omega)$. In Sec. VI, we summarize our results and reemphasize our main conclusions.

II. MEMORY-FUNCTION APPROACH

Our starting point is the t-J model,

$$H=-\sum_{i,j,s} t_{ij}\tilde{c}^{\dagger}_{js}\tilde{c}_{is}+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{1}{4}n_in_j\right), \qquad (1)$$

on a square lattice, and we consider both the nearest-neighbor (nn) hopping $t_{ij}=t$ as well as the next nn $t_{ij}=t'$ hopping. Strong correlations among electrons are incorporated via projected operators, e.g., $\tilde{c}^{\dagger}_{is}=(1-n_{i,-s})c^{\dagger}_{is}$, which do not allow for double occupance of sites. We assume furtheron $J=0.3t$, as relevant to cuprates.

Within the memory-function approach of Mori[14] to dynamical response functions, the dynamical spin susceptibility $\chi_{\mathbf{q}}(\omega)$ can be expressed in the following form:

$$\chi_{\mathbf{q}}(\omega)=-\langle\langle S^z_{\mathbf{q}};S^z_{\mathbf{q}}\rangle\rangle_{\omega}=\frac{-\eta_{\mathbf{q}}}{\omega^2+\omega M_{\mathbf{q}}(\omega)-\omega^2_{\mathbf{q}}},\qquad(2)$$

which is well suitable for the analysis of collective magnetic response, emerging both as the resonant mode in the SC phase and as an overdamped mode in the normal phase in cuprates.

In order to evaluate the quantities entering Eq. (2), we follow the formalism of memory functions,[14] defining the scalar products and projections in terms of static response functions

$$(A|B)=\chi^0_{AB}=-i\int_0^{\infty}dt\langle[A(t),B]\rangle,\qquad(3)$$

and the action of the Liouville superoperator $\mathcal{L}A\equiv[H,A]=-i\dot{A}$. Within this framework, we can express

$$\eta_{\mathbf{q}}=-i\langle[S^z_{-\mathbf{q}}\dot{S}^z_{\mathbf{q}})]\rangle,\qquad(4a)$$

$$M_{\mathbf{q}}(\omega)=\frac{1}{\eta_{\mathbf{q}}}\left(Q\ddot{S}^z_{\mathbf{q}}\left|\frac{1}{Q\mathcal{L}Q-\omega}\right|Q\ddot{S}^z_{\mathbf{q}}\right),\qquad(4b)$$

where $\chi^0_{\mathbf{q}}=\chi_{\mathbf{q}}(\omega=0)$ is the static susceptibility and

$$\omega^2_{\mathbf{q}}=\frac{\eta_{\mathbf{q}}}{\chi^0_{\mathbf{q}}}=\int\omega\chi''_{\mathbf{q}}(\omega)d\omega\Big/\int\frac{\chi''_{\mathbf{q}}(\omega)}{\omega}d\omega\qquad(5)$$

is the second frequency moment of $\chi''_{\mathbf{q}}(\omega)/\omega$, the spectral shape function. Q is a projector which removes from an operator A any component of A proportional to either $S^z_{\mathbf{q}}$ or $\dot{S}^z_{\mathbf{q}}$ in the sense of the scalar product,[14] i.e.,

$$QA=A-\frac{(S^z_{\mathbf{q}}|A)}{\chi^0_{\mathbf{q}}}S^z_{\mathbf{q}}-\frac{(\dot{S}^z_{\mathbf{q}}|A)}{\eta_{\mathbf{q}}}\dot{S}^z_{\mathbf{q}}.\qquad(6)$$

In order to proceed, we write down the EQM for the spin operators $S^z_{\mathbf{q}}$. By evaluating $\mathcal{L}S^z_{\mathbf{q}}$ it is straightforward to explicitly express $\eta_{\mathbf{q}}$ in Eq. (4a) as

$$\eta_{\mathbf{q}}=\frac{1}{4N}\sum_{\mathbf{k},s}[\epsilon^0_{\mathbf{q+k}}+\epsilon^0_{\mathbf{q-k}}-2\epsilon^0_{\mathbf{k}}]\langle\tilde{c}^{\dagger}_{\mathbf{k}s}\tilde{c}_{\mathbf{k}s}\rangle+\frac{1}{2N}\sum_{\mathbf{k}}[J_{\mathbf{q+k}}+J_{\mathbf{q-k}}-2J_{\mathbf{k}}]\langle S^+_{\mathbf{k}}S^-_{-\mathbf{k}}\rangle.\qquad(7)$$

In the region $\mathbf{q}\sim\mathbf{Q}$ that we are primarily concerned with, $\eta_{\mathbf{q}}$ is closely related to the internal energy, i.e., $\eta_{\mathbf{Q}}\sim-\langle H\rangle/N$. This indicates that $\eta_{\mathbf{q}}$ does neither substantially depend on temperature T nor on $\mathbf{q}$, while the dependence on hole concentration $c_h=1-\langle n_i\rangle$ (at low doping) $\eta\sim 2ac_h|t|+2bJ$ is as well modest, where $a\sim b\sim\mathcal{O}(1)$.

Before proceeding to the discussion and the evaluation of the damping function $\Gamma_{\mathbf{q}}(\omega)$, we note that the theory requires an additional input, i.e., in Eq. (2) we need $\chi^0_{\mathbf{q}}$ (or $\omega_{\mathbf{q}}$). Since the latter quantity can be quite sensitive (in particular, T dependent) even in the normal state, we rather fix it with the fluctuation-dissipation sum rule in the paramagnetic phase,

$$\frac{1}{\pi}\int_0^{\infty}d\omega\ \mathrm{cth}\frac{\omega}{2T}\chi''_{\mathbf{q}}(\omega)=\langle S^z_{-\mathbf{q}}S^z_{\mathbf{q}}\rangle=C_{\mathbf{q}},\qquad(8)$$

where in addition

$$\frac{1}{N}\sum_{\mathbf{q}}C_{\mathbf{q}}=\frac{1-c_h}{4}.$$

Static correlation functions $C_{\mathbf{q}}$ are much better known within the t-J model,[17] in particular one can relate $C_{\mathbf{Q}}\propto\xi^2$. The latter is also known experimentally, e.g., in $La_{2-x}Sr_xCO_4$,[18] where $\xi^2\sim c_h$. Also, it is expected that $C_{\mathbf{q}}$ in doped cuprates saturate approaching low T.

Let us now briefly comment on the behavior of the spin response in $\chi_{\mathbf{q}}(\omega)$, [Eq. (2)]. We note that $\omega_{\mathbf{q}}$ is indeed related to the dispersion of the collective mode provided that the mode damping $\gamma_{\mathbf{q}}$ is small enough, i.e., $\gamma_{\mathbf{q}}\sim M''_{\mathbf{q}}(\omega_{\mathbf{q}})<\omega_{\mathbf{q}}$. The dispersion of such an underdamped mode is entirely determined by the static correlation functions via Eq. (8),

$$\omega_{\mathbf{q}}=\frac{\eta_{\mathbf{q}}}{2C_{\mathbf{q}}},\qquad(9)$$

provided that $T<\omega_{\mathbf{q}}$.

In the opposite case $\gamma_{\mathbf{q}}>\omega_{\mathbf{q}}$, we are dealing with an overdamped mode, as seems to be generally the case for the magnetic response near the AFM wave vector $\mathbf{q}\sim\mathbf{Q}=(\pi,\pi)$ in the normal state of cuprates.[2–5] In such a case, $\omega_{\mathbf{q}}$ is not simply related to the dispersion of (some) collective mode. It is likewise not as simply related via the sum rule, [Eq. (8)] to $C_{\mathbf{q}}$ as in Eq. (9) because it must also self-consistently satisfy the (nontrivial) constraint (5).

III. EQUATIONS OF MOTION

The evaluation of $\ddot{S}^z_{\mathbf{q}}=-\mathcal{L}^2S^z_{\mathbf{q}}$ is also straightforward, but results in a rather lengthy expression, so it is convenient to split the action into separate terms involving different powers of kinetic and exchange terms, i.e.,

$$\mathcal{L}^2=\mathcal{L}^2_t+\mathcal{L}^2_I+\mathcal{L}^2_J,$$

$$\mathcal{L}^2_I=[\mathcal{L}_t,\mathcal{L}_J]_+.\qquad(10)$$

Moreover, since in the final expression spin and particle currents are involved, we also introduce the local current operators connecting sites j and k,

$$J^{\mu}_{jk}=i(S^{\mu}_{kj}-S^{\mu}_{jk}),\quad \mu=x,y,z,\qquad(11)$$

where

$$S^{\mu}_{jk}=\frac{1}{2}\sum_{ss'}\tilde{c}^{\dagger}_{js}(\sigma^{\mu})_{ss'}\tilde{c}_{ks'}. \tag{12}$$

Here σ^x, etc., are the usual 2×2 Pauli matrices. Finally, taking care of the projected character of fermionic operators, the equation of motion for $\mathbf{S}_j$ in the site representation then yields

$$\mathcal{L}_t^2\mathbf{S}_j=\sum_k t^2_{jk}[(1-n_k)\mathbf{S}_j-(1-n_j)\mathbf{S}_k]+\sum_{l\neq j} t_{jk}t_{kl}\mathcal{T}_{jk}\mathbf{S}_{jl} -\sum_{l\neq k} t_{jk}t_{jl}\mathcal{T}_{jl}\mathbf{S}_{lk}+\sum_{l\neq j} t_{jk}t_{kl}\mathbf{J}_{jl}\times\mathbf{S}_k+\mathrm{H.c.}, \tag{13a}$$

$$\mathcal{L}_I^2\mathbf{S}_j=-\frac{1}{2}\sum_{l\neq k} J_{jk}t_{jl}\mathbf{J}_{jl}\times\mathbf{S}_k+\frac{1}{2}\sum_{l\neq j} J_{jk}t_{kl}\mathbf{J}_{kl}\times\mathbf{S}_j +\frac{1}{2}\sum_{l\neq k} t_{jk}H_{jl}\mathbf{S}_{jk}-\frac{1}{2}\sum_{l\neq k} t_{jk}H_{kl}\mathbf{S}_{kj}+\mathrm{H.c.}, \tag{13b}$$

$$\mathcal{L}_J^2\mathbf{S}_j=\imath\sum_{l\neq k} J_{jk}J_{jl}[(\mathbf{S}_k\cdot\mathbf{S}_l)\mathbf{S}_j-(\mathbf{S}_j\cdot\mathbf{S}_k)\mathbf{S}_l] +\imath\sum_{l\neq j} J_{jk}J_{kl}[(\mathbf{S}_j\cdot\mathbf{S}_l)\mathbf{S}_k-(\mathbf{S}_j\cdot\mathbf{S}_k)\mathbf{S}_l]. \tag{13c}$$

Here $\mathcal{T}_{jk}$ and the local spin bond energy H_{jk} are

$$\mathcal{T}_{jk}=n_j(1-n_k)+\mathcal{P}_{jk},$$

$$H_{jk}=J_{jk}(\mathcal{P}_{jk}-n_jn_k), \tag{14}$$

where $\mathcal{P}_{jk}=1/2n_jn_k+2\mathbf{S}_j\cdot\mathbf{S}_k$ defines the spin interchange operator.

Let us start the analysis with the term $\mathcal{L}_J^2\mathbf{S}_j$. First, following Mori's formalism, we should project out from the right-hand side (rhs) of Eq. (13c) terms proportional to $\mathbf{S}_j$ itself. On substituting $\mathbf{S}_j\cdot\mathbf{S}_k$ and similar terms with their thermal averages $\langle\mathbf{S}_j\cdot\mathbf{S}_k\rangle$ and performing the transformation to $\mathbf{q}$ space, it follows

$$\mathcal{L}_J^2S^z_{\mathbf{q}}=\omega^2_{\mathbf{q},\mathrm{RPA}}S^z_{\mathbf{q}}+\text{corrections}, \tag{15}$$

where $\omega^2_{\mathbf{q},\mathrm{RPA}}$ is the usual RPA AFM spin-wave dispersion. Fluctuations which contribute to damping are contained in "corrections." Therefore $Q\mathcal{L}_J^2\mathbf{S}^z_{\mathbf{q}}\approx$corrections. It is well known, however, that for an undoped system at $T\sim 0$, the damping of spin modes is much smaller than the frequency of excitations $\omega_{\mathbf{q}}$, provided that $q\xi\gg 1$, where the AFM correlation length $\xi\sim\exp(\mathrm{const}/T)$.[19,20] The argument can be extended to doped systems, and at least for small doping the contribution to damping from $\mathcal{L}_J^2S^z_{\mathbf{q}}$ should remain subleading.

The role of $\mathcal{L}_I^2$ cannot be *a priori* neglected at $\omega\to 0$. However, within the same approximation as described below, the last two terms cancel each other, whereas the first two terms, i.e., currents coupled to the local magnetization, contribute to vertex corrections in $M_{\mathbf{q}}(\omega)$ and are again subleading in relevance.

Then, the main contribution to the damping function $\Gamma_{\mathbf{q}}(\omega)=M''_{\mathbf{q}}(\omega)$ in the regime of interest, i.e., at $\mathbf{q}\sim\mathbf{Q}$, low $T\sim 0$ and low to intermediate doping, should result from the kinetic term $\mathcal{L}_t^2S^z_{\mathbf{q}}$. Namely, in the normal state the damping $\Gamma_{\mathbf{q}}(\omega)$ should approach a constant $\gamma_{\mathbf{q}}$ for $\omega\to 0$ as in a Fermi liquid (although anomalous). Such a damping can arise only from the coupling to fermionic degrees of freedom and the decay of spin fluctuations via the kinetic term H_t into electron-hole excitations.

The complicated form of Eq. (13a) reflects the well-known involved nature of correlated hopping in a strongly correlated system, i.e., with a reshuffling of spins along the hole path, due to the action of the spin interchange operator $\mathcal{P}_{jk}$. Since the main goal is to obtain the coupling to nonlocal fermionic degrees, we replace the operators $\mathcal{P}_{ij},\mathcal{T}_{ij}$ in Eq. (13a) by their thermodynamical averages P_{ij},T_{ij}, respectively. This results in an effective hopping renormalization, which can be quite substantial, since in a Neél state one would get, e.g., $P_1=0$ while in heavily doped system $P_1\sim 1/2-c_h$. For the doping regime of interest, i.e., $0.1\lesssim c_h\lesssim 0.25$, one can on the basis of numerical results for the static correlation functions within the *t-J* model simplify $T_1\sim c_h$. Finally, applying the projector Q, whereupon the first two terms in Eq. (13a) drop out, we obtain

$$Q\mathcal{L}_t^2\mathbf{S}_j\sim\sum_{l\neq j} t_{jk}\tilde{t}_{kl}\mathbf{S}_{jl}-\sum_{l\neq k} t_{jk}\tilde{t}_{jl}\mathbf{S}_{lk}+\mathrm{H.c.}, \tag{16}$$

where $\tilde{t}_{ij}\approx t_{ij}T_{ij}$ are the effective hopping parameters and the coupling of the bond current $\mathbf{J}_{jl}$ to the neighboring spin $\mathbf{S}_k$ has again been neglected. Performing the transformation into the $\mathbf{q}$ space, it follows

$$Q\mathcal{L}_t^2S^z_{\mathbf{q}}\sim\frac{1}{2\sqrt{N}}\sum_{\mathbf{k}s} w_{\mathbf{kq}}s\tilde{c}^{\dagger}_{\mathbf{k}s}\tilde{c}_{\mathbf{k}+\mathbf{q},s}, \tag{17}$$

$$w_{\mathbf{kq}}=(\epsilon^0_{\mathbf{k}}-\epsilon^0_{\mathbf{k}+\mathbf{q}})(\tilde{\epsilon}^0_{\mathbf{k}}-\tilde{\epsilon}^0_{\mathbf{k}+\mathbf{q}})-\zeta_{\mathbf{q}}.$$

Here $\epsilon^0_{\mathbf{k}}$ is the "free" band dispersion with hopping t_{ij}, whereas $\tilde{\epsilon}^0_{\mathbf{k}}$ is defined with renormalized hopping parameters $\tilde{t}_{ij}$. $\zeta_{\mathbf{q}}$ is determined by the condition $\Sigma_{\mathbf{k}}w_{\mathbf{kq}}=0$.

IV. DAMPING FUNCTION

Equation (17) represents the decay of spin variables into fermions in a doped system and the resulting $M_{\mathbf{q}}(\omega)$ is, in fact, closely related to the irreducible particle-hole bubble.[8,12] We evaluate $M_{\mathbf{q}}(\omega)$ by performing a decoupling (in the normal state) in the lowest approximation,

$$\Gamma_{\mathbf{q}}(\omega)=\frac{1}{2\eta_{\mathbf{q}}\omega}\int d\omega'[f(\omega')-f(\omega+\omega')]R_{\mathbf{q}}(\omega,\omega'), \tag{18}$$

with

$$R_{\mathbf{q}}(\omega,\omega')=\frac{\pi}{N}\sum_{\mathbf{k}} w_{\mathbf{kq}}^2 A_{\mathbf{k}}(\omega')A_{\mathbf{k+q}}(\omega+\omega'), \quad (19)$$

where $A_{\mathbf{k}}(\omega)$ are electron spectral functions and $f(\omega)$ is the Fermi function. At low doping an alternative decoupling of fermionic operators directly in the site representation, Eq. (13a), neglecting the coherence between different sites might be more appropriate, since in underdoped systems spectral functions exhibit pronounced incoherent behavior. This yields

$$\tilde{R}_{\mathbf{q}}(\omega,\omega')\approx\pi\zeta_{\mathbf{q}}^2\mathcal{N}(\omega')\mathcal{N}(\omega+\omega'), \quad (20)$$

where $\mathcal{N}(\omega)=(2/N)\Sigma_{\mathbf{k}}A_{\mathbf{k}}(\omega)$ is the electron density of states (DOS). The form [Eqs. (19), (20)] is particularly appealing since by Eq. (18) the damping becomes proportional to the c-axis conductivity, i.e.,

$$\Gamma_{\mathbf{q}}(\omega)\propto\sigma_c(\omega), \quad (21)$$

which can be well represented within the same form.[21,22]

In the present study, we assume some simple form for spectral functions $A_{\mathbf{k}}(\omega)$. In the normal state, we insert an effective coherent band crossing the Fermi energy, i.e.,

$$A_{\mathbf{k}}(\omega)\sim Z_{\mathbf{k}}\delta(\omega-\epsilon_{\mathbf{k}}^{\mathrm{eff}}). \quad (22)$$

Such a form yields at $T\to 0$ and small ω the damping $\Gamma_{\mathbf{Q}}(\omega\to 0)\sim$const from Eq. (18), using either expression (20) or (19), provided that the Fermi surface crosses the AFM zone boundary. We can estimate the size of normal-state damping as

$$\Gamma_{\mathbf{Q}}\sim\frac{\pi\zeta_{\mathbf{Q}}^2\bar{Z}^2}{2\tilde{W}^2\eta_{\mathbf{Q}}}. \quad (23)$$

The doping dependence enters $\Gamma_{\mathbf{Q}}$ in several ways. There is a direct contribution from the effective hopping $\tilde{t}_{ij}$ in $w_{\mathbf{kq}}^2$, Eq. (17). On the other hand, the effective band width $\tilde{W}$ and the quasiparticle weight $\bar{Z}$ also depend on c_h. Alternatively, there is the proportionality to c_h which is evident from the relation of $\Gamma_{\mathbf{q}}$ with σ_c,[21] Eq. (21). Thus, at low doping the damping can be quite small, $\gamma_{\mathbf{Q}}\ll t$. Nevertheless, from the available numerical data we obtain the damping still too large, $\gamma_{\mathbf{Q}}>\omega_{\mathbf{Q}}$, to allow for an underdamped collective mode in the normal state.

V. DYNAMICAL SUSCEPTIBILITY AND RESONANT PEAK

In order to get un underdamped resonant mode at ω_r as observed experimentally,[1–5] one needs a depleted damping $\Gamma_{\mathbf{Q}}(\omega_r)$. The latter can evidently arise in the SC state, $T<T_c$, from the SC gap. Whether the (three-dimensional) t-J model develops a SC phase at low temperature is as yet unclear, although there are strong indications from numerical results that in two-dimensional quantum fluctuations are not strong enough to suppress the off-diagonal long-range order.[23] We proceed our analysis phenomenologically and introduce an effective d-wave gap

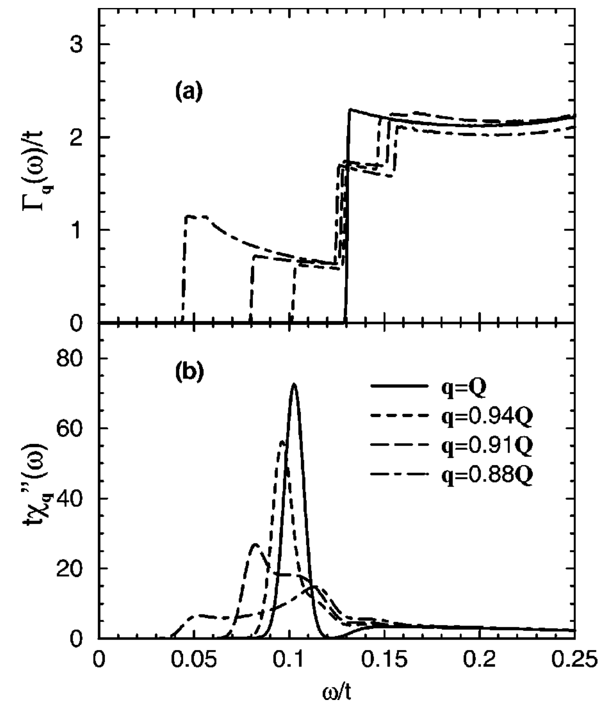

FIG. 1. (a) Damping function $\Gamma_{\mathbf{q}}(\omega)$ at optimal doping $c_h\sim 0.2$ for various $\mathbf{q}\|\mathbf{Q}$ for a d-wave SC, (b) corresponding to spin response $\chi''_{\mathbf{q}}(\omega)$. Note that $t\sim 400$ meV. The resonance peaks are artificially broadened with $\delta=0.01t$.

$$\Delta_{\mathbf{k}}=\frac{\Delta_0}{2}(\cos k_x-\cos k_y) \quad (24)$$

into the spectral functions $A_{\mathbf{k}}(\omega)$. However, due to assumed broken symmetry, Eq. (18) must be supplemented by contributions from anomalous spectral functions $F_{\mathbf{q}}(\omega)$ (Refs. 8,24) as well, leading for $T\sim 0$ and $\omega>0$ to

$$\Gamma_{\mathbf{q}}(\omega)\sim\frac{\pi}{2\eta_{\mathbf{q}}\omega N}\sum_{\mathbf{k}} Z_{\mathbf{k}}Z_{\mathbf{k+q}}w_{\mathbf{kq}}^2(u_{\mathbf{k}}v_{\mathbf{k+q}}-v_{\mathbf{k}}u_{\mathbf{k+q}})^2 \times[f(E_{\mathbf{k}})-f(E_{\mathbf{k}}-\omega)][\delta(\omega-E_{\mathbf{k}}-E_{\mathbf{k+q}})], \quad (25)$$

where $u_{\mathbf{k}}$, etc., are the usual BCS coherence amplitudes[24] and

$$E_{\mathbf{k}}=\sqrt{(\epsilon_{\mathbf{k}}^{\mathrm{eff}}-\mu)^2+\Delta_{\mathbf{k}}^2}. \quad (26)$$

The SC gap eventually leads to the vanishing of $\Gamma_{\mathbf{Q}}(\omega<\omega_{\mathbf{Q}}^*)=0$, where $\omega_{\mathbf{Q}}^*\sim 2\Delta_{\mathbf{k}^*}<2\Delta_0$, and $\mathbf{k}^*$ is the position of the "hot spot" along the AFM zone boundary.

A. Optimum-doping regime

Such an analysis with a d-wave SC gap is particularly appropriate for the situation close to optimum doping. The resulting $\Gamma_{\mathbf{q}}(\omega)$ is presented in Fig. 1(a) for several $\mathbf{q}$ along the zone diagonal. Selecting $c_h\sim 0.2$, we choose the other parameters to correspond to cuprates as follows: effective band with $\tilde{t}=0.3t$, $\tilde{t}'=-0.1t$, $\bar{Z}=0.4$, and the SC gap Δ_0

$\sim 0.1t$. Note that $\Gamma_{\mathbf{q}}(\omega)$ has a single step at $\mathbf{q}=\mathbf{Q}$. For $\mathbf{q}\neq\mathbf{Q}$, it develops two steps and the threshold $\omega^*_{\mathbf{q}}\to 0$ closes for $\tilde{q}=|\mathbf{q}-\mathbf{Q}|>q^*\sim 0.5$. This is a mechanism for the onset of strong damping of the collective mode for $\tilde{q}>q^*$. Another important feature is the size of "normal-state" damping $\gamma_{\mathbf{Q}}=\Gamma_{\mathbf{Q}}(\omega>\omega^*_{\mathbf{Q}})$, which we calculate explicitly. Note that $\gamma_{\mathbf{Q}}\gg\omega_r$ prevents any coherent feature in the normal state.

The corresponding $\chi''_{\mathbf{q}}(\omega)$ is presented in Fig. 1(b). Since in the optimum-doping regime $q^*\ll\xi^{-1}$, $C_{\mathbf{q}}$ should only weakly depend on $\mathbf{q}$ for $\tilde{q}<q^*$. We choose $C_{\mathbf{q}}\sim 0.4$, being consistent with results within the t-J model[17] which by Eq. (8) yields $\omega_{\mathbf{q}}\sim 0.38t$. At $\mathbf{q}=\mathbf{Q}$ the resonant mode is undamped since $2\Delta_0>\omega_r$. However, due to large $\Gamma_{\mathbf{Q}}(\omega>\omega^*_{\mathbf{Q}})$ the resonant frequency is significantly renormalized,

$$\frac{\omega_r}{\omega_{\mathbf{Q}}}=\left[1+\frac{M'_{\mathbf{Q}}(\omega)}{\omega}\bigg|_{\omega=\omega_r}\right]^{-1/2}, \tag{27}$$

while its intensity $I_{\mathbf{Q}}$ is simultaneously reduced,

$$I_{\mathbf{Q}}\sim\frac{\omega_r}{\omega_{\mathbf{Q}}}C_{\mathbf{Q}}. \tag{28}$$

The ratio for our case is $\omega_r/\omega_{\mathbf{Q}}\sim 0.25$. The rest of the spectral weight is distributed over a shallow but very broad continuum. Moving away from $\mathbf{Q}$ the mode gets overdamped and merges with a broad continuum for $\tilde{q}>q^*$. In Fig. 1(b), we observe a downward dispersion of the resonant peak,[25] consistent with experiments.[3,26] The latter is due to the closing of the gap in $\Gamma_{\mathbf{q}}(\omega)$ as $\tilde{q}\to q^*$, which shifts the resonant peak downward, before eventually entering the heavily overdamped regime.

B. Low-doping regime

Analyzing the regime of low doping, it appears more appropriate to use the incoherent approximation, Eq. (20). It is crucial that the normal-state damping $\gamma_{\mathbf{Q}}$ also decreases with doping. On the other hand, it seems clear that for underdoped cuprates the experimental data in the SC phase cannot be explained with a single gap only. Neutron-scattering results for $\chi''_{\mathbf{Q}}(\omega)$ in the underdoped YBCO (Ref. 2) indicate the appearance of the resonance at $T<T_c$, possibly even at $T>T_c$.[3] However, in contrast to optimum doping, the mode at ω_r appears quite broad although still underdamped.[2] The drop in $\chi''_{\mathbf{Q}}(\omega<\omega_c)$, where $\omega_c<\omega_r$, can be again interpreted with a coherent SC gap in $\Gamma_{\mathbf{Q}}(\omega)$, but with a substantially diminished SC gap $\omega_c\sim 2\Delta_0<\omega_r$. Since the 'normal' damping is still too large, i.e., $\gamma_{\mathbf{Q}}>\omega_r$, we need to assume also the appearance of a pseudogap in the DOS below some $\omega\sim\omega_{pg}$ for $T<T^*$, where $T^*>T_c$. This is well consistent with the behavior of $\sigma_c(\omega)$ in underdoped cuprates[27] where the pseudogap appears at $T<T^*$, well above T_c.

In Fig. 2(a), we present characteristic $\Gamma_{\mathbf{Q}}(\omega)$, calculated at $T\sim 0$ for $c_h\sim 0.1$ with corresponding $\Delta_0\sim 0.01t$ and $\eta_{\mathbf{Q}}\sim 0.5t$ whereas $t\mathcal{N}(\omega>\omega_{pg})\sim 0.15$, as inferred from numerical results for the t-J model.[22] An additional pseudogap

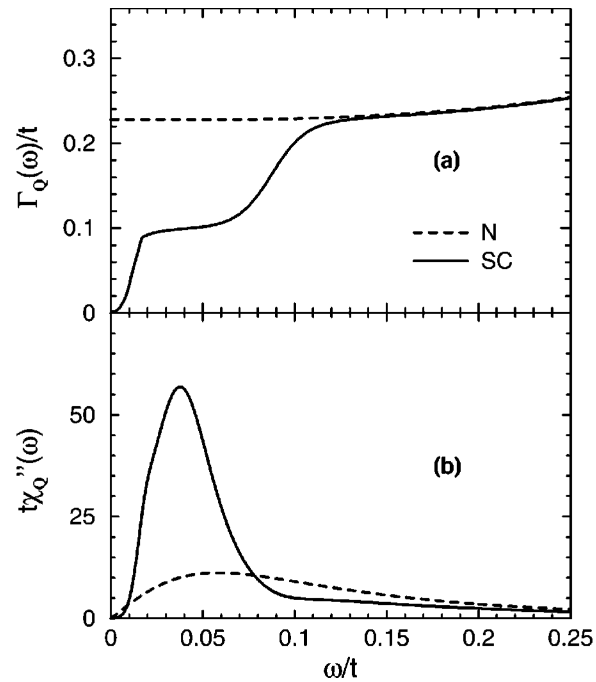

FIG. 2. (a) $\Gamma_{\mathbf{Q}}(\omega)$ in underdoped regime, $c_h\sim 0.1$. Dashed curve: normal-state regime beyond the pseudogap temperature, $T\sim 0.05t>T^*$. Full curve: SC regime, $T\ll T_c$. Here, damping is assumed proportional to $\sigma_c(\omega)$ with a SC gap $\Delta_0\sim 0.01t$. (b) Corresponding to $\chi''_{\mathbf{Q}}(\omega)$.

reduction for $\omega<\omega_{pg}\sim 0.1t$ is assumed, consistent with experimental data.[27] By further specifying $C_{\mathbf{Q}}\sim 1.0$,[17] $\chi''_{\mathbf{Q}}(\omega)$ is completely determined via Eq. (8) and is shown in Fig. 2(b). In the normal state, but above the pseudogap $T>T^*$, $\chi''_{\mathbf{Q}}(\omega)$ reveals an overdamped form. Still, a substantial part of the sum rule is exhausted in the window, $\omega<\omega_{\mathbf{Q}}$. It should be also pointed out that in the normal state the role of temperature $T>0$ is essential, as it brings about—via the sum rule (8)—a shift in $\omega_{\mathbf{Q}}(T)$ with T.

From Fig. 2(b), it is evident that also in the SC state several features are different, given below, when compared to the regime of intermediate to large doping in Fig. 1(b).

(a) The resonant peak is damped even for $T<T_c$, but still underdamped.

(b) The spin response and the sum rule for $\chi''_{\mathbf{Q}}(\omega)$ are essentially exhausted within $\omega<\omega_{pg}$. Since in the underdoped regime normal $\gamma_{\mathbf{Q}}$ is also reduced, peak position given by Eq. (27) is only moderately renormalized and $\omega_r\sim\omega_{\mathbf{Q}}$. Consequently, for the underdamped mode using the sum rule, we obtain $\omega_r\propto\xi^{-2}\propto c_h$.

(c) A spin-gap shoulder appears for $\omega<\omega_c$ below which there are no spin excitations.[2]

VI. SUMMARY AND DISCUSSION

To summarize, our analysis of the dynamical spin response and resonance peak in cuprates within the memory-function approach can qualitatively, and at low doping even quantitatively, reproduce the spectra as measured in neutron-scattering experiments.[1–4] The central point of the present theory is the evaluation of the damping function $\Gamma_{\mathbf{q}}(\omega)$, using the EQM where we consider the decay of a spin fluctuation into electron-hole excitations as the dominant process. In the normal state, we obtain a large damping $\gamma_{\mathbf{Q}}>\omega_{\mathbf{Q}}$ increasing with doping, leading generally to an overdamped AFM collective mode. Here the renormalization due to $T_{ij}\ll 1$ in Eq. (17) is essential. Namely, without this reduction the damping would be much too large. In particular, it would prevent the matching of the sum rule [Eq. (8)] with any pronounced short-range AFM order, e.g., $C_{\mathbf{Q}}>0.5$.

Addressing the resonance peak in the SC state, we find that in optimally doped samples it can arise only inside the frequency gap $\sim 2\Delta_0$. The peak exhibits a downward dispersion and a significant reduction in intensity. It is also strongly renormalized in comparison to the characteristic frequency $\omega_{\mathbf{Q}}$. On the other hand, the incoherent part of spin fluctuations extends over a broad frequency range $\sim\widetilde{W}$ and accounts for $>75\%$ of the integrated intensity, $\int\chi''_{\mathbf{Q}}(\omega)d\omega$.

In the underdoped (weakly doped) case, however, the sum rule at $T=0$ is nearly exhausted within the peak width. As a consequence, we obtain in this regime $\omega_r\propto c_h$, quite consistent with experiments.[2] Moreover, in contrast to optimum doping with a single SC gap, in underdoped samples two energy scales seem to play the role in the SC state.[2,3] The coherent SC gap Δ_0 appears to be below ω_r, hence there is a full spin gap for $\omega<2\Delta_0$, while the resonant peak seems to be broadened but still underdamped for $T<T^*$.[4] The proportionality to σ_c, Eq. (21), results in gradual closing of the pseudogap with doping.

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