Influence of the pseudogap on the superconductivity-induced phonon renormalization in high-T_c superconductors

S. Varlamov and G. Seibold
Institut für Physik, BTU Cottbus, PBox 101344, D-03013 Cottbus, Germany

(Received 12 November 2001; published 11 March 2002)

We investigate the influence of a *d*-density wave (DDW) gap on the superconductivity-induced renormalization of phonon frequency and linewidth. The results are discussed with respect to Raman and inelastic neutron scattering experiments. It turns out that the DDW gap can enhance the range of frequencies for $q=0$ phonon softening depending on the underlying band structure. Moreover we show that an anisotropic "*d*-wave" pseudogap can also contribute to the *q*-dependent linewidth broadening of the 340 cm^{-1} phonon in $YBa_2Cu_3O_7$.

DOI: 10.1103/PhysRevB.65.132504 PACS number(s): 74.25.Jb, 74.25.Gz, 74.25.Kc

The origin of the pseudogap is presently a strongly debated issue in the field of high-T_c superconductivity and has been detected by numerous techniques in all the cuprates.[1] One of the ideas which received considerable attention involves the existence of preformed pairs.[2] This idea finds support in continuous evolution of angle-resolved photoemission spectra (ARPES) from the normal to the superconducting (SC) state.[3] However, another appealing scenario suggests that the pseudogap could (not only) arise from pairing in the particle-particle channel, but also from different scattering mechanisms (such as CDW fluctuations) which become singular near optimal doping. Indeed there is increasing experimental evidence[4,5] that the peculiar properties of the cuprates, both in the normal and the SC phase are related to the occurrence of a quantum critical point (QCP) located near (slightly above) the optimal charge carrier concentration. Besides singular scattering at the QCP a further direct consequence of this scenario is the prediction of an ordered state in the underdoped regime. Various types of orderings have been proposed each of them breaking different kinds of symmetries. For example, Castellani *et al.*[6] have proposed incommensurate charge-density waves (ICDW) which break translational invariance. Varma[7] considers circulating currents which (in addition to time-reversal symmetry) break a rotational invariance of the copper oxygen lattice but preserve translational invariance. In one of the latest proposals Chakravarty *et al.*[8] have investigated *d*-density wave order. This state is made of staggered currents which break parity and time-reversal symmetry as well as translational invariance by one lattice constant and rotation by $\pi/2$. All of these proposals have in common that the corresponding order parameter induces a gap in the single-particle spectrum which has the same anisotropy as observed in ARPES experiments. For the circulating current state this has been shown in Ref. 9 and for the ICDW phase in Ref. 10. In the case of the DDW state the pseudogap anisotropy is explicitly put in the quasiparticle Hamiltonian.

In this paper we consider the influence of an anisotropic single-particle gap on the frequency shift and linewidth of phonons in the SC state. Strong phonon self-energy effects in high-T_c cuprates have been analyzed first by Zeyher and Zwicknagel[11] within Eliashberg theory. For an isotropic *s*-wave superconductor they obtained softening for phonons with frequencies $\omega<2\Delta_0$ and hardening for phonons with $\omega>2\Delta_0$. In addition the linewidth of the phonon mode is only affected for $\omega>2\Delta_0$ where it is additionally broadened due to the opening of the SC (*s*-wave) gap. The Zeyher-Zwicknagel approach has been generalized to anisotropic gap functions and dispersions relevant for the cuprates in Refs. 12,13. The main difference with respect to the *s*-wave model is the appearance of an additional line broadening for mode frequencies $\omega<2\Delta_0$ since in a *d*-wave superconductor the density of states (DOS) remains finite for energies within the maximum SC gap.

Our investigations are based on the DDW state since from the formal point of view this scenario offers a simple way of introducing an anisotropic gap into the problem. However, we want to stress that most of the results presented below should also (at least qualitatively) hold for other QCP proposals as long as the corresponding pseudogap leads to an analogous quasiparticle dispersion. In this context it is interesting to note that a DDW-type gap has also been considered for the ICDW scenario.[14] The starting point is the following Hamiltonian:

$$H=\sum_{\mathbf{k}\sigma}[\epsilon_{\mathbf{k}}-\mu]c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+i\sum_{\mathbf{k}\sigma}\chi_{\mathbf{k}}c^\dagger_{\mathbf{k}+\mathbf{Q}\sigma}c_{\mathbf{k}\sigma}$$
$$+\sum_{\mathbf{k}}\Delta_{\mathbf{k}}[c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}+c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}], \tag{1}$$

where $\chi_{\mathbf{k}}=\chi_0[\cos(k_x)-\cos(k_y)]/2$ and $\Delta_{\mathbf{k}}=\Delta_0[\cos(k_x)-\cos(k_y)]/2$ denote the DDW and SC gap, respectively, and $\mathbf{Q}=(\pi,\pi)$. The dispersion $\epsilon_{\mathbf{k}}$ will be specified later. In the basis $\Psi^\dagger_k=(c^\dagger_{\mathbf{k}\uparrow},c_{-\mathbf{k}\downarrow},c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow},c_{-\mathbf{k}-\mathbf{Q}\downarrow})$ the Hamiltonian (1) is given by

$$H_{\mathbf{kk}}=\begin{pmatrix}(\tilde{\varepsilon}_k-\tilde{\mu}_k) & \Delta_k & i\chi_k & 0\\ \Delta_k & -(\tilde{\varepsilon}_k-\tilde{\mu}_k) & 0 & i\chi_k\\ -i\chi_k & 0 & -(\tilde{\varepsilon}_k+\tilde{\mu}_k) & -\Delta_k\\ 0 & -i\chi_k & -\Delta_k & (\tilde{\varepsilon}_k+\tilde{\mu}_k)\end{pmatrix},$$

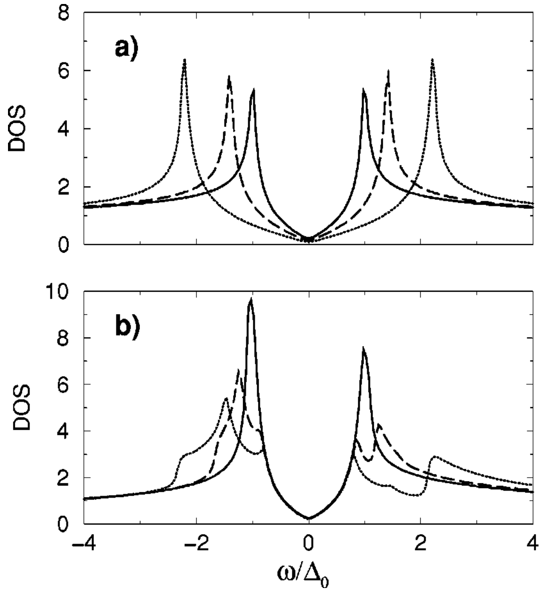

FIG. 1. Density of states in the superconducting state ($\Delta_0 = 23$ meV) for three values of pseudogap. $\chi_0/\Delta_0 = 0$: solid curve, $\chi_0/\Delta_0 = 1$: dashed curve, $\chi_0/\Delta_0 = 2$: dotted curve. (a) Nearest-neighbor tight-binding model at half filling. (b) Energy dispersion from Ref. 16.

where $\tilde{\varepsilon}_k = (\varepsilon_k - \varepsilon_{k+Q})/2$ and $\tilde{\mu}_k = \mu - (\varepsilon_k + \varepsilon_{k+Q})/2$. Diagonalization yields the four eigenvalues $\pm E_{1,2}(k) = \pm\sqrt{(\tilde{E}_k \pm |\tilde{\mu}_k|)^2 + \Delta_k^2}$, where $\tilde{E}_k = \sqrt{\tilde{\varepsilon}_k^2 + \chi_k^2}$. Note that the wave vector is now within the reduced zone of the DDW state.[8]

The superconductivity induced phonon renormalization is obtained from the imaginary-time ordered charge-charge correlation function $\Pi(q,i\omega) = \langle T_\tau \rho_q(i\omega)\rho_{-q}(-i\omega)\rangle$ via $\delta\omega = g^2\Pi(\mathbf{q},\omega + i\delta)$ and the correlator is analytically continued to real frequencies at the end of the calculation. Throughout the paper we restrict ourselves to a momentum independent electron-phonon coupling constant g in order to focus on the essential contribution from the pseudogap anisotropy.[15]

We start our analysis by calculating the renormalization of $q=0$ phonons. In this case the charge susceptibility reads

$$\Pi(q=0,i\omega) = \frac{1}{N}\sum_{\substack{k\\ s=1,2}} \frac{\Delta_k^2[1-2n_s(k)]}{E_s(k)} \times \frac{4}{\{(i\omega)^2 - [2E_s(k)]^2\}},$$

where $n_s(k) = (e^{\beta E_s(k)} + 1)^{-1}$. Note that within our approach the $q=0$ phonon self-energy is only finite in the SC state for arbitrary value of the pseudogap. In order to investigate the influence of the pseudogap on the phonon renormalization above T_c one should include vertex corrections to $\Pi(q=0,i\omega)$ which, however, is beyond the scope of the present paper.

Obviously the underlying dispersion plays a significant role in determining the properties of $\Pi(q=0,\omega)$. Figure 1 shows the density of states (DOS) for two model band dispersions which will be considered below. The DOS is evaluated in the SC state ($\Delta_0 = 23$ meV for all following results) and for three values of the pseudogap. Figure 1(a) corresponds to $\varepsilon_k^a = -2t[\cos(k_x) + \cos(k_y)]$ with $t = 0.5$ eV, i.e., complete nesting for the DDW scattering vector at half-filling. Due to particle-hole symmetry the chemical potential μ is not altered in this case upon increasing the pseudogap. Thus for $\mu = 0$ χ_k and Δ_k work cooperatively and the DOS shows a single "leading edge" gap at energy $2\sqrt{\Delta_0^2 + \chi_0^2}$. Figure 1(b) shows the DOS for a tight-binding dispersion ε_k^b recently proposed by Norman[16] in order to analyze neutron-scattering and ARPES data in the SC state of underdoped bilayer cuprates. In this case the gap edges of SC gap and pseudogap are separated since the former opens at the chemical potential whereas the pseudogap is related to the energy where the dispersion is most susceptible to DDW scattering. Moreover the DDW state induces a Fermi surface which consists of four pockets centered around $(\pm\pi/2, \pm\pi/2)$. With increasing DDW gap the pockets shrink towards the nodes thus decreasing the effective SC gap in the DOS [see Fig. 1(b)].

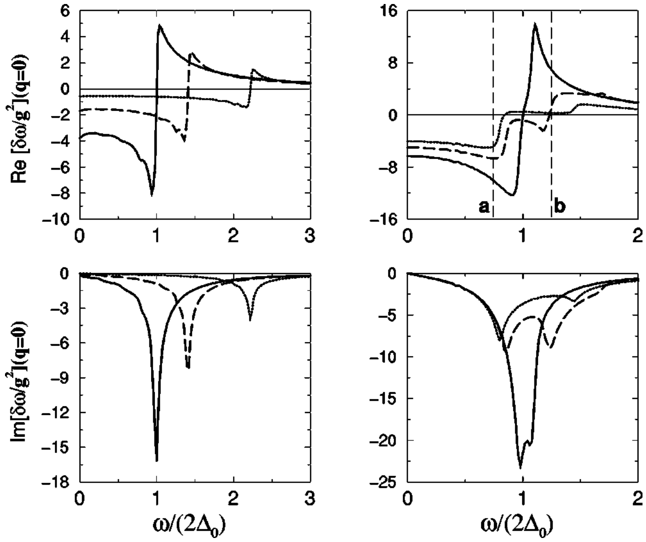

FIG. 2. Real and imaginary part of $\Pi(q=0,\omega)$ corresponding to the DOS shown in Fig. 1(a) (left panel) and Fig. 1(b) (right panel). Labeling of the curves is the same than in Fig. 1. The dashed lines in the upper right plot indicate the phonon frequencies discussed in the text.

For both dispersions Fig. 2 depicts the real and imaginary part of $\Pi(q=0,\omega)$ as a function of $\omega/(2\Delta_0)$ and for zero temperature. In case of zero pseudogap the frequency shift and linewidth broadening correspond to the results of Refs. 12,13, i.e., crossover from hardening to softening at frequencies $\omega \approx 2\Delta_0$. In addition the d-wave gap results in a linewidth broading also for $\omega < 2\Delta_0$ due to the finite density of states in the SC gap. However, consider the case of finite DDW gap and the underlying dispersion ε_k^a (left panel). It turns out that the sign change in $\delta\omega$ now occurs at frequencies $2\sqrt{\Delta_0^2 + \chi_0^2}$ following the behavior in the DOS. Moreover with increasing pseudogap the phonon linewidth broadening rapidly decreases and correspondingly also the maximum phonon frequency shift. In case of the dispersion ε_k^b (right panel) the situation is more complex and can be

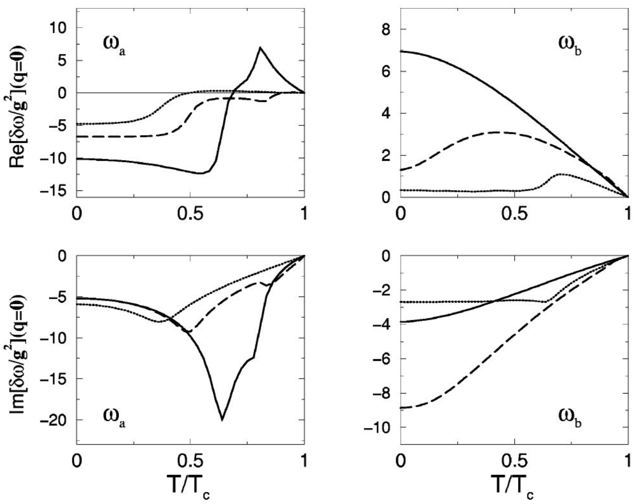

FIG. 3. Temperature dependence of frequency shift and linewidth broadening for two frequences $\omega_{a,b}=2\Delta_0\pm\Delta_0/2$ (left and right panel). Labeling of the curves is the same than in Fig. 1.

analyzed best by first considering the linewidth broadening which follows closely the behavior of the DOS. Upon increasing the DDW gap $\mathrm{Im}\,\Pi(q=0,\omega)$ develops a double peak structure,[17] where the low energy excitation is due to SC and the other one is due to the DDW "leading edge" in the DOS. This structure is reflected in $\mathrm{Re}\,\Pi(q=0,\omega)$ by the two step like features below and above $2\Delta_0$. It turns out that at least up to $\chi_0/\Delta_0=1$ the DDW gap enlarges the frequency range where phonon softening occurs. In addition the "hardening peak" becomes strongly suppressed by a finite value of the pseudogap most notably exemplified in case of $\chi_0/\Delta_0=2$ where $\mathrm{Re}\,\Pi(q=0,\omega)$ is practically zero above $\omega\sim 2\Delta_0$.

We now turn to the analysis of the temperature dependence of the phonon renormalization which we evaluate for the dispersion ε_k^b. Figure 3 shows the real and imaginary part of $\Pi(q=0,\omega)$ for the two frequencies $\omega_{a,b}=2\Delta_0\pm\Delta_0/2$ [indicated by dashed lines in Fig. 2(b)]. For simplicity, we adopt the BCS temperature dependence for both SC and DDW order parameters, i.e., $\Delta_0(T)=\sqrt{1-(T/T_c)^2}$, $T_c=80$ K and $\chi_0(T)=\sqrt{1-(T/T^*)^2}$, $T^*=150$ K [note that the temperature dependence of $\chi_0(T)$ has no significant influence on the result]. For zero DDW gap the a phonon initially hardens close to T_c where the "effective" SC gap is well below ω_a in agreement with Ref. 13. This hardening becomes completely suppressed upon increasing the DDW gap, however, there is still significant softening for $T\to 0$. Correspondingly the peak in $\mathrm{Im}\,\Pi(q=0,\omega)$ is also reduced by the opening of the pseudogap. As already discussed above the hardening of the b phonon is much more affected by the DDW gap. In fact the frequency shift is almost completely suppressed for $\chi_0/\Delta_0=2$ where also the strongly reduced DOS in the pseudogap reduces the phonon scattering and thus the corresponding linewidth.

Our results can be compared with doping dependent Raman scattering experiments where upon underdoping the increasing pseudogap should have a significant influence on the phonon renormalization. The most pronounced features are found for the 340 cm^{-1} phonon in $YBa_2Cu_3O_{7-x}$ which undergoes a strong softening and hardening of the 440 and 500 cm^{-1} modes below the SC transition temperature. The particular role of doping for the Raman modes below T_c was investigated by Altendorf *et al.*[18] and more recently by Limonov *et al.*[19] It turns out that the superconductivity induced changes in linewidth and frequency for the 340 cm^{-1} B_{1g} mode depend very sensitively on the charge carrier concentration near optimal doping. With increasing underdoping the phonon renormalization becomes rapidly suppressed in contrast to the overdoped regime where the data of Ref. 19 do not show a pronounced difference of frequency shift to the optimally doped case. Only the linewidth broadening gradually decreases from the overdoped to the optimally doped sample and vanishes for the underdoped system. Analagous behavior is observed for the 430 and 500 cm^{-1} modes which show hardening for the optimal and overdoped samples while frequency shifts are suppressed in the underdoped regime. Thus these features can be (at least qualitatively) accounted for by evaluating the phonon renormalization with an anisotropic pseudogap as described above.

We now proceed in calculating the influence of the DDW gap on the q-dependent phonon renormalization in the SC state (based on dispersion ε_k^b). For simplicity we restrict ourselves to zero temperature where the charge-charge correlation function is given by

$$\Pi(q,i\omega)=\frac{1}{2N}\sum_{\substack{k\\ s,t=1,2}}\Theta_{s,t}\Omega_{s,t}\frac{E_s(k+q)+E_t(k)}{(i\omega)^2-[E_s(k+q)+E_t(k)]^2}.$$

The coherence factors read

$$\Theta_{s,t}=1+(-1)^{s+t}\frac{\tilde{\varepsilon}_k\tilde{\varepsilon}_{k+q}+\chi_k\chi_{k+q}}{\tilde{E}_k\tilde{E}_{k+q}}$$

and

$$\Omega_{s,t}=1-\frac{[(-1)^s\tilde{E}_k-|\tilde{\mu}_k|][(-1)^t\tilde{E}_{k+q}-|\tilde{\mu}_{k+q}|]-\Delta_k\Delta_{k+q}}{E_s(k)E_t(k+q)}.$$

Since we are interested in the change of phonon frequency and linewidth upon entering the SC state we consider in the following the difference $\Pi^{\Delta>0}(q,i\omega)-\Pi^{\Delta=0}(q,i\omega)$. Figure 4 depicts the corresponding real and imaginary part for $\omega_a=2\Delta_0-\Delta_0/2$ along the $[1,0]-$ and $[1,1]$ direction for different values of χ_0. Note that the peaklike structures at small q are due to the two dimensionality of the Fermi surface (see, e.g., Refs. 20,21) and they are only observable

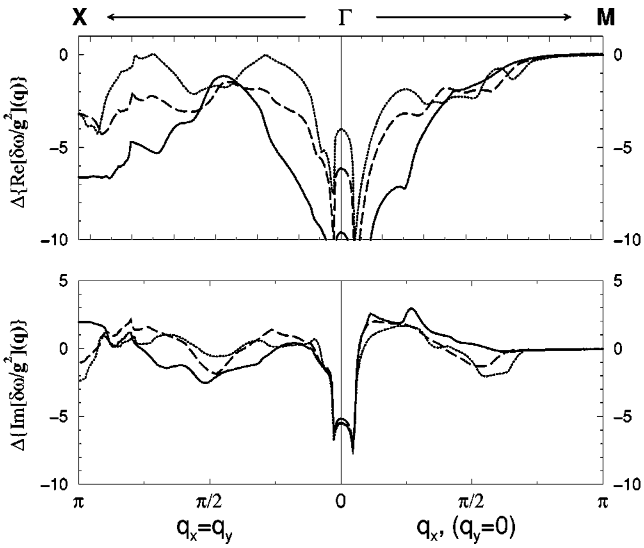

FIG. 4. SC induced change in the q-dependent frequency shift and linewidth broadening for $\omega_a = 2\Delta_0 - \Delta_0/2$. Labeling of the curves is the same than in Fig. 1.

when the condition $q_z = 0$ is fulfilled. However, since the latter is experimentally hard to realize we disregard these features in our following analysis.

Consider first the $(0,0) \rightarrow (\pi,0)$ $(\Gamma \rightarrow M)$ scan where the pseudogap induced change in $\mathrm{Re}\,\Pi(q,\omega)$ is most significant for wave vectors up to $q \sim (\pi/2,0)$. In fact, for zero DDW gap the system is rather susceptible for perturbations within this wave vector range since the corresponding scattering acts in the high-density $(\pi,0)$ region of the underlying dispersion. However, it is exactly this part of the Brillouin zone where the DDW state induces a gap which in turn leads to the decrease in the charge susceptiblity for $q_x < \pi/2$. As a consequence the most pronounced change in the SC induced phonon frequency shift now occurs at around $q \approx (\pi/2,0)$ which reflects itself in an increase of the linewidth around the same wave vector. For the $(0,0) \rightarrow (\pi,\pi)$ $(\Gamma \rightarrow X)$ scan the same arguments than above can be applied in order to understand the suppression of small q frequency shifts upon increasing the DDW gap. Moreover, along the diagonals also the large wave vector phonon renormalization is affected. Thus the opening of the pseudogap strongly reduces the SC induced frequency change over large parts of the $\Gamma \rightarrow X$ direction.

Therefore, our results can account for some of the anomalies of the 340 cm^{-1} phonon observed by inelastic neutron scattering.[22,23] Most interestingly it was found that at low temperature the SC induced change in phonon frequency is largest along the (1,0) direction for wave vectors up to $q \sim (\pi/2,0)$. Then the softening progressively vanishes towards the zone boundary and as a consequence the linewidth aquires a maximum at $q \approx (\pi/2,0)$. On the other hand, much smaller softening and no linewidth broadening has been detected along the diagonal direction. Thus from our analysis one may deduce that the measured linewidth broadening along the (1,0) direction is at least partially due to the presence of the pseudogap. This feature together with the reduced frequency renormalization of phononic Raman modes upon underdoping supports the point of view, that the pseudogap also persists below T_c and may not (only) originate from pair fluctuations.

Obviously for a quantitative comparison a more detailed analysis for the q-dependent electron-phonon coupling is necessary which for the 340 cm^{-1} mode has been done in Ref. 24. In addition, we have restricted ourselves to the purely two-dimensional BCS case. However, at least the qualitative features of our investigations should be robust with respect to these approximations and may provide a basis for a more quantitative analysis of phonon renormalizations under the presence of an anisotropic pseudogap.

The authors would like to thank A. Bill for helpful discussions and a critical reading of the manuscript.

[1] T. Timusk and B. Statt, Phys. Rep. **62**, 61 (1999).
[2] M. Randeria *et al.*, Phys. Rev. Lett. **62**, 981 (1989).
[3] H. Ding *et al.*, Nature (London) **382**, 51 (1996).
[4] J.L. Tallon *et al.*, Phys. Status Solidi B **215**, 531 (1999); J.L. Tallon, G.V.M. Williams, and J.W. Loram, Physica C **338**, 9 (2000).
[5] G.S. Boebinger *et al.*, Phys. Rev. Lett. **77**, 5417 (1996).
[6] C. Castellani *et al.*, Phys. Rev. Lett. **75**, 4650 (1995).
[7] C.M. Varma, Phys. Rev. B **55**, 14 554 (1997).
[8] S. Chakravarty *et al.*, Phys. Rev. B **63**, 094503 (2001); C. Nayak, *ibid.* **62**, 4880 (2000); **62**, R6135 (2000).
[9] C.M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).
[10] G. Seibold *et al.*, Eur. Phys. J. B **13**, 87 (2000).
[11] R. Zeyher and G. Zwicknagel, Solid State Commun. **66**, 617 (1988); Z. Phys. B: Condens. Matter **78**, 175 (1990).
[12] E.J. Nicol *et al.*, Phys. Rev. B **47**, 8131 (1993).
[13] A. Bill *et al.*, Phys. Rev. B **52**, 7637 (1995).
[14] L. Benfatto *et al.*, Eur. Phys. J. B **17**, 95 (2000).
[15] The coupling constant g should be considered as an effective one, i.e., already reduced by vertex corrections.
[16] M.R. Norman, Phys. Rev. B **63**, 092509 (2001). We have chosen the parameter set ''$tb3$'' in this paper.
[17] Note that for zero pseudogap the double peak structure in the linewidth is due to the small separation of van Hove singularity and SC ''leading gap'' edge.
[18] E. Altendorf *et al.*, Phys. Rev. B **47**, 8140 (1993).
[19] M.F. Limonov *et al.*, Phys. Rev. B **61**, 12 412 (2000); M. Limonov *et al.*, *ibid.* **62**, 11 859 (2000).
[20] F. Marsiglio, Phys. Rev. B **47**, 5419 (1993).
[21] A. Bill *et al.*, J. Supercond. **9**, 493 (1996).
[22] N. Pyka *et al.*, Phys. Rev. Lett. **70**, 1457 (1993).
[23] D. Reznik *et al.*, Phys. Rev. Lett. **75**, 2396 (1995).
[24] T.P. Devereaux *et al.*, Phys. Rev. B **59**, 14 618 (1999).