

Magnetic Resonance in the Spin Excitation Spectrum of Electron-Doped Cuprate Superconductors

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We study the emergence of a magnetic resonance in the superconducting state of the electron-doped cuprate superconductors. We show that the recently observed resonance peak in the electron-doped superconductor $\text{Pr}_{0.88}\text{LaCe}_{0.12}\text{CuO}_{4-\delta}$ is consistent with an overdamped spin exciton located near the particle-hole continuum. We present predictions for the magnetic-field dependence of the resonance mode as well as its temperature evolution in those parts of the phase diagram where $d_{x^2-y^2}$ -wave superconductivity may coexist with an antiferromagnetic spin-density wave.

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Recently, inelastic neutron scattering (INS) experiments on the electron-doped high-temperature superconductors (HTSC) $\text{Pr}_{0.88}\text{LaCe}_{0.12}\text{CuO}_{4-\delta}$ (PLC_{0.12}CO) [1] observed a resonance peak in the superconducting (SC) state, a phenomenon similar to that observed in the hole-doped cuprates [2–4]. While the resonance frequency in PLC_{0.12}CO, $\omega_{\text{res}} \approx 11$ meV, obeys the same scaling with T_c as that in the hole-doped HTSC, there exist two significant differences. First, the resonance is confined to a small momentum region around $\mathbf{Q} = (\pi, \pi)$, where it is almost dispersionless. Second, angle-resolved photoemission (ARPES) experiments on PLC_{0.11}CO [5] estimated, based on measurements of the leading edge gap, a maximum SC gap located at the “hot spots” [the Fermi surface (FS) points connected by \mathbf{Q}] of $\Delta_{\text{hs}} \approx 5$ meV. Assuming the same SC gap in PLC_{0.12}CO, this would suggest that the resonance is located slightly above the onset of the particle-hole (p - h) continuum given by $2\Delta_{\text{hs}}$, a result which would challenge the interpretation of the resonance as a spin exciton [4,6–9]. However, the uncertainties in ARPES and INS experiments are currently such that it is not possible to determine the relative magnitude of ω_{res} and $2\Delta_{\text{hs}}$ and thus ascertain the validity of the spin-exciton scenario.

In this Letter we address this issue and study the emergence of a resonance mode in the SC state of electron-doped HTSC. We show that the experimental features of the resonance in PLC_{0.12}CO can be explained within a spin-exciton scenario. In particular, we demonstrate that the position of the hot spots close to the Brillouin zone (BZ) diagonal [10,11] combined with the momentum dependence of the fermionic interaction leads to an almost dispersionless resonance that is confined to a small momentum region around \mathbf{Q} . Moreover, while the resonance is always located below the p - h continuum in systems with a quasiparticle lifetime, $1/\Gamma \rightarrow \infty$, we show that the maximum of the resonance’s intensity can be shifted to frequen-

cies above the p - h continuum when $1/\Gamma$ is sufficiently small. In this case, the form of the spin susceptibility is more reminiscent of the *magnetic coherence effect* in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [12,13] than of the resonance observed in the hole-doped HTSC. We present two predictions for further experimental tests of the spin-exciton scenario. First, we show that a magnetic field in the ab plane leads to an energy splitting of the resonance which for typical fields is sufficiently large to be experimentally observable in the electron-doped HTSC. Second, we predict that in those parts of the phase diagram, where $d_{x^2-y^2}$ -wave superconductivity (d SC) coexists with an antiferromagnetic spin-density wave (SDW) [14–16] and $T_N < T_c$, the resonance evolves into the Goldstone mode of the SDW state as T_N is approached.

The starting point for our study of the resonance mode in the electron-doped cuprates is the Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger + \text{H.c.}, \quad (1)$$

where $c_{\mathbf{k},\sigma}^\dagger$ creates an electron with spin σ and momentum \mathbf{k} , and $\Delta_{\mathbf{k}}$ is the SC gap with $d_{x^2-y^2}$ -wave symmetry. The normal state tight binding dispersion

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - \mu \quad (2)$$

with $t = 250$ meV, $t'/t = -0.4$, $t''/t = 0.1$, and $\mu/t = -0.2$ reproduces the position of the hot spots and the underlying FS [Fig. 1(a)] as inferred from ARPES [5].

Despite the same FS topology in the electron-doped and hole-doped cuprates, the angular dependence of the superconducting gap along the FS is qualitatively different in these systems. Based on a scenario in which superconductivity arises from the exchange of antiferromagnetic spin fluctuations, it was argued that the maximum SC gap is achieved near the hot spots [11,17,18]. In the hole-doped

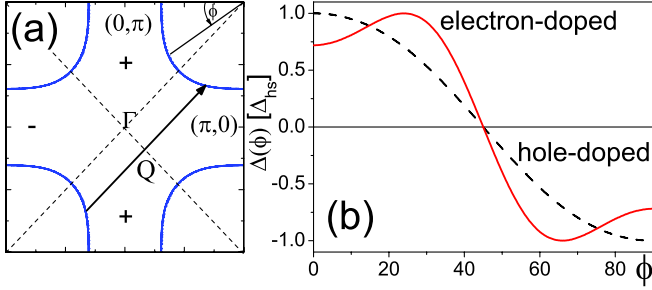


FIG. 1 (color online). (a) Fermi surface in optimally electron-doped cuprates. The arrow indicates the scattering of quasiparticles by \mathbf{Q} . (b) Angular dependence of the SC gap for electron and hole-doped HTSC.

cuprates, the hot spots are located close to $\mathbf{q} = (\pm\pi, 0)$ and $(0, \pm\pi)$, resulting in a SC $d_{x^2-y^2}$ -wave gap that varies monotonically along the FS, as shown in Fig. 1(b). In contrast, in the electron-doped cuprates, the hot spots are located much closer to the zone diagonal [Fig. 1(a)], leading to a nonmonotonic behavior of the SC gap [11,18], in agreement with ARPES experiments [5]. A good fit of $\Delta_{\mathbf{k}}$ to the experimental data is achieved via the inclusion of a higher harmonic, such that $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y) + \frac{\Delta_1}{2}(\cos 2k_x - \cos 2k_y)$, where $\Delta_1/\Delta_0 = 0.63$ ensures that the maximum of $|\Delta_{\mathbf{k}}|$ along the FS is located at the hot spots, as shown in Fig. 1(b) [19]. Since the magnitude of the SC gap in PLC_{0.12}CO is still unknown, we use $\Delta_0 = 10$ meV which yields $\Delta_{\text{hs}} = 5$ meV thus reproducing the ARPES estimate of the SC gap at the hot spots of PLC_{0.11}CO. Note that the results shown below are robust against (reasonable) changes in the band structure, as long as Δ_{hs} remains unchanged.

Similar to the hole-doped HTSC [4,6–8] the resonance peak in the SC state of the electron-doped cuprates can be understood by considering the dynamical spin susceptibility within the random phase approximation (RPA)

$$\chi(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{1 - U(\mathbf{q})\chi_0(\mathbf{q}, \omega)}, \quad (3)$$

where $U(\mathbf{q})$ is the fermionic four-point vertex and $\chi_0(\mathbf{q}, \omega)$ is the free-fermion susceptibility given by the sum of two single bubble diagrams consisting of either normal or anomalous Green functions. While momentum independent as well as momentum dependent forms of $U(\mathbf{q})$ were used in the hole-doped cuprates [4,6–8], the close proximity of the (commensurate) antiferromagnetic and SC phases in the electron-doped HTSC suggests that $U(\mathbf{q})$ is momentum dependent, with a maximum at $\mathbf{Q} = (\pi, \pi)$ [20]. Here, we use $U_{\mathbf{q}} = -\frac{U_0}{2}(\cos q_x + \cos q_y)$ which reproduces a nearly dispersionless resonance mode around \mathbf{Q} . The form of χ_0 in the hole-doped and electron-doped HTSC is qualitatively similar and has been extensively discussed for the former [4,6–8]. For momenta \mathbf{q} near \mathbf{Q} and $\Gamma = 0^+$, $\text{Im}\chi_0$ is zero at low frequencies and exhibits a discontinuous jump at the onset frequency of the p - h continuum $\Omega_c(\mathbf{q}) = |\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|$, where both \mathbf{k} and

$\mathbf{k} + \mathbf{q}$ lie on the FS [for $\mathbf{q} = \mathbf{Q}$ one has $\Omega_c(\mathbf{Q}) = 2\Delta_{\text{hs}}$]. The discontinuity in $\text{Im}\chi_0$, which is a direct consequence of $\text{sgn}(\Delta_{\mathbf{k}}) = -\text{sgn}(\Delta_{\mathbf{k}+\mathbf{q}})$ and hence the $d_{x^2-y^2}$ -wave symmetry of the SC gap, leads to a logarithmic singularity in $\text{Re}\chi_0$. As a result, the resonance conditions (i) $U_{\mathbf{Q}}\text{Re}\chi_0(\mathbf{Q}, \omega_{\text{res}}) = 1$ and (ii) $\text{Im}\chi_0(\mathbf{Q}, \omega_{\text{res}}) = 0$ can be fulfilled simultaneously at $\omega_{\text{res}} < \Omega_c$ for any $U_{\mathbf{Q}} > 0$, leading to the emergence of a resonance peak as a spin exciton. Note that for finite Γ , condition (i) can only be satisfied if $U_{\mathbf{Q}}$ exceeds a critical value, and condition (ii) is replaced by $U_{\mathbf{Q}}\text{Im}\chi_0(\mathbf{Q}, \omega_{\text{res}}) \ll 1$.

In Fig. 2, we present $\text{Im}\chi(\mathbf{Q}, \omega)$ resulting from Eq. (3). Since the INS data suggest that the resonance is located close to the p - h continuum, we have chosen $U_0 = 0.854$ eV such that for $\Gamma \rightarrow 0$ (not shown), the resonance is located at $\omega_{\text{res}} = 9.8$ meV $= 0.98\Omega_c$. For small $\Gamma = 0.5$ meV [Fig. 2(a)], the resonance broadens but only exhibits a negligible frequency shift. However, for larger $\Gamma = 3$ meV [Fig. 2(b)], the resonance has not only become much broader but its peak intensity has also shifted to $\omega_{\text{res}} \approx 11$ meV $= 1.1\Omega_c$ well above the onset of the p - h continuum. In this case, neither of the resonance conditions is satisfied, and $\text{Im}\chi$ is more reminiscent of the magnetic coherence effect in La_{2-x}Sr_xCuO₄ [12,13] than of the resonance in the hole-doped HTSC. Hence, when the resonance is located close to the p - h continuum, its form depends rather sensitively on Γ .

The observed spectral weight in $\text{Im}\chi$ at frequencies much below Ω_c [1] is consistent with a shorter lifetime $1/\Gamma$, arising, for example, from disorder effects. Whether the INS data are better described by the results shown in Fig. 2(a) (albeit with a larger Δ_{hs} such that the experimen-

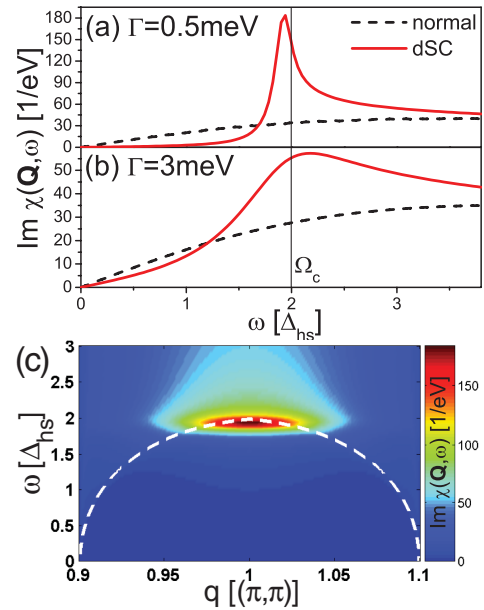


FIG. 2 (color online). $\text{Im}\chi(\mathbf{Q}, \omega)$ for $U_0 = 0.854$ eV and (a) $\Gamma = 0.5$ meV, and (b) $\Gamma = 3$ meV. (c) Contour plot of $\text{Im}\chi$ in the (ω, \mathbf{q}) plane for the parameters in (a), together with $\Omega_c(\mathbf{q})$ (dashed white line).

tally determined $\omega_{\text{res}} = 11$ meV corresponds to $0.98\Omega_c$, or in Fig. 2(b), is presently unclear, mainly due to experimental resolution effects which are in general difficult to account for. Moreover, since the resonance's maximum intensity is affected by its distance to the p - h continuum, the band structure, the magnitude of the SC gap, and $1/\Gamma$, we expect it to be smaller in the electron-doped HTSC than in the hole-doped cuprates.

In Fig. 2(c) we present a contour plot of $\text{Im}\chi$ for $\Gamma = 0.5$ meV along $\mathbf{q} = \eta(\pi, \pi)$ together with the momentum dependence of $\Omega_c(\mathbf{q})$, the onset of the p - h continuum. The resonance is almost dispersionless and exists only in a small momentum region ($0.96\mathbf{Q} \lesssim \mathbf{q} \lesssim 1.04\mathbf{Q}$) around \mathbf{Q} , in agreement with experiment [1]. This effect arises from the momentum dependence of $U(\mathbf{q})$, combined with the fact that the resonance at \mathbf{Q} is located only slightly below the p - h continuum, which leads to a ‘‘merging’’ of the resonance with the p - h continuum at small deviations from \mathbf{Q} . The momentum connecting the nodal points, $\mathbf{q}_n \approx 0.9\mathbf{Q}$, where $\Omega_c(\mathbf{q})$ reaches zero, is much closer to \mathbf{Q} than in the hole-doped systems where $\mathbf{q}_n \approx 0.8\mathbf{Q}$, leading to an additional narrowing of the dispersion.

The phase diagram of the electron-doped HTSC, and a SC gap that is much smaller than in the hole-doped cuprates, provide further opportunities for testing the nature of the resonance peak. Consider, for example, the effects of a magnetic field H in the ab plane, which enters the calculation of χ only through the Zeeman splitting of the electronic bands, while orbital effects are absent [21]. The field lifts the degeneracy of the transverse and longitudinal components of χ_0 which are given by

$$\begin{aligned} \chi_0^{\pm\mp}(\mathbf{q}, i\omega_n) &= -\frac{1}{N} \sum_{\mathbf{k}} \left\{ c^+ \frac{f_{\mathbf{k}+\mathbf{q}}^{\pm} - f_{\mathbf{k}}^{\mp}}{i\omega_n + \xi_{\mathbf{k}+\mathbf{q}}^{\pm} - \xi_{\mathbf{k}}^{\mp}} \right. \\ &\quad + \frac{c^-}{2} \frac{1 - f_{\mathbf{k}+\mathbf{q}}^{\mp} - f_{\mathbf{k}}^{\mp}}{i\omega_n - \xi_{\mathbf{k}+\mathbf{q}}^{\mp} - \xi_{\mathbf{k}}^{\mp}} \\ &\quad \left. - \frac{c^-}{2} \frac{1 - f_{\mathbf{k}+\mathbf{q}}^{\pm} - f_{\mathbf{k}}^{\pm}}{i\omega_n + \xi_{\mathbf{k}+\mathbf{q}}^{\pm} + \xi_{\mathbf{k}}^{\pm}} \right\}, \\ \chi_0^{zz}(\mathbf{q}, i\omega_n) &= -\frac{1}{4N} \sum_{\mathbf{k}} \left\{ c^+ \frac{f_{\mathbf{k}+\mathbf{q}}^+ - f_{\mathbf{k}}^+ + f_{\mathbf{k}+\mathbf{q}}^- - f_{\mathbf{k}}^-}{i\omega_n + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}}} \right. \\ &\quad + c^- \frac{1 - f_{\mathbf{k}+\mathbf{q}}^- - f_{\mathbf{k}}^+}{i\omega_n - E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}}} \\ &\quad \left. - c^- \frac{1 - f_{\mathbf{k}+\mathbf{q}}^+ - f_{\mathbf{k}}^-}{i\omega_n + E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{q}}} \right\}, \end{aligned} \quad (4)$$

where $\chi_0^{zz} = (\chi_0^{\uparrow\uparrow} + \chi_0^{\downarrow\downarrow} + \chi_0^{\uparrow\downarrow} + \chi_0^{\downarrow\uparrow})/4$, $\xi_{\mathbf{k}}^{\pm} = E_{\mathbf{k}} \pm H$, $f_{\mathbf{k}}^{\pm} = f(\xi_{\mathbf{k}}^{\pm})$ is the Fermi function, $c^{\pm} = \frac{1}{2} \times (1 \pm \frac{\varepsilon_{\mathbf{k}} \varepsilon_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}} \Delta_{\mathbf{k}+\mathbf{q}}}{E_{\mathbf{k}} E_{\mathbf{k}+\mathbf{q}}})$, and $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ (we set $g\mu_B S = 1$). The RPA result for the full susceptibility is

$$\begin{aligned} \chi &= \frac{1}{2} \left(\frac{\chi_0^{\pm}}{1 - U_{\mathbf{q}} \chi_0^{\pm}} + \frac{\chi_0^{\mp}}{1 - U_{\mathbf{q}} \chi_0^{\mp}} \right) \\ &\quad + \frac{\chi_0^{zz} + \frac{1}{2} U_{\mathbf{q}} (\chi_0^{\uparrow\uparrow} \chi_0^{\downarrow\downarrow} - \chi_0^{\uparrow\downarrow} \chi_0^{\downarrow\uparrow})}{(1 - U_{\mathbf{q}} \chi_0^{\uparrow\uparrow})(1 - U_{\mathbf{q}} \chi_0^{\downarrow\downarrow}) - U_{\mathbf{q}}^2 \chi_0^{\uparrow\downarrow} \chi_0^{\downarrow\uparrow}}. \end{aligned} \quad (5)$$

The Zeeman term in the denominators of χ_0 shifts $\Omega_c(\mathbf{q})$ in χ_0^{\mp} (χ_0^{\pm}) by $+2H \approx 1$ meV ($-2H$), while $\Omega_c(\mathbf{q})$ remains unaffected in χ_0^{zz} [22]. This effect leads to a splitting of the resonance into three peaks [23], as shown in Fig. 3 for $H = 8$ T $\ll H_{c2}^{ab}(T=0) \approx 50$ T [24] [for the results in Fig. 2(b), the magnetic-field effects are negligible]. If the resonance is located close to the p - h continuum [Fig. 3(a)], the splitting results in an asymmetric resonance, while for a resonance located well below Ω_c , $\text{Im}\chi$ exhibits a symmetric splitting [Fig. 3(b)]. Hence, the resonance's asymmetry is an indication for the proximity of the p - h continuum. The current experimental resolution at a frequency of 10 meV is about 1 meV [25], such that the predicted splitting of the resonance should be experimentally observable, in contrast to the hole-doped HTSC.

One of the most important questions regarding the nature of the resonance mode in the hole-doped cuprates is whether with decreasing doping, the resonance mode transforms into the Goldstone mode of the antiferromagnetic parent compounds. Important insight into this question can be provided by those electron-doped cuprates, in which superconductivity coexists with a commensurate SDW [14–16]. Extending the spin-exciton scenario to such a coexistence phase [26], we find that the spin response at (π, π) only possesses a Goldstone mode at zero energy but no additional resonance at higher energies. Since the existence of a Goldstone mode requires the condition $U_{\mathbf{Q}} \text{Re}\chi_0(\mathbf{Q}, \omega) = 1$ to be satisfied at $\omega = 0$, and since $\text{Re}\chi_0(\mathbf{Q}, \omega)$ increases monotonically with frequency from $\omega = 0$ up to Ω_c , the resonance conditions can only be satisfied once, namely at $\omega_{\text{res}} = 0$. In contrast, in a ‘‘pure’’ SC state, the resonance is necessarily located at $\omega_{\text{res}} \neq 0$. Moreover, the results of recent experiments [16,25] suggest the existence of electron-doped HTSC with $T_N < T_c$. For these materials, it follows from the above discussion that the resonance of the pure SC state shifts downward in energy with decreasing temperature, until it reaches zero energy at T_N and forms the Goldstone mode. Within the spin-exciton scenario, this requires that $U(\mathbf{q})$ increases with decreasing temperature. In order to

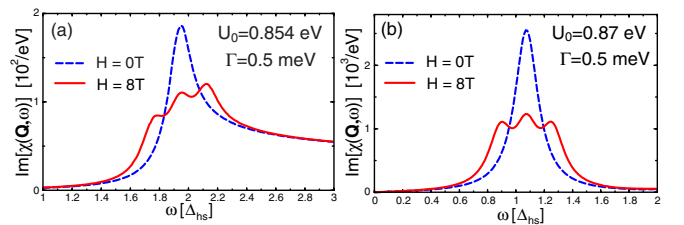


FIG. 3 (color online). $\text{Im}\chi(\mathbf{Q}, \omega)$ for $H = 0$ T (dashed blue curve) and $H = 8$ T (solid red curve) at $T = 2$ K.

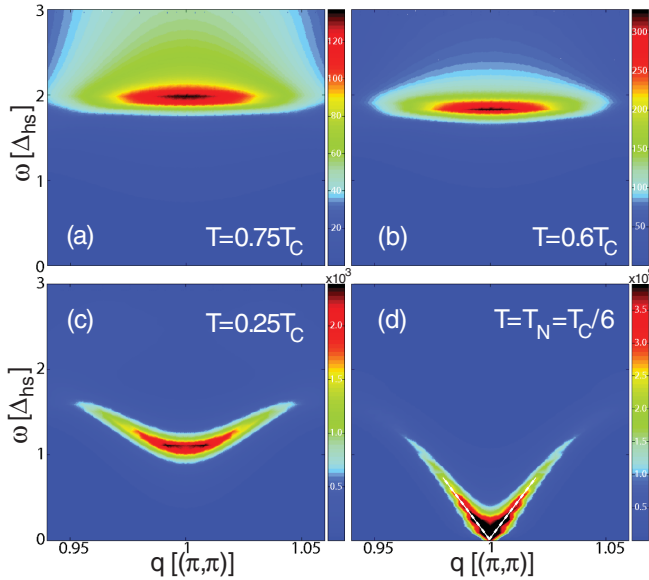


FIG. 4 (color online). Contour plots of $\text{Im}\chi$ (in units of $1/\text{eV}$) for $\Gamma = 0.5 \text{ meV}$ at four different temperatures and $U_0(T) = 0.8784 \text{ eV} - 0.0014 \text{ eV/K}T$. The white dashed line in (d) represents the dispersion of the Goldstone mode.

exemplify the resonance's temperature evolution, we consider a system with $T_N < T_c$ (for concreteness we chose $T_N = T_c/6$). We assume (somewhat arbitrarily) that U_0 varies linearly with temperature while the momentum dependence of $U(\mathbf{q})$ remains unchanged, such that the resonance at \mathbf{Q} and $T = 0.75T_c$ is located at $\omega_{\text{res}} \approx 0.92\Omega_c$, while for $T = T_N$, we have $\omega_{\text{res}} = 0$. In Fig. 4, we present the contour plots of $\text{Im}\chi$ for four different temperatures. While the resonance shifts downwards with decreasing temperature, it remains nearly dispersionless over some temperature range below T_c [see Figs. 4(a) and 4(b)]. However, upon decreasing temperature even further [Fig. 4(c)], the “flat” dispersion evolves continuously into an upward dispersion whose minimum is located at \mathbf{Q} . Finally, at T_N [Fig. 4(d)], the minimum of the dispersion at \mathbf{Q} reaches zero energy and the resonance becomes the Goldstone mode of the SDW state [27]. The qualitative features of this evolution are independent of the specific temperature dependence of U_0 , as long as $U(\mathbf{q})$ decreases sufficiently fast with deviation from (π, π) .

In summary, we studied the emergence of a magnetic resonance mode in the SC state of the electron-doped HTSC. We show that the recently observed resonance peak in $\text{PLC}_{0.12}\text{CO}$ is likely an overdamped spin exciton located near the p - h continuum. We discuss the magnetic-field dependence of the resonance as well as its temperature evolution in those parts of the phase diagram where $d\text{SC}$ may coexist with an antiferromagnetic SDW.

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