Low-Doping Anomalies in High-T_c Cuprate Superconductors as Evidence of a Spin-Fluctuation-Mediated Superconducting State

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We present a theoretical study of the impact of spin fluctuations on electronic properties when these fluctuations are soft and strong, as in low-doped cuprates. We show that they play a triple role: they mediate d pairing, destroy the coherence of antinodal electrons, and create a spin density wave pseudogap. The competition between these effects is responsible for numerous electron anomalies close to those observed experimentally in the low-doping superconducting state.

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The microscopic mechanism of high-T_c superconductivity is still not known. The enigmatic low-doping superconducting (SC) state anomalies are actually the subject of intense debate and a test for any proposed mechanism. Taken as a whole, these anomalies seem currently incompatible with all existing scenarios. The most important anomalies are: (i) the opposite behaviour with doping of the maximum electron gap $\Delta^{\max}$ [1–3] and of the SC order parameter (OP) [4] (and T_c); (ii) the vanishing with underdoping of the antinodal electron contribution to the Cooper pair density [5]; (iii) the existence of two distinct energy scales, related to the nodal and antinodal electrons and behaving with doping in a divergent way [1,2,5]; (iv) the strange form of electron density of states (DOS) in which the lowest energy feature is not SC peaks but a kink occurring at positive energies [2]. And finally, most striking and difficult to explain is the loss of electron coherence in a large $\mathbf{k}$ space area near the antinode [1,3,5]: In the popular scenario of Fermi surface (FS) pockets around nodes formed due to some additional "hidden" static order, electrons should remain well defined everywhere, even for $\mathbf{k}$ near the antinode, the δ function peak in electron spectral functions simply moving away from the Fermi level. The loss of electron coherence seems also to be incompatible with any pairing through a glue boson since, even in strong-coupling dynamic theories, the near FS electrons usually remain well defined [6]. On the other hand, the latter scenario is strongly suggested by the existence in different electronic properties of low energy features, such as kink, dip, etc. [observed by angle resolved photoemission spectroscopy (ARPES), scanning tunneling microscopy (STM), optical conductivity], which are supposed to be related to the glue boson's characteristic energy. Moreover, the scenario with spin fluctuations (SFs) as a glue boson is strongly supported by the d symmetry of pairing and it can explain some important details in the observed electronic properties near optimal doping [7–10].

In this Letter, we show that the low-doping SC state anomalies, whose origin is critical for our understanding of the high-T_c pairing mechanism, find unexpectedly a natural explanation within the SF scenario. The key point is that SFs, when they are soft and strong (as in the low-doped cuprates [11,12]), not only mediate a SC attraction but at the same time destroy the electron coherence for some part of the FS (impossible under conventional phonon-mediated superconductivity). This occurs in the $\mathbf{k}$ region where the electron gap is high compared to SF characteristic energy, i.e., around the antinode. This region increases with SF softening and strengthening, i.e., with underdoping in cuprates. Finally, a new SC state emerges with properties very different from those of conventional superconductors and close to those observed experimentally in the low-doped cuprates. All anomalies of this state are summarized at the end of this Letter.

The results are obtained using a dynamic strong-coupling approach [8]. The dynamic equations are given by

$$G^N(\mathbf{k},\omega)=\frac{\omega+\epsilon_{\mathbf{k}}+(\Sigma^N_{\mathbf{k}-\omega})^*}{D_{\mathbf{k}\omega}},\qquad G^A(\mathbf{k},\omega)=\frac{\Sigma^A_{\mathbf{k}\omega}}{D_{\mathbf{k}\omega}},$$
$$D_{\mathbf{k}\omega}=\omega^2Z^2_{\mathbf{k}\omega}-(\epsilon_{\mathbf{k}}+\Sigma^+_{\mathbf{k}\omega})^2-(\Sigma^A_{\mathbf{k}\omega})^2, \tag{1}$$

$$\Sigma^{N,A}_{\mathbf{k}\omega}=-\frac{\tilde{g}^2}{N}\sum_{\mathbf{p}}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}\mathrm{Im}K_r(\mathbf{p},\omega')$$
$$\times\mathrm{Im}G^{N,A}_r(\mathbf{p}+\mathbf{k},\epsilon)\frac{1+n^B_{\omega'}-n^F_{\epsilon}}{\omega'+\epsilon-\omega-i\delta\mathrm{sgn}(\omega)}. \tag{2}$$

G^N and Σ^N are the normal (diagonal) Green function and self-energy, respectively, and G^A and Σ^A are the anomalous (off-diagonal) ones in the Gorkov-Nambu presentation; K is the spin Green function; r stands for "retarded"; $\epsilon_{\mathbf{k}}$ is the bare electron spectrum that we will take as $\epsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y-2t''(\cos 2k_x+\cos 2k_y)-\mu$ to describe the CuO_2 plane symmetry; $Z_{\mathbf{k}\omega}=1-\Sigma^-_{\mathbf{k}}(\omega)/\omega$ is the renormalization factor; $\Sigma^{\pm}_{\mathbf{k}\omega}=(\Sigma^N_{\mathbf{k}\omega}\pm\Sigma^N_{\mathbf{k}-\omega})/2$ are the even and odd parts of Σ^N; and $\tilde{g}$ is the effective interaction. Equations (1) and (2) are integral in energy and momentum equations with respect to Σ^N and Σ^A that should be solved self-consistently. Note that, contrary to the case of phonon-mediated superconductivity, one has

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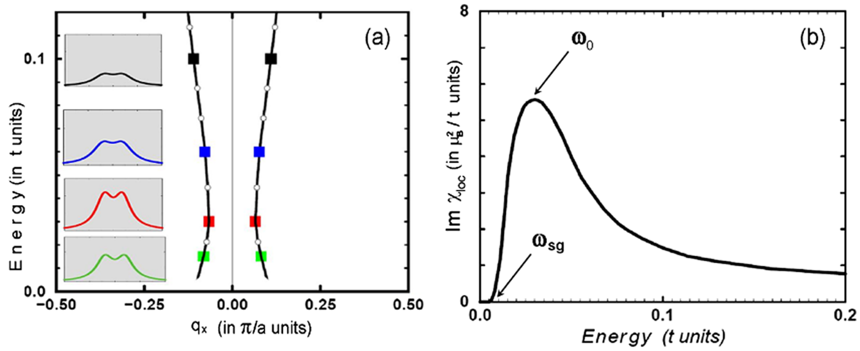

FIG. 1 (color online). The model for the input SF spectrum. The dispersion [shown in (a)], the momentum profiles around (π, π) [shown in the insets (a)], and the form and intensity of local susceptibility [shown in (b)] are taken close to those in experimental spectra at very low doping [11,12]. Energies are in t units; note that, for the cuprates, $t \sim 300$–400 meV.

no right to use their simplified version, Eliashberg equations (with integrals only in energy) [6], valid only when both the normal state electrons and SC pairing are isotropic, which is not the case for cuprates (with highly anisotropic FS and d pairing).

When the equations are solved, the quasiparticle ("electron") spectrum is determined, as usual, by poles of the Green functions, i.e., by solutions of the equation $D_{\mathbf{k}\omega} = 0$ on the real axis. We note that, in the dynamic theory of conventional superconductors, this equation always has a solution for the FS electrons and that their damping $\gamma_{\mathbf{k}}$ is always zero [6]. The situation is different for the SF-mediated SC state. Three different regimes can exist for FS electrons: regimes I and II with coherent electrons (in I, $\gamma_{\mathbf{k}} = 0$; in II, $\gamma_{\mathbf{k}}$ is finite) and regime III in which coherent electrons disappear. To demonstrate this, let us first use the simplified "Einstein" model for SFs, $\mathrm{Im}K_r(\mathbf{p}, \omega) = -IA_{\mathbf{p}}[\delta(\omega - \omega_r) - \delta(\omega + \omega_r)]$ [with $A_{\mathbf{p}}$ maximum at $\mathbf{p} = \mathbf{Q} = (\pi, \pi)$] that roughly reproduces the most important properties of the observed SFs and leads to the d symmetry of pairing [8]. Zeros of $\mathrm{Re}D_{\mathbf{k}\omega}$ on the real axis, if they exist, are given by the equation $\omega = \pm\Delta_{\mathbf{k}}(\omega)$ with the energy-dependent real gap $\Delta_{\mathbf{k}}(\omega) = \mathrm{Re}\Sigma^A_{\mathbf{k}\omega}/\mathrm{Re}Z_{\mathbf{k}\omega}$. (We omitted for simplicity the term $\epsilon_{\mathbf{k}} + \Sigma^+_{\mathbf{k}\omega}$, which is negligible for FS electrons after the renormalization of $\mathbf{k}_F$.) With this model, the expressions for $\mathrm{Im}\Sigma^{N,A}$ roughly reduce to $|\mathrm{Im}\Sigma^{N,A}(\omega)| \sim N(\omega - \omega_r \mathrm{sgn}\omega)$, where $N(\omega)$ is the electron DOS that for d pairing behaves linearly for low $|\omega|$ and has a logarithmic singularity at $\pm\Delta^{\max}$. Therefore, $|\mathrm{Im}\Sigma^{N,A}|$ is 0 for $|\omega|$ below ω_r, increases continuously above, and reaches ∞ at $\omega_c = \omega_r + \Delta^{\max}$. As for $\mathrm{Re}\Sigma^{N,A}$ (related to $\mathrm{Im}\Sigma^{N,A}$ by the Kramers-Kronig relation), they behave in such a way that $\Delta_{\mathbf{k}}(\omega)$ is practically constant for $|\omega|$ below ω_r, increases rather rapidly for higher $|\omega|$, and becomes singular (namely, it jumps) at $|\omega| = \omega_c$. It is clear therefore that, if $\Delta_{\mathbf{k}}(0)/\omega_r \ll 1$, the equation $\mathrm{Re}D_{\mathbf{k}\omega} = 0$ has always a solution, while $\gamma_{\mathbf{k}} = 0$—one gets regime I. [The solution occurs at $\omega = \Delta_{\mathbf{k}} \equiv \Delta_{\mathbf{k}}(\omega = \Delta_{\mathbf{k}})$.] If $\Delta_{\mathbf{k}}(0)/\omega_r > 1$, then there is still a pole of the Green function but the damping is nonzero—regime II occurs. The higher $\Delta_{\mathbf{k}}(0)/\omega_r$, the higher the pole (i.e., the quasiparticle) energy $\Delta_{\mathbf{k}}$, with respect to $\Delta_{\mathbf{k}}(0)$, and the stronger the relative damping $\gamma_{\mathbf{k}}/\Delta_{\mathbf{k}}$. Thus, when the pole energy approaches the energy ω_c, where $|\mathrm{Im}\Sigma^{N,A}| \to \infty$ and therefore $\gamma_{\mathbf{k}} \to \infty$, the coherent quasiparticles disappear. In fact, as shown by the numerical calculations, when $\Delta_{\mathbf{k}}(0)/\omega_r \gg 1$, the loss of electron coherence happens in a slightly different way: The solution of the equation $\mathrm{Re}D_{\mathbf{k}\omega} = 0$ disappears even before the electron gap value $\Delta_{\mathbf{k}}$ reaches ω_c. (This happens due to the high contribution of the imaginary parts $\mathrm{Im}\Sigma^A$ and $\mathrm{Im}Z$ to $\mathrm{Re}D_{\mathbf{k}\omega}$ in this energy range.) This is regime III. We see that it is the smallness of the spin mode energy and its high intensity I [since $\Delta_{\mathbf{k}}(0)$ increases with increasing I] that favor this regime, both effects taking place in cuprates with underdoping. More generally, one should speak about the high value of effective coupling $\Lambda \propto \tilde{g}^2 I/\omega_r$. [Note that $\Lambda \to \infty$ when the system is in the limit of instability at the origin of the boson softening, antiferromagnetic (AFM) instability here.] Another factor that governs the electron belonging to different regimes is the location of $\mathbf{k}$ on the FS: Indeed, for d symmetry, with $\Delta_{\mathbf{k}}(0)$ increasing progressively [from 0 to $\Delta_A(0)$] along the FS from the node to the antinode, near-node electrons are necessarily in regime I while antinodal electrons can be in regimes I, II, or III, depending on the $\Delta_A(0)/\omega_r$ ratio. In the latter (most interesting) case, the FS electrons pass progressively from regime III to regime I through regime II, i.e., restore progressively their coherence, when going from antinode to node. It is clear from the above discussion that the $\mathbf{k}$ space area where the coherent quasiparticles exist (we will call it the FS arc) decreases with decreasing $\omega_r/\Delta_A(0)$. In other words, the FS arc shrinks with the spin mode softening and strengthening, i.e., with underdoping in cuprates. This is exactly what is observed experimentally; see, e.g., Ref. [1]. Note that the regime of incoherent electrons cannot appear for the s pairing since, in this case, $\mathrm{Im}\Sigma^{N,A}_{\omega}$, and therefore the electron damping, is zero, not until $|\omega| = \omega_r$ but until $|\omega| = \omega_r + \Delta$. As a result, there is always a solution for the equation $\omega = \Delta(\omega)$ and no damping for FS electrons. [In fact, the extreme limit $\Lambda \to \infty$ in

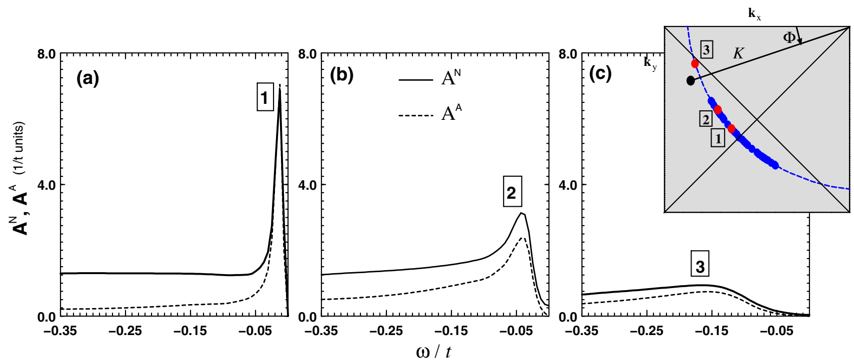

FIG. 2 (color online). Evolution along the FS of the diagonal (A^N) and off-diagonal (A^A) electron spectral functions (the numbers in the boxes correspond to the locations of $\mathbf{k}_F$ on the FS, shown in the inset). Note the progressive disappearance of the coherent peak when moving from node to antinode.

the phonon-mediated superconductivity was studied in the early 1990s (see, e.g., Ref. [13] and references therein), and it was found that, while $\Delta(0)/\omega_r$ increases as $\sqrt{\Lambda}$, the poles of the Green function, i.e., coherent electrons, are always preserved.]

To see whether this new regime can indeed occur in the low-doped cuprates, we perform below a detailed study using a more realistic model for SFs. Although different theories exist for the low-doping SFs (see, e.g., Ref. [14]), we prefer to use for the input SFs a model that reproduces closely the experimentally observed spectrum [11,12]. The model takes into account the SF dispersion and presents the spectrum as a series of plateaus with an incommensurate $\mathbf{q}$ profile [Fig. 1(a)] and local susceptibility $\mathrm{Im}\chi_{\mathrm{loc}}(\omega) = \frac{1}{N}\sum_{\mathbf{q}}\mathrm{Im}\chi(\mathbf{q}, \omega)$, shown in Fig. 1(b) ($\mathbf{q}$ is defined as $\mathbf{q} = \mathbf{Q} - \mathbf{p}$). (The SF spectrum is cut off at $\omega = 0.2t$.) The characteristic energy, ω_0, with maximal $\mathrm{Im}\chi_{\mathrm{loc}}$, is taken very low and the intensity at $\omega = \omega_0$ rather high (as in experimental spectra), so that one would expect to find regime III for antinodal electrons. [A SC spin gap ω_{sg} (that is normally present in the SC state SFs) is introduced formally while taken extremely low to correspond to the low-doping neutron data [11,12] in which such a gap is not seen at least down to 3 meV.] Note that, from the theoretical point of view, the softening and strengthening are natural properties of SFs near AFM instability or more generally of any critical fluctuations near a quantum critical point (QCP). The state with soft SFs as in Fig. 1 can be considered as a dynamic spin density wave (SDW) state, the energy ω_0 playing the role of the distance from the AFM QCP. For the electron system, we choose the parameters $t'/t = -0.3$, $t''/t = 0.05$, and $\mu/t = -0.6$ to get the FS close to the observed one. For the effective interaction, we take $\tilde{g} = 5t \sim 1.5$ eV of the same order as in other theories treating electron-spin coupling (see, e.g., Ref. [9]).

The self-consistent solution of Eqs. (1) and (2) gives the following results: first, we find that the equation $\mathrm{Re}D_{\mathbf{k}\omega} = 0$ has no solution for antinodal electrons; this occurs in the same way as for the Einstein model, the energy ω_0 playing the role of ω_r. As a consequence, the spectral functions $A^N_{\mathbf{k}}(\omega) = -\frac{1}{\pi}\mathrm{Im}G^N_r(\mathbf{k}, \omega)$ have an incoherent form for the antinodal electrons, and a coherent peak emerges progressively in approaching the nodal region; see Fig. 2. The reason for such a behavior, evident from the analysis performed for the Einstein model, is a passage from regime III through II to I when going from the antinodal to the nodal region. Note that the evolution of the spectral function form along the FS in Fig. 2 is exactly the same as that observed experimentally (ARPES) (see, e.g., Fig. 1 in Ref. [1]). If one associates the energy positions of $A^N_{\mathbf{k}}(\omega)$ peaks for different $\mathbf{k}_F$ with electron gap along the FS, as usually made in ARPES, one gets the electron gap angular dependence shown in Fig. 3(a). It exhibits two distinct regimes, in the near-node and near-antinode regions, with a rapid crossover between them, a behavior very close to that observed experimentally by ARPES [1,15] and STM [2]. The gap in these regimes has a different origin: For the near-node electrons, the peak positions in $A^N_{\mathbf{k}}(\omega)$ coincide with zeros of $\mathrm{Re}D_{\mathbf{k}\omega}$ and the gap is a SC gap in its standard definition. The near-antinode electron gap given by hardly pronounced maxima in $A^N_{\mathbf{k}}(\omega)$ is not a SC gap in the usual sense. It originates from a subtle interplay between three factors: the two orders, static with respect to superconductivity and dynamic with respect to SDW and the incoherence of the antinodal electrons, due to which the form of $A^N_{\mathbf{k}}(\omega)$ is determined not so much by $\mathrm{Re}D_{\mathbf{k}\omega}$- but rather by $\mathrm{Im}D_{\mathbf{k}\omega}$-behavior. The existence of these two distinct gap regimes results in the appearance of *two characteristic gaps*: the maximum gap of coherent electrons, $\Delta^{\mathrm{arc}} \sim \omega_0$, and the overall maximum gap (the antinodal one), Δ^{max}, the two appearing as characteristic energies in different macroscopic properties. They can behave in a divergent way: Δ^{arc} compulsorily decreases with underdoping as does ω_0, while Δ^{max} can increase due to an increase of SF intensity.

Now, let us study the electronic properties describing the SC order. As we deal with anisotropic pairing, we determine the momentum- and angle-dependent OPs,

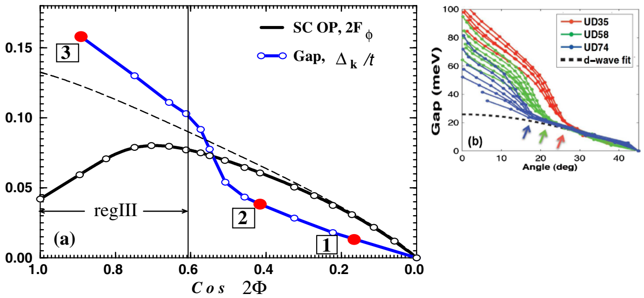

FIG. 3 (color online). (a) Angular dependence of the electron gap and the SC OP; the solid red points correspond to $\mathbf{k}_F$ in Figs. 2(a)–2(c). Note two anomalies: the presence of two distinct regimes for the electron gap and especially the decrease of F_ϕ towards the antinode. (The dashed black line shows $2F_\phi$ for the static d wave pairing.) (b) Gap from STM [2].

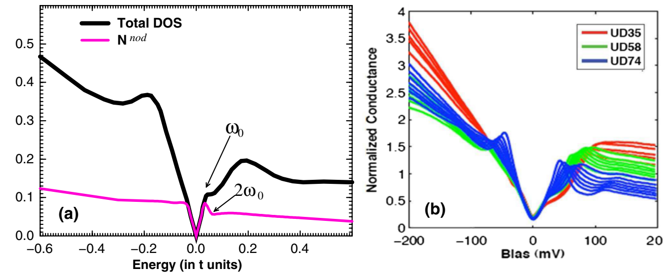

FIG. 4 (color online). Electron DOS in the low-doping SC state: (a) present theory and (b) STM data for different samples [2].

$F_{\mathbf{k}} \equiv \langle \psi_{\mathbf{k}\sigma}(t)\psi_{-\mathbf{k}\bar{\sigma}}(t)\rangle$ and $F_\phi = \int KdKF_{(K,\phi)}$ (K and ϕ are polar coordinates of vector $\mathbf{k}$; see the inset in Fig. 2). Using the theorem for operator averages in the Green function formalism, we get $F_{\mathbf{k}} = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} A_{\mathbf{k}}^A(\omega) n_\omega^F$, where we introduce the off-diagonal spectral function $A_{\mathbf{k}}^A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}G_r^A(\mathbf{k}, \omega)$. It evolves along the FS in the same way (and due to the same reason) as the diagonal spectral function A^N; see Fig. 2. As a result, in the near-node region, where electrons are coherent, F_ϕ increases with $\cos 2\phi$, being determined by the d symmetry of pairing. In the near-antinode region, F_ϕ decreases towards the antinode, being mainly determined by the progressive disappearance of the coherent peak in $A_{\mathbf{k}}^A(\omega)$; see Fig. 3(a). In this way, in the antinodal region, the electron gap and the SC OP turn out to behave in the opposite way, extremely unusual for a SC state feature but very similar to that observed in the low-doping cuprates [15,16]. The enigmatic opposite behavior with underdoping of the SC OP and maximum (antinodal) electron gap could, in our opinion, have the same origin. Note that the suppression of the SC OP near the antinode seen in Fig. 3(a) is the same effect as the suppression of Cooper pair density in the antinodal region observed by Raman spectroscopy [5].

Finally, let us see what is the form of the electron DOS in this regime in view of the strange form observed experimentally in the low-doping SC state. The calculated DOS $N(\omega) = \frac{1}{N}\sum_{\mathbf{k}} A_{\mathbf{k}}^N(\omega)$ is shown in Fig. 4(a). Like the observed DOS, it has only weakly pronounced peaks at $\pm\Delta^{\max}$ that are a natural consequence of the incoherence of antinodal electrons. Less expected is a kink at $\omega > 0$. Analysis shows that it is related to the near-node electron DOS properties. Such a DOS, defined as $N^{\rm nod}(\omega) = \int_{\phi_0}^{\pi/4} d\phi N_\phi(\omega)$ (with ϕ_0 close to $\pi/4$), exhibits a peak at ω_0 and a pseudogap just above; see Fig. 4(a), where we take $\phi_0 = 0.7\pi/4$ [$N_\phi(\omega) = \int dKKA_{(K,\phi)}^N(\omega)$]. The physical origin of these features is a proximity to SDW instability: We remind readers that, in the case of the static SDW order, a pseudogap related to $(\pi/2, \pi/2)$ electrons opens in the electron DOS at positive ω in addition to the one at negative ω related to $(0, \pi)$ electrons and extending over the Fermi level (for the hole-type FS) [17]. [These pseudogaps are related to the topological properties of the FS of 2D electrons on a square lattice with respect to the $\mathbf{q} = \mathbf{Q}$ wave vector, namely, to the existence of two topological QCPs, at $(0, \pi)$ and $(\pi/2, \pi/2)$ [18].] A similar effect takes place in our case as a consequence of the dynamic SDW order, with ω_0 characterizing a distance from static SDW order. The dynamic SDW pseudogap due to $(\pi/2, \pi/2)$ electrons opens in the nodal DOS at ω_0 and develops around $2\omega_0$ [19]. Although its existence in the near-node DOS is in no way related to the regime for antinodal electrons, only when the latter are in regime III is this pseudogap seen in the total DOS. Indeed, when $\Delta^{\max} \sim \omega_0$ (regimes I, II corresponding to the weakly underdoped cuprates), the SC peaks at $\pm\Delta^{\max}$ are strongly pronounced and occur in the same energy range as the nodal SDW pseudogap hiding it. On the contrary, when $\Delta_A \gg \omega_0$, the peak at ω_0 represents the lowest energy scale and appears in the total DOS as a kink at positive ω. This is exactly what is observed by STM in the underdoped cuprates [2] [Fig. 4(b)], where moreover the kink energy shows the same tendency of decrease with underdoping as in our theory.

In summary, we found that strong and soft SFs turn out to be destroyers rather than glue for SC pairing. The more SF intensity is concentrated at low energies, i.e., the higher the ratio $\Delta^{\max}/\omega_0$, the more their first role dominates. The emerging SC state is very different from the conventional one and is characterized by numerous anomalies, close to those observed in cuprates at low doping. First, coherent electron quasiparticles disappear in a large part of $\mathbf{k}$ space (around the antinode) that increases with SF softening and strengthening, i.e., with underdoping. Second, two different characteristic energy scales emerge related to the maximum gap of coherent electrons and to the overall maximum gap. They behave in a different way, the former being proportional to the SF's characteristic energy ω_0 and therefore decreasing with underdoping. Third, the SC OP behaves in a highly unconventional way, being determined by pairing symmetry only for the near-node electrons; otherwise, it decreases towards the antinode despite the d

symmetry of pairing. Such a behavior leads to the weakening of SC order in approaching AFM instability, opposite to the conventional phonon-induced SC order near structural instability [20]. Fourth, the electron DOS becomes sensitive to details in the near-node electron spectrum and shows a kink at positive energies related to the dynamic nodal SDW pseudogap.

In this scenario, the destructive role of SFs weakens and the effectiveness of pairing restores progressively with increasing the distance from the AFM QCP, i.e., with increasing doping, due to the increase of $\omega_0/\Delta^{\max}$. The effectiveness is fully restored once ω_0 exceeds $\Delta^{\max}$. Starting from this doping, the strength of pairing and T_c are, as usual, mainly determined by glue boson intensity. Since the SF's intensity continues to decrease with doping, the SC OP should decrease, as well, so that the doping where $\omega_0 \sim \Delta^{\max}$ will turn out to be an optimal doping for superconductivity.

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