

# Spin fluctuations in cuprates as the key to high $T_c$

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**Abstract.** Spin fluctuations represent the lowest established energy scale in cuprates and are crucial for the understanding of anomalous normal state properties and superconductivity in these materials [1]. The memory-function approach to the spin response in the  $t$ - $J$  model is described. Combined with numerical results for small systems it is able to explain the anomalous scaling at low doping and the crossover to the Fermi-liquid-like behavior in overdoped systems. Within the superconducting phase the theory reproduces the resonant peak and its peculiar double dispersion. Such spin fluctuations are then used as the input for the theory of superconductivity within the  $t$ - $J$  model, where we show that an important role is played also by the next-nearest-neighbour hopping parameter  $t'$ .

**Keywords:** cuprates, spin fluctuations, non-Fermi liquid, resonant peak, superconductivity

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## INTRODUCTION

The phase diagram of cuprates still represents one of the major challenges in solid state physics, both for theoreticians and experimentalists. Besides superconductivity (SC) and antiferromagnetic (AFM) ordering, several regimes with distinct electronic properties have been identified within the normal metallic phase. In this contribution, we are concerned with the spin dynamical response in cuprates which has been intensively studied using the inelastic neutron scattering (INS) [2, 3] and NMR relaxation experiments [4].

There is an abundant evidence that in underdoped cuprates magnetic properties are not following the usual Fermi-liquid (FL) scenario within the metallic state above the SC transition  $T > T_c$ . It should be reminded that within a normal FL the dynamical spin susceptibility  $\chi''_{\mathbf{q}}(\omega)$  is essentially  $T$ -independent at low  $T < T_{FL}$ . From the point of spin response one can use the latter criterion as the working definition of the Fermi-liquid temperature  $T_{FL}$ . Note that in usual metals  $T_{FL} \gg 1000$  K, in striking contrast to underdoped cuprates with  $T_{FL} < T_c$  [2, 4]. Evidence for the non-Fermi-liquid (NFL) behavior are INS results for the  $\mathbf{q}$ -integrated spin susceptibility which exhibit in a broad  $\omega, T$  range an anomalous, but universal  $\chi''_L(\omega) \propto f(\omega/T)$ , established in underdoped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) [5, 2], as well as in  $\text{YBaCu}_3\text{O}_{6+x}$  (YBCO) [6]. Similar conclusions arise from evident  $T$ -dependence of  $^{63}\text{Cu}$  NMR spin-lattice relaxation rate  $1/T_1T$  and of the spin-spin relaxation rate  $1/T_{2G}$  [4].

Cuprates at optimum doping, and even more in the overdoped regime, approach closer the usual FL description. INS reveals only weak spin response at low energies  $\omega$  in the normal state (NS) at  $T > T_c$ , characteristic for metals with a broader band. Also, NMR relaxation rates  $1/T_1T$  and  $1/T_{2G}$  are weakly  $T$ -dependent, again consistent with the FL scenario. Analogous message arises from the analysis of cuprates doped with nonmagnetic Li and Zn [7], where the impurity-induced spin susceptibility varies as

$\propto 1/(T + T_K)$ , whereby the characteristic (Kondo-type) temperature is  $T_K \sim 0$  in the underdoped regime and increasing fast with doping in the overdoped regime.

While in the NS the dynamical spin response  $\chi''_{\mathbf{q}}(\omega)$  is in general compatible with an overdamped collective mode, the prominent feature appearing in the SC phase is the magnetic resonant mode. First observed in optimally doped YBCO [8], it has been in the last decade the subject of numerous INS experiments [3]. The resonant response, in spite of evident differences between YBCO and LSCO systems, as well as changes with doping, reveals some surprisingly universal characteristics. The peak intensity is highest at the commensurate wavevector  $\mathbf{Q} = (\pi, \pi)$ , while its frequency  $\omega_r$  increases with doping up to the optimum doping. In addition, one component of the resonant mode disperses downwards [9], while another branch apparently emerging from the same peak shows an upward dispersion [10, 11, 12].

It seems a plausible (although surprisingly not generally accepted) conclusion, that the understanding of spin dynamics is the key for the proper description of the anomalous properties of cuprates, and to the mechanism of high  $T_c$  in particular. The main argument remains, that up to now the spin fluctuations represent the lowest (experimentally well established) energy scale in cuprates, both in the NS as well as in the SC state. Namely, the peak in the spin response (as measured by INS) in the normal state appears in underdoped cuprates at  $\omega_p \sim T_c$ , moving even lower with decreasing  $T$ . Moreover, the collective mode  $\omega_r$  in the SC phase lies even below the SC gap  $\omega_r < 2\Delta_0$ . On the other hand, low spin-fluctuation energy scale also sets a clear limit to the FL behavior since FL can become normal only for  $T, \omega$  which are below this scale.

A comprehensive theoretical description of spin fluctuations in cuprates and their implications on other properties, in particular their role in the mechanism of SC, is still lacking. A FL behavior in the overdoped regime far from a metal-insulator transition seems plausible, nevertheless a solid theoretical approach is missing even in this regime. A crossover from a strange metal to a coherent metal phase has been predicted within some theoretical approach. Quite fashionable and frequently invoked interpretation is given in terms of the quantum critical point (QCP) at optimum doping  $c_h^*$  (masked, however, at low  $T$  by the SC phase), dividing the FL phase at  $c_h > c_h^*$  from a (singular) non-Fermi-liquid (NFL) metal at  $c_h < c_h^*$ . Such a scenario is established, e.g. theoretically in spin systems [13] and experimentally in some heavy-fermion compounds, but remains controversial in cuprates. The obvious argument against the QCP scenario is the absence of a critical length scale, e.g., AFM correlation length  $\xi(T \rightarrow 0) \rightarrow \infty$  as well as the absence of the phase with the AFM long-range order for  $c_h < c_h^*$  (sometimes put in connection with the pseudogap scale  $T^*$ ). In the underdoped cuprates the spin fluctuation seem to follow quite well the phenomenological scenario of the marginal FL [14], which got so far only partially a solid theoretical foundation. The main distinction to the QCP scenario is the absence of a critical length scale, which is in agreement with low-energy INS revealing at low  $T$  the saturation of the inverse AFM correlation length  $\kappa = 1/\xi$ , at least in YBCO [3] and in LSCO at low doping [5, 2].

With respect to the most challenging problem, the mechanism of SC in cuprates, the role of strong correlations and the antiferromagnetic (AFM) state of the reference insulating undoped compound has been recognized very early [15]. Still, up to date there is no general consensus whether ingredients as embodied within the prototype single-band models of strongly correlated electrons are sufficient to explain the onset

of high  $T_c$ . Even within the frequently invoked  $t$ - $J$  model, being the subject of this paper, proposed mechanism of SC and the methods for the evaluation of corresponding  $T_c$  differ with respect to the fact whether the attractive interaction is mainly local and instantaneous [16] or the retardation effects are important [17]. Recognizing the very low spin-fluctuation scale, we will advocate in the following the latter for spin-fluctuation scenario, emerging in contrast to previous approaches directly from the strongly correlated  $t$ - $J$  model.

In the following we present some of our recent theoretical results on spin fluctuations in cuprates and their relation to SC. The analysis within the  $t$ - $J$  model, as relevant for cuprates, is mostly based on the general memory-function approach and the equations-of-motion (EQM) method. The latter has been first applied to the  $t$ - $J$  model to explain anomalous (MFL-type) properties of NS spectral function [18] and then extended to low-doping regime [19] and SC [20]. Spin dynamical response  $\chi_{\mathbf{q}}(\omega)$  has been considered within analogous treatment to yield the overdamped mode in the NS and resonant peak dispersion in the SC state [21], the anomalous  $\omega/T$  scaling in the underdoped regime [22], the influence of nonmagnetic impurities [23], the NFL-FL crossover in spin dynamics [24], and double dispersion of resonant peak [25]. The extracted knowledge on spin fluctuations is used as an input the theory of SC [26].

## NFL - FL CROSSOVER IN THE NORMAL STATE

To be specific, we consider in the following the spin dynamics within the framework of the extended  $t$ - $J$  model, which has been shown to represent surprisingly well several electronic properties of cuprates, both qualitatively and quantitatively [27],

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

including in general both the NN hopping  $t_{ij} = t$  and the NNN hopping  $t_{ij} = t'$ , and involving the projected fermionic operators,  $\tilde{c}_{is} = (1 - n_{i,-s}) c_{is}$ .

We will first argue [22] that the anomalous  $\omega/T$  scaling and the related NFL behavior of the magnetic response can be understood as a consequence of few simple ingredients which appear to be valid for doped AFM in the normal state: a) the collective mode is strongly overdamped, whereby the damping is nearly  $\omega$ - and  $T$ - independent at low  $\omega$ , and b) there is no long-range spin order at low  $T$ , so that static spin correlations saturate with a finite  $\xi$ .

Within the memory function approach the dynamical spin susceptibility  $\chi_{\mathbf{q}}(\omega) = -\langle\langle S_{\mathbf{q}}^z; S_{\mathbf{q}}^z \rangle\rangle_{\omega}$  can be generally expressed [21, 22] in the form

$$\chi_{\mathbf{q}}(\omega) = \frac{-\eta_{\mathbf{q}}}{\omega^2 + \omega M_{\mathbf{q}}(\omega) - \omega_{\mathbf{q}}^2}, \quad (2)$$

suitable for the analysis of the magnetic response, as present in undoped and moderately doped AFM [21].  $\omega_{\mathbf{q}}$  represents the frequency of the collective mode provided that the mode damping is small, i.e.,  $\Lambda_{\mathbf{q}} \sim M_{\mathbf{q}}''(\omega_{\mathbf{q}}) < \omega_{\mathbf{q}}$ . In the opposite case, i.e.  $\Lambda_{\mathbf{q}} > \omega_{\mathbf{q}}$  the

mode is overdamped. Still, the advantage of the form (2) is that it can fulfill basic sum rules even for an approximate  $M_{\mathbf{q}}''$ . Thermodynamic quantities entering Eq. (2) can be expressed as

$$\eta_{\mathbf{q}} = -i \langle [S_{-\mathbf{q}}^z, \dot{S}_{\mathbf{q}}^z] \rangle, \quad \omega_{\mathbf{q}}^2 = \eta_{\mathbf{q}} / \chi_{\mathbf{q}}^0, \quad (3)$$

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

$\eta_{\mathbf{q}}$  is the spin stiffness and can be expressed in terms of the static correlation functions, in particular within  $t$ - $J$  model  $\eta_{\mathbf{Q}} = -\langle H \rangle / N$ .  $\chi_{\mathbf{q}}^0$  (or  $\omega_{\mathbf{q}}$ ) remains to be determined, even for known  $M_{\mathbf{q}}(\omega)$ . It is quite a sensitive quantity, hence it is safer to fix it by the sum rule (fluctuation - dissipation relation)

$$\frac{1}{\pi} \int_0^{\infty} d\omega \operatorname{cth} \frac{\omega}{2T} \chi_{\mathbf{q}}''(\omega) = \langle S_{-\mathbf{q}}^z S_{\mathbf{q}}^z \rangle = C_{\mathbf{q}}, \quad (4)$$

given in terms of equal time spin correlations, which are expected to be much more robust. Moreover  $C_{\mathbf{q}}$  are bound by the constraint  $(1/N) \sum_{\mathbf{q}} C_{\mathbf{q}} = (1 - c_h) / 4$ , where  $c_h$  is an effective hole doping.

Let us now state two basic assumptions: a) static correlations are taken to follow a Lorentzian form, i.e.  $C_{\mathbf{q}} = C / (\kappa^2 + \tilde{q}^2)$  where  $\tilde{\mathbf{q}} = \mathbf{q} - \mathbf{Q}$ .  $\kappa$  is assumed to be a noncritical quantity, which on approaching low  $T$  saturates at a finite value. As already noted, this is consistent with the neutron scattering data for weakly doped LSCO [5] and YBCO [6]. It is also consistent with numerical results for the  $t$ - $J$  model at finite doping. b) The damping is also assumed to be a constant,  $M_{\mathbf{q}}''(\omega) \sim \Lambda$ , i.e., (roughly) independent of  $\omega$ ,  $\tilde{\mathbf{q}}$  and  $T$ , or at least not critically dependent on these variables. The support for this assumption comes from our numerical results on small systems, using the finite- $T$  Lanczos method (FTLM) [27], for the  $t$ - $J$  model on small lattices with up to 20 sites. Calculating  $\chi_{\mathbf{q}}''(\omega)$  and extracting then  $M_{\mathbf{q}}''(\omega)$  with the help of Eq.(2), one can conclude [22] that in spite of widely different  $\chi_{\mathbf{q}}''(\omega)$  the damping function  $M_{\mathbf{q}}''(\omega)$  is nearly constant in a broad range of  $\omega < t$  and almost independent of  $\mathbf{q}$ . Moreover, for doped systems with  $c_h > 0$  data are consistent with a finite (and quite large) extrapolated value  $\Lambda_{\mathbf{Q}}(T \rightarrow 0)$ . In the normal state this leads to an overdamped collective mode vicinity of  $\mathbf{q} = \mathbf{Q}$ , i.e.,  $\omega_{\mathbf{Q}} < \Lambda$ , as generally observed in INS experiments [1, 2, 3],

$$\chi_{\mathbf{q}}''(\omega) \sim \frac{\eta}{\Lambda} \frac{\omega}{(\omega^2 + \Gamma_{\mathbf{q}}^2)}, \quad \Gamma_{\mathbf{q}} = \frac{\omega_{\mathbf{q}}^2}{\Lambda}, \quad (5)$$

and  $\Gamma_{\mathbf{q}} < \omega_{\mathbf{q}}$ . At low  $T \rightarrow 0$ , Eq.(4) leads now to a nontrivial restriction for  $\omega_{\mathbf{q}}$  and  $\Gamma_{\mathbf{q}}$ . The relevant quantity is the peak frequency  $\omega_p = \Gamma_{\mathbf{Q}}(T \rightarrow 0)$ , which determines the characteristic  $T = 0$  spin-fluctuation scale as well as  $T_{FL}$ .

The crucial parameter appears to be

$$\zeta = C\pi\Lambda / (2\eta\kappa^2), \quad \omega_p \sim \Lambda e^{-2\zeta}, \quad (6)$$

which exponentially renormalizes  $\omega_p$ . Since  $C \sim O(1)$  and  $\eta \sim 0.6t$  at low doping,  $\zeta$  is effectively governed by the ratio  $\Lambda/\kappa^2$ . It is easy to imagine the situation that  $\zeta \gg 1$  in the underdoped cuprates, leading to very low  $\omega_p \ll \Lambda$  and even  $\omega_p < T_c$ . On the other

hand, in the overdoped case  $\Lambda/\kappa^2 \sim 1$  and  $\omega_p$  becomes large as in usual FL systems. Due to exponential dependence in Eq.(6) it is also plausible that the crossover from the NFL regime with extremely small  $\omega_p$  and FL behavior is quite abrupt [24], resembling the QCP scenario.

In order to extract the characteristic energy scale  $\omega_{FL}$  of spin fluctuations directly from numerical FTLM results [24], we use an alternative definition,

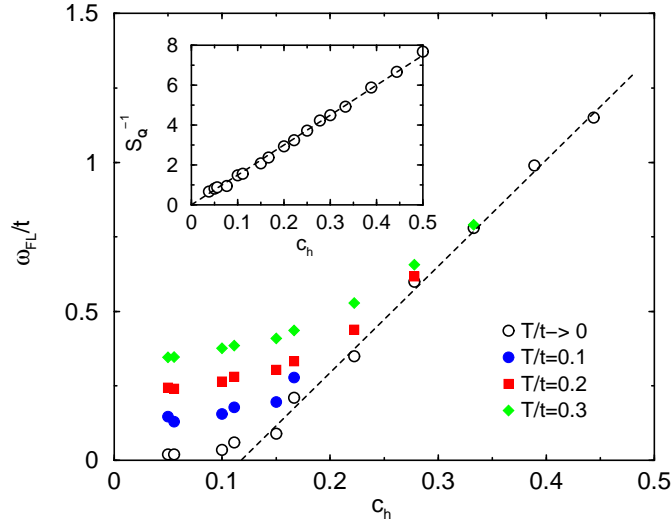
$$\omega_{FL}(T) = S_{\mathbf{Q}}/\chi_{\mathbf{Q}}(T) \quad (7)$$

with the corresponding  $T = 0$  limit  $\omega_{FL}(0)$ . Note that  $\omega_{FL}(0) = \langle \omega \rangle$  is just the first frequency moment of the shape function  $\chi_{\mathbf{Q}}''(\omega)/\omega$ ,

$$\omega_{FL}(0) = \langle \omega \rangle = \frac{2}{\pi\chi_{\mathbf{Q}}} \int_0^{\infty} \chi_{\mathbf{Q}}''(\omega)d\omega. \quad (8)$$

On the other hand, one can extract  $\omega_{FL}$  also from experiments, in particular from NMR  $1/T_{2G}$  relaxation data [4], which give rather straightforward information on  $\chi_{\mathbf{Q}}(T)$ .

In Fig. 1 we show FTLM results for  $\omega_{FL}(c_h)$  at  $0.1t \leq T \leq J$ . Besides we also present values extrapolated to  $T \rightarrow 0$ . Note that in the considered  $T$  window  $S_{\mathbf{Q}}(T)$  is essentially  $T$ -independent, following well the linear variation  $1/S_{\mathbf{Q}} = Kc_h$ . In contrast, the FL scale  $\omega_{FL}$  reveals a nonuniform variation with doping. Again, for  $c_h > c_h^*$ ,  $\omega_{FL}$  is already rather  $T$ -independent for  $T < J$ . On the other hand, in the regime  $c_h < c_h^*$  we find a strong  $T$ -dependence of  $\omega_{FL}$  even at lowest reliable  $T$ , where  $\omega_{FL} \sim T + \omega_{FL}(0)$ . We can summarize results in Fig. 1 as follows: a) in the overdoped regime  $\omega_{FL}(0) \sim \alpha(c_h - c_{h0})$  with  $c_{h0} \sim 0.12$  and a large slope  $\alpha \sim 3.5t \sim 1.4$  eV, b) in the underdoped regime our results indicate on a smooth crossover to very small  $\omega_{FL}(0) \ll J$ .



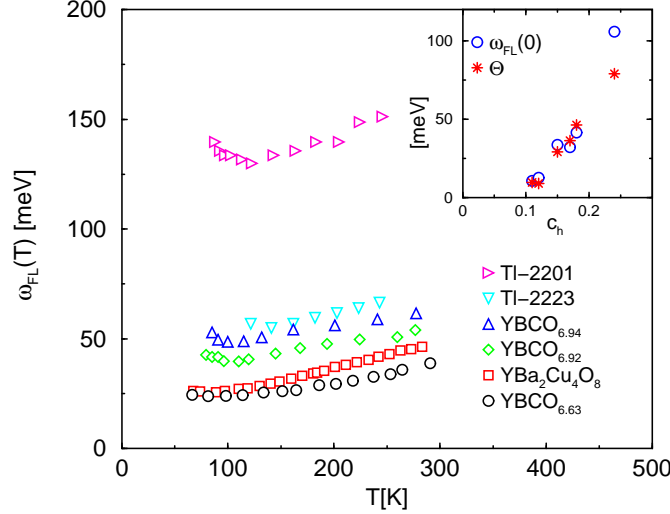
**FIGURE 1.** FL scale  $\omega_{FL}/t$  vs.  $c_h$ , obtained for the  $t$ - $J$  model using the FTLM for  $T > 0$  and their  $T \rightarrow 0$  extrapolated values. The inset shows  $T = 0$  results for  $1/S_{\mathbf{Q}}$  vs.  $c_h$ . Dashed lines are guide to the eye only.

Let us estimate  $\chi_{\mathbf{Q}}(T)$  and consequently  $\omega_{FL}$  directly from experiments on cuprates. Within the normal state the results for the NMR spin-spin relaxation time  $T_{2G}$ , obtained

from the  $^{63}\text{Cu}$  spin-echo decay, can be related to static  $\chi_{\mathbf{q}}$  [28]. Assuming that  $\chi_{\mathbf{q}}$  is peaked at commensurate  $\mathbf{q} = \mathbf{Q}$  and can be described by a Lorentzian form with a width  $\kappa \ll \pi$ , one gets a simplified relation

$$\frac{1}{T_{2G}} \sim 0.083 \kappa F(\mathbf{Q}) \chi_{\mathbf{Q}}. \quad (9)$$

$1/T_{2G}$  relaxation rates have been measured and summarized in Ref. [4], i.e., from underdoped to optimally doped YBCO with  $0.63 < x < 1$ , underdoped  $\text{YBa}_2\text{Cu}_4\text{O}_8$ , nearly optimum doped  $\text{Tl}_2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$  (Tl-2223) and the overdoped  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  (Tl-2201), whereby the normalization with corresponding  $F(\mathbf{Q})$  has been already taken into account. Relevant  $\kappa$  is the one appropriate for low- $\omega$  spin dynamics and measured directly by INS. For YBCO data are taken from Ref.[29], which allows us to evaluate  $\chi_{\mathbf{Q}}(T)$  from Eq.(9).  $S_{\mathbf{Q}}$  is so far not experimentally accessible, so we assume here the  $t$ - $J$  model results to finally extract corresponding  $\omega_{FL}(T)$  as presented in Fig. 2 for various cuprates. Derived  $\omega_{FL}(0)$  are well in agreement with model result in Fig. 1, in particular regarding the large slope in the overdoped regime and a clear change of scale between the underdoped and overdoped cuprates.



**FIGURE 2.**  $\omega_{FL}$  vs.  $T$ , for various cuprates. The inset shows the extrapolated scales  $\omega_{FL}(0)$  and  $\Theta$  (defined by  $1/\chi_{\mathbf{Q}} \propto T + \Theta$ ) vs. doping  $c_h$ .

## DISPERSION OF THE RESONANT MODE

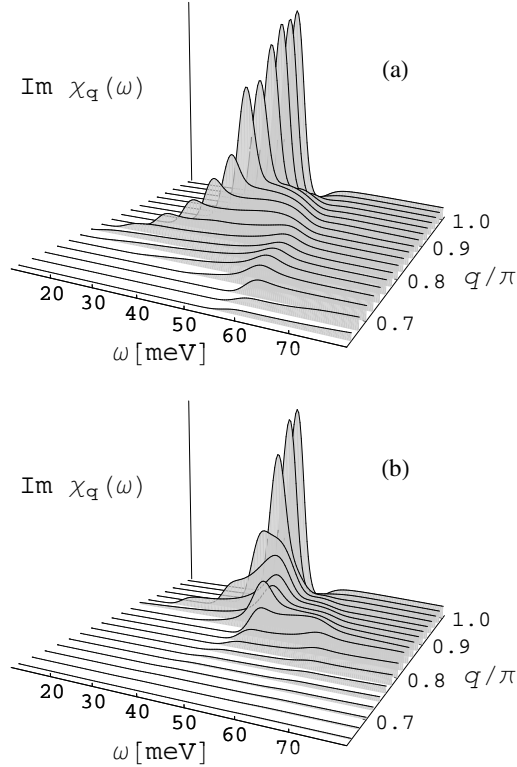
Using the method of equations of motion within the  $t$ - $J$  model it has been shown that the collective spin fluctuations decay into electron-hole excitations [21, 25]. This leads to the lowest-order mode-coupling approximation for the damping in the NS,

$$\Lambda_{\mathbf{q}}(\omega) = \frac{\pi}{2\eta_{\mathbf{q}}\omega N} \int d\omega' [f(\omega') - f(\omega + \omega')] \sum_{\mathbf{k}} w_{\mathbf{k}\mathbf{q}}^2 A_{\mathbf{k}}(\omega') A_{\mathbf{k}+\mathbf{q}}(\omega + \omega'), \quad (10)$$

where  $w_{\mathbf{kq}}$  is the effective spin-fermion coupling [21] and  $A_{\mathbf{k}}(\omega)$  is the single-particle spectral function. Provided the existence of ‘hot spots’ where the FS crosses the AFM zone boundary (being the case for cuprates at low to intermediate doping) we assume that in the NS low- $\omega$  quasiparticles (QP) with dispersion  $\varepsilon_{\mathbf{k}}$  and weight  $Z_{\mathbf{k}}$  determine the spectral function  $A_{\mathbf{k}}(\omega) = Z_{\mathbf{k}}\delta(\omega - \varepsilon_{\mathbf{k}})$ . This results in a rather constant  $\Lambda_{\mathbf{q}}(\omega)$ . The form of Eq. (10) is anyhow quite generic for the damping of the collective magnetic mode in a metallic system, since the lowest-energy decay processes naturally involve the electron-hole excitations close to the FS. Similar expressions appear also in theories based on the RPA approach [30, 31]. Within the SC phase, Eq. (10) has to be generalized to include the anomalous spectral functions [30] leading to [21, 25]

$$\Lambda_{\mathbf{q}}(\omega) \sim \frac{\pi}{2\omega N} \sum_{\mathbf{k}} \tilde{w}_{\mathbf{kq}}^2 (u_{\mathbf{k}}v_{\mathbf{k+q}} - v_{\mathbf{k}}u_{\mathbf{k+q}})^2 [f(E_{\mathbf{k}}) - f(E_{\mathbf{k}} - \omega)] \delta(\omega - E_{\mathbf{k}} - E_{\mathbf{k+q}}), \quad (11)$$

where  $\tilde{w}_{\mathbf{kq}}^2 = w_{\mathbf{kq}}^2 Z_{\mathbf{k}}Z_{\mathbf{k+q}}/\eta_{\mathbf{q}}$ , while  $u_{\mathbf{k}}, v_{\mathbf{k}}$  are the usual BCS coherence amplitudes and  $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ . For the SC gap we assume the  $d_{x^2-y^2}$  form,  $\Delta_{\mathbf{q}} = \Delta_0(\cos q_x - \cos q_y)/2$ . Thus we end up with few adjustable parameters at chosen  $c_h$ :  $\kappa$  in the Lorentzian form for  $C_{\mathbf{q}}$ , the effective coupling  $\bar{w}$  and the maximum SC gap  $\Delta_0$  [21, 25].



**FIGURE 3.**  $\chi''_{\mathbf{q}}(\omega)$  at intermediate doping  $c_h = 0.15$  for momenta: a) along the  $x$  direction  $\mathbf{q} = q(1,0)$ , and b) along the zone diagonal  $\mathbf{q} = q(1,1)$ .

At intermediate doping the collective mode is heavily overdamped in the NS. The

indication for the latter is low intensity of the INS in the relevant low-energy window. For the presented case [25] we fix the 'optimum' doping at  $c_h = 0.15$  and  $\kappa \sim 1.25$ . The SC gap is roughly known from experiments  $\Delta_0 = 40$  meV. The remaining input is  $\Gamma_{\mathbf{Q}}$  within the NS. For the appearance of the upper resonant branch it is crucial that  $\Gamma_{\mathbf{Q}}$  is not too large, as seems to be inherent within the RPA [30, 31].

In Fig. 3 we display  $\chi_{\mathbf{q}}''(\omega)$  for momenta both along the two  $\mathbf{q}$  directions. Following observations can be made [25]: a) results reveal two branches emerging from the same coherent resonant mode at  $\omega_r \sim 41$  meV. Intensity plots of both branches within the  $\mathbf{q}$  plane are square-like around AFM  $\mathbf{Q}$ , however with quite pronounced anisotropy. b) For the downward branch the intensities are strongest along the  $(1,0)$  direction. c) The development is more sensitive for  $\omega > \omega_r$ , still the situation with the upward branch is just opposite to the downward one. The dispersion is stronger along the  $(1,0)$  direction. d) Above the damping threshold  $\omega > 2\Delta_0$  the upward branch merges into an incoherent response broad both in  $\mathbf{q}$  as well as in  $\omega$ . The incoherent part still exhausts most of the intensity sum rule, Eq. (4), even for  $\mathbf{q} = \mathbf{Q}$ .

## SPIN-FLUCTUATION MECHANISM OF SUPERCONDUCTIVITY

The projection in fermionic operators in the  $t$ - $J$  model, Eq.(1), leads to a nontrivial EQM, which can be in the  $\mathbf{k}$ -basis written as

$$[\tilde{c}_{\mathbf{k}s}, H] = [(1+c_h)\frac{\varepsilon_{\mathbf{k}}^0}{2} - (1-c_h)J]\tilde{c}_{\mathbf{k}s} + \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} m_{\mathbf{kq}} [sS_{\mathbf{q}}^z \tilde{c}_{\mathbf{k}-\mathbf{q},s} + S_{\mathbf{q}}^{\mp} \tilde{c}_{\mathbf{k}-\mathbf{q},-s} - \frac{1}{2}\tilde{n}_{\mathbf{q}}\tilde{c}_{\mathbf{k}-\mathbf{q},s}], \quad (12)$$

where  $m_{\mathbf{kq}} = 2J\gamma_{\mathbf{q}} + \varepsilon_{\mathbf{k}-\mathbf{q}}^0$  is the effective spin-fermion coupling, while  $\varepsilon_{\mathbf{k}}^0 = -4t\gamma_{\mathbf{k}} - 4t'\gamma'_{\mathbf{k}}$  is the bare band dispersion on a square lattice, and  $\gamma_{\mathbf{q}} = (\cos k_x + \cos k_y)/2$ ,  $\gamma'_{\mathbf{q}} = \cos k_x \cos k_y$ . To keep similarity with the spin-fermion phenomenology [17] we use the symmetrized coupling [21]

$$\tilde{m}_{\mathbf{kq}} = 2J\gamma_{\mathbf{q}} + (\varepsilon_{\mathbf{k}-\mathbf{q}}^0 + \varepsilon_{\mathbf{k}}^0)/2. \quad (13)$$

EQM, Eq. (12), are used to derive the approximation for the Green's function (GF) matrix  $G_{\mathbf{k}s}(\omega) = \langle\langle \Psi_{\mathbf{k}s} | \Psi_{\mathbf{k}s}^{\dagger} \rangle\rangle_{\omega}$  for the spinor  $\Psi_{\mathbf{k}s} = (\tilde{c}_{\mathbf{k},s}, \tilde{c}_{-\mathbf{k},-s}^{\dagger})$ . We follow the method, as applied to the normal state (NS) GF by present authors [18, 19], and generalized to the SC pairing in Ref.[20, 26]. In general, we can represent the GF matrix in the form

$$G_{\mathbf{k}s}(\omega)^{-1} = \frac{1}{\alpha} [\omega\tau_0 - \hat{\zeta}_{\mathbf{k}s} + \mu\tau_3 - \Sigma_{\mathbf{k}s}(\omega)], \quad (14)$$

where  $\alpha = \sum_i \langle\langle \tilde{c}_{is}, \tilde{c}_{is}^{\dagger} \rangle\rangle_+ / N = (1+c_h)/2$  is the normalization factor,  $\mu$  is the chemical potential, and the frequency matrix  $\hat{\zeta}_{\mathbf{k}s} = \langle\langle [\Psi_{\mathbf{k}s}, H], \Psi_{\mathbf{k}s}^{\dagger} \rangle\rangle_+ / \alpha$ , which generates a renormalized band  $\tilde{\zeta}_{\mathbf{k}} = \zeta_{\mathbf{k}s}^{11} = \bar{\zeta} - 4\eta_1 t \gamma_{\mathbf{k}} - 4\eta_2 t' \gamma'_{\mathbf{k}}$  and the mean-field SC gap

$$\Delta_{\mathbf{k}}^0 = \zeta_{\mathbf{k}s}^{12} = -\frac{4J}{N\alpha} \sum_{\mathbf{q}} \gamma_{\mathbf{k}-\mathbf{q}} \langle\langle \tilde{c}_{-\mathbf{q},-s} \tilde{c}_{\mathbf{q},s} \rangle\rangle. \quad (15)$$



To evaluate  $\Sigma_{\mathbf{k}s}(\omega)$  we use the lowest-order mode-coupling approximation, analogous to the treatment of the SC in the spin-fermion model [17]. Taking into account EQM, Eq. (12), and by decoupling fermionic and bosonic degrees of freedom, one gets

$$\Sigma_{\mathbf{k}s}^{11(12)}(i\omega_n) = \frac{-3}{N\alpha\beta} \sum_{\mathbf{q},m} \tilde{m}_{\mathbf{kq}}^2 G_{\mathbf{k}-\mathbf{q},s}^{11(12)}(i\omega_m) \chi_{\mathbf{q}}(i\omega_n - i\omega_m) \quad (16)$$

where  $i\omega_n = i\pi(2n+1)/\beta$  and  $\beta = 1/T$ , whereby we have neglected the charge-fluctuation contribution.

In order to analyze the low-energy behavior in the SC state, we use the QP approximation for the spectral function matrix where the QP energies are  $E_{\mathbf{k}} = (\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}s}^2)^{1/2}$ , while NS parameters, i.e., the QP weight  $Z_{\mathbf{k}}$  and the QP energy  $\varepsilon_{\mathbf{k}}$ , are determined from  $G_{\mathbf{k}s}(\omega \sim 0)$ , Eq. (14). By defining normalized  $F_{\mathbf{q}}(i\omega_l) = \chi_{\mathbf{q}}(i\omega_l)/\chi_{\mathbf{q}}^0$ , and rewriting the MF gap, Eq. (15), in terms of the spectral function, we can display the gap equation in a BCS-like form form,

$$\Delta_{\mathbf{k}s} = \frac{1}{N} \sum_{\mathbf{q}} [4J\gamma_{\mathbf{k}-\mathbf{q}} - 3\tilde{m}_{\mathbf{k},\mathbf{k}-\mathbf{q}}^2 \chi_{\mathbf{k}-\mathbf{q}}^0 C_{\mathbf{q},\mathbf{k}-\mathbf{q}}] \frac{Z_{\mathbf{k}}^0 Z_{\mathbf{q}}^0 \Delta_{\mathbf{q}s}}{2E_{\mathbf{q}}} \text{th}\left(\frac{\beta E_{\mathbf{q}}}{2}\right), \quad (17)$$

where  $C_{\mathbf{kq}} = I_{\mathbf{kq}}(i\omega_n \sim 0)/I_{\mathbf{k}}^0$  plays the role of the cutoff function with

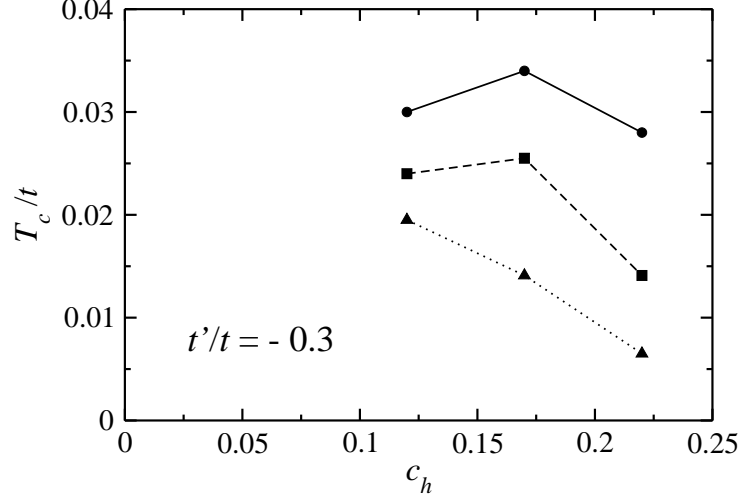
$$I_{\mathbf{kq}}(i\omega_n) = \frac{1}{\beta} \sum_m F_{\mathbf{q}}(i\omega_n - i\omega_m) \frac{1}{\omega_m^2 + E_{\mathbf{k}s}^2}, \quad (18)$$

and  $I_{\mathbf{k}}^0 = \text{th}(\beta E_{\mathbf{k}}/2)/(2E_{\mathbf{k}})$ .

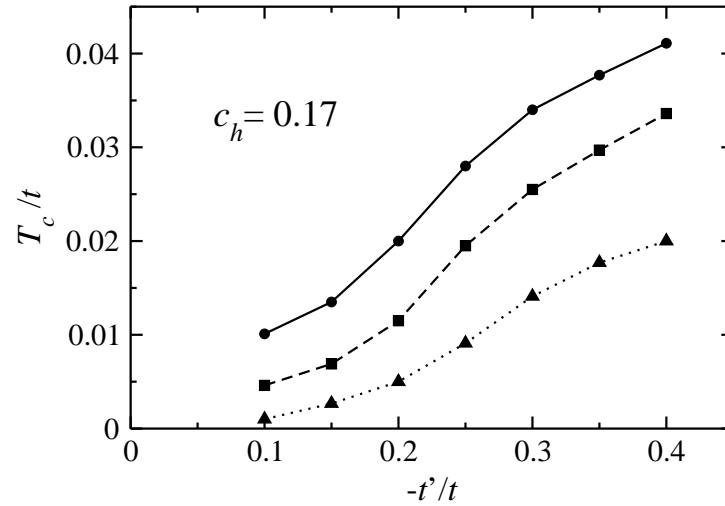
Eq. (17) represents the BCS-like expression which we use to evaluate  $T_c$ . To proceed we need the input of two kinds: a)  $\chi_{\mathbf{q}}(\omega)$ , and b) the NS QP properties  $Z_{\mathbf{k}}, \varepsilon_{\mathbf{k}}$ . As discussed in Sec. II the NS spin dynamics at  $\mathbf{q} \sim \mathbf{Q}$  is generally overdamped in the whole doping regime [3]. Hence we use the form, Eq.(5). We end up with parameters  $\chi_{\mathbf{Q}}^0, \Gamma_{\mathbf{Q}}, \kappa$ , which are dependent on  $c_h$ , but in general as well vary with  $T$ . Although one can attempt to calculate them as described in Sec. III [21], we use here the experimental input for cuprates, as discussed in Sec. II [24]. For the NS  $A_{\mathbf{k}}(\omega)$  and corresponding  $Z_{\mathbf{k}}, \varepsilon_{\mathbf{k}}$  we solve Eq. (16) for  $\Sigma_{\mathbf{k}}^{11} = \Sigma_{\mathbf{k}}$  as in Ref. [19], with the same input for  $\chi_{\mathbf{q}}(\omega)$ . The main message remains [26] that soft AFM fluctuations with  $\mathbf{q} \sim \mathbf{Q}$  lead through Eq. (16) to a reduction of  $Z_{\mathbf{k}}$ , which is  $\mathbf{k}$ -dependent. A pseudogap appears along the AFM zone boundary and the FS is effectively truncated in the underdoped regime with  $Z_{\mathbf{k}_F} \ll 1$  near the saddle points  $(\pi, 0)$  (in the antinodal part of the FS) [19, 26].

Close to half-filling and for  $\chi_{\mathbf{q}}^0$  peaked at  $\mathbf{q} \sim \mathbf{Q}$  both terms in the gap equation, Eq. (17), favor the  $d_{x^2-y^2}$  SC. The mean-field part  $\Delta_{\mathbf{k}}^0$ , Eq. (15), involves only  $J$  which induces a nonretarded local attraction, playing the major role in the RVB-type theories [15, 16]. In contrast, the spin-fluctuation part represents a retarded interaction due to the cutoff function  $C_{\mathbf{kq}}$ , determined by  $\Gamma_{\mathbf{k}-\mathbf{q}}$ . The largest contribution to the SC pairing naturally arises from the antinodal part of the Fermi surface. Meanwhile, in the same region also  $Z_{\mathbf{k}}$  is smallest thus reducing the pairing strength, in particular in the underdoped regime.

One can question the relative role of the hopping parameters  $t, t'$  and the exchange  $J$  in the coupling, Eq. (13). While our derivation within the  $t$ - $J$  model is straightforward, an analogous analysis within the Hubbard model using the projections to the lower and the upper Hubbard band, respectively, would not yield the  $J$  term within the lowest order since  $J \propto t^2$ . This stimulates us to investigate in the following also separately the role of  $J$  term in Eq. (17), both through the MF term, Eq. (15), and the coupling  $\tilde{m}_{\mathbf{k}\mathbf{q}}$ , Eq. (13).



**FIGURE 4.**  $T_c/t$  vs. doping  $c_h$  for  $t'/t = -0.3$ , calculated for various versions of Eq. (17): a) full result (full line), b) with neglected MF term (dashed line), and c) in addition to b) modified  $\tilde{m}_{\mathbf{k}\mathbf{q}}$  without the  $J$  term (dotted line).



**FIGURE 5.**  $T_c/t$  vs.  $-t'/t$  for fixed 'optimum' doping  $c_h = 0.17$  and different versions of Eq. (17), as in Fig. 2.

Results for the NS spectral properties reveal that the coupling to AFM fluctuations partly change the shape of the Fermi surface, more pronounced is however the effect on the QP weight.  $Z_{\mathbf{k}}$  is reduced along the AFM zone boundary away from the nodal points. In Fig. 4 we present final results for  $T_c$ , as they follow from the gap equation, Eq. (17). It is evident that the spin-fluctuation contribution is dominant over the mean-field term.

When discussing the role of the  $J$  term in the coupling, Eq. (13), we note that in the most relevant region, i.e., along the AFM zone boundary  $\tilde{m}_{\mathbf{k}\mathbf{Q}} = 2J - 4t' \cos^2 k_x$ . Thus, for hole doped cuprates,  $t' < 0$  term and  $J$  term enhance each other in the coupling, and neglecting  $J$  in  $\tilde{m}_{\mathbf{k}\mathbf{q}}$  reduces  $T_c$ , although at the same time relevant  $Z_{\mathbf{k}}$  is enhanced.

Finally, in Fig. 5 we present results, as obtained for fixed intermediate doping  $c_h = 0.17$ , but different  $t'/t < 0$ , as relevant for hole-doped cuprates [32]. As expected the dependence on  $t'$  is pronounced, since the latter enters directly the coupling  $\tilde{m}_{\mathbf{k}\mathbf{Q}}$ , Eq.(13). It is instructive to find an approximate BCS-like formula which simulates our results. The latter involves the characteristic cut-off energy  $\Gamma_{\mathbf{Q}}$ , while other relevant quantities are the electron density of states  $\mathcal{N}_0$  and  $Z_m$  being the minimum  $Z_{\mathbf{k}}$  on the FS (in the antinodal point). Then, we get a reasonable fit to our numerical results with the expression,

$$T_c \sim 0.5\Gamma_{\mathbf{Q}} e^{-2/(\mathcal{N}_0 V_{eff})}, \quad (19)$$

where the effective interaction is given by  $V_{eff} = 3Z_m(2J - 4t')^2\chi_{\mathbf{Q}}$ .

Probably the most interesting novel result on SC is a pronounced dependence of  $T_c$  on  $t'$  which is also consistent with the evidence from different families of cuprates [32]. One can give a plausible explanation of this effect. In contrast to NN hopping  $t$ , the NNN  $t'$  represents the hopping within the same AFM sublattice, consequently in a double unit cell fermions couple directly to low-frequency AFM paramagnons. Calculated  $T_c$  are in a reasonable range of values in cuprates. We also note that rather modest 'optimum'  $T_c$  value within presented spin-fluctuation scenario emerge due to two competing effects in Eqs. (17),(19): large  $\tilde{m}_{\mathbf{k}\mathbf{q}}$  and  $\chi_{\mathbf{Q}}$  enhance pairing, while at the same time through a reduced  $Z_{\mathbf{k}}$  and cutoff  $\Gamma_{\mathbf{Q}}$  they limit  $T_c$ . At the same time, INS experiments [3] reveal that in underdoped cuprates the resonant peak at  $\omega \sim \omega_r$  takes the dominant part of intensity of  $\mathbf{q} \sim \mathbf{Q}$  mode which becomes underdamped possibly even for  $T > T_c$ . Thus it is tempting to relate  $\Gamma_{\mathbf{Q}}$  to  $\omega_r$  and to claim  $T_c \sim a\omega_r$ , as indeed observed in cuprates [3].

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