

# Supplemental Material to the article “On Gap Wave Vector Dependence in $\text{Pr}_{0.89}\text{LaCe}_{0.11}\text{CuO}_4$ ”

The expression for dynamic spin susceptibility of the electron-doped cuprates is written as follows

$$\chi_{sp}(\omega, \mathbf{q}) = \frac{\chi_q \zeta_{hJ} + (J_1 K_1 (4 - \gamma_{\mathbf{q}}) - \chi_{hJ}) \zeta_q}{(1 + \lambda_q) \zeta_{hJ} + (\omega^2 - \Omega_{\mathbf{q}}^2 - \frac{1}{2} J_1 h_1 (4 - \gamma_{\mathbf{q}}) - \lambda_{hJ}) \zeta_q}. \quad (1)$$

The formula for dynamic charge susceptibility is

$$\chi_{ch}(\omega, \mathbf{q}) = \frac{\chi_q \zeta_h - \chi_h \zeta_q}{(1 - \eta_q) \zeta_h - (\omega/2 - \eta_h) \zeta_q}. \quad (2)$$

Functions  $\chi_q, \chi_{hJ}, \chi_h, \zeta_q, \zeta_{hJ}, \zeta_h, \lambda_q, \lambda_{hJ}, \eta_q, \eta_h, \Omega_{\mathbf{q}}$  are determined as:

$$\chi_q = \frac{1}{N} \sum_{\mathbf{k}} \chi_{kq}, \quad \chi_{hJ} = \frac{1}{N} \sum_{\mathbf{k}} M_{k,q} \chi_{kq}, \quad \chi_h = \frac{1}{N} \sum_{\mathbf{k}} (h_{\mathbf{k}+\mathbf{q}} - h_{\mathbf{k}}) \chi_{kq}, \quad (3)$$

$$\zeta_q = \frac{1}{N} \sum_{\mathbf{k}} \zeta_{kq}, \quad \zeta_{hJ} = \frac{1}{N} \sum_{\mathbf{k}} M_{k,q} \zeta_{kq}, \quad \zeta_h = \frac{1}{N} \sum_{\mathbf{k}} (h_{\mathbf{k}+\mathbf{q}} - h_{\mathbf{k}}) \zeta_{kq}, \quad (4)$$

$$\lambda_q = \frac{1}{N} \sum_{\mathbf{k}} \lambda_{kq}, \quad \lambda_{hJ} = \frac{1}{N} \sum_{\mathbf{k}} (h_{\mathbf{k}+\mathbf{q}} - h_{\mathbf{k}}) \lambda_{kq}, \quad (5)$$

$$\eta_q = \frac{1}{N} \sum_{\mathbf{k}} \eta_{kq}, \quad \eta_h = \frac{1}{N} \sum_{\mathbf{k}} (h_{\mathbf{k}+\mathbf{q}} - h_{\mathbf{k}}) \eta_{kq}, \quad (6)$$

$$\Omega_{\mathbf{q}}^2 = 2J_1^2 \alpha |K_1| (2 - \gamma_{\mathbf{q}}/2) (\Delta_{sp} + 2 + \gamma_{\mathbf{q}}/2), \quad (7)$$

in which we used the following notations:

$$\chi_{kq} = \frac{n_{\mathbf{k}}^h - n_{\mathbf{k}+\mathbf{q}}^h}{\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}, \quad (8)$$

$$\zeta_{kq} = \frac{1}{\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}, \quad (9)$$

$$\lambda_{kq} = \pi_{kq} + \left(\frac{1}{2} J'_{\mathbf{q}} + P T'_{\mathbf{k}, \mathbf{k}+\mathbf{q}}\right) \chi_{kq} \quad (10)$$

$$\eta_{kq} = \frac{1}{2} \pi_{kq}^h + \left(\frac{1}{4} J'_{\mathbf{q}} + \frac{P}{2} T'_{\mathbf{k}, \mathbf{k}+\mathbf{q}} - G_{\mathbf{q}}\right) \chi_{kq}, \quad (11)$$

$$\pi_{kq} = \frac{h'_{\mathbf{k}+\mathbf{q}} P f_{\mathbf{k}} - h'_{\mathbf{k}} P f_{\mathbf{k}+\mathbf{q}}}{\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}, \quad (12)$$

$$\pi_{kq}^h = \frac{h'_{\mathbf{k}} n_{\mathbf{k}}^h - h'_{\mathbf{k}+\mathbf{q}} n_{\mathbf{k}+\mathbf{q}}^h}{\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}, \quad (13)$$

$$t'_{\mathbf{k}} = \sum_m t_{lm} (1 - F_{lm}^t) e^{-i\mathbf{k}\mathbf{R}_{lm}}, \quad (14)$$

$$T_{\mathbf{k}}'' = \sum_{f, m \neq l} \frac{t_{lf} t_{fm}}{U} (1 - F_{lm}^T) e^{-i\mathbf{k}\mathbf{R}_{lf} - i\mathbf{k}\mathbf{R}_{fm}}, \quad (15)$$

$$J'_{\mathbf{q}} = J_1 (1 - F_1^J) \gamma_{\mathbf{q}}, \quad (16)$$

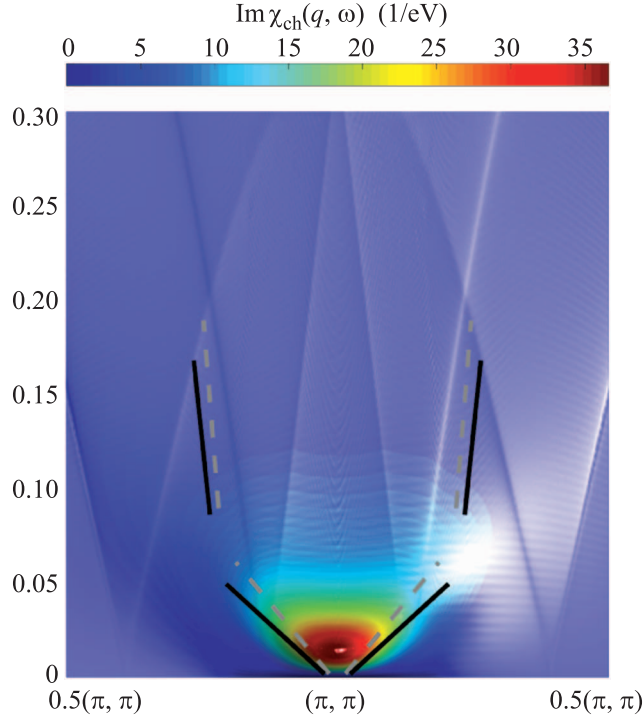


Figure 1: The imaginary part of the spin susceptibility, calculated along the diagonal of the Brillouin zone near  $Q = (\pi, \pi)$ . Black and gray segments correspond to the experimental results from the paper M. Fujita, K. Shigiya, J. Kaminaga, M. Nakagawa, M. Enoki, and K. Yamada, *J. Phys. Soc. Jpn.* **80**, SB029 (2011).

$$T'_{\mathbf{k}, \mathbf{k}+\mathbf{q}} = \frac{t_1^2}{U}(1 - F_1^T)\gamma_{2\mathbf{k}+\mathbf{q}}, \quad (17)$$

$$G_{\mathbf{q}} = \frac{2\pi d e^2}{\varepsilon_{\perp} a^2 \sqrt{A^2 - 1}}, \quad (18)$$

$$A = \left( 2 \frac{\varepsilon_{\parallel}}{\varepsilon_{\perp}} \frac{\sin^2(q_x a/2)}{(a/d)^2} + 2 \frac{\varepsilon_{\parallel}}{\varepsilon_{\perp}} \frac{\sin^2(q_y a/2)}{(a/d)^2} + 1 \right), \quad (19)$$

$$M_{k,q} = \frac{1}{2}(\bar{J}_{\mathbf{k}+\mathbf{q}} - \bar{J}_{\mathbf{k}} - 2\omega)(h_{\mathbf{k}+\mathbf{q}} - h_{\mathbf{k}}) - J_1 \frac{t_1^2}{U} L_{k,q}, \quad (20)$$

$$L_{k,q} = K_1(\gamma_{\mathbf{q}} - 4)\gamma_{2\mathbf{k}+\mathbf{q}} + \frac{1 - \delta_0}{2}(\gamma_{2\mathbf{k}+2\mathbf{q}} + \gamma_{2\mathbf{k}} - 2\gamma_{2\mathbf{k}+\mathbf{q}}). \quad (21)$$

$n_{\mathbf{k}}^h$  denotes the number of quasi-particles in the hole representation;  $n_{\mathbf{k}}^h = P f_{\mathbf{k}}^h$ ,  $P = (1 + \delta_0)/2$ ,  $f_{\mathbf{k}}^h = 1/(1 + e^{-\varepsilon_{\mathbf{k}}/k_B T})$ .

The energy of quasi-particles, is written as

$$\varepsilon_{\mathbf{k}} = -\mu + 2t(\cos k_x a + \cos k_y a) + 4t' \cos k_x a \cos k_y a + 2t''(\cos 2k_x a + \cos 2k_y a). \quad (22)$$

The effective hopping parameters of quasi-particles “dressed with charge and spin correlations” are expressed in terms of the bare hopping parameters of electrons between the first ( $t_1$ ), second ( $t_2$ ) and third neighbors ( $t_3$ ) in the following way

$$t = t_1 \left( P + \frac{1 + 2F_1^t}{4P} K_1 \right) + \left( J_1 \frac{F_1^J}{2P} + 3 \frac{t_1^2}{U} (1 + F_1^T) \right) \langle X_0^{0,\sigma} X_1^{\sigma,0} \rangle, \quad (23)$$

$$t' = t_2 P + 2 \frac{t_1^2}{U} \left( \frac{2 + F_1^T}{2} K_1 - \frac{1 - \delta_0}{2} P \right), \quad (24)$$

$$t'' = t_3 P + \frac{t_1^2}{U} \left( \frac{2 + F_1^T}{2} K_1 - \frac{1 - \delta_0}{2} P \right). \quad (25)$$

$K_1 = 4 \langle S_0^z S_1^z \rangle$  denotes spin-spin correlation function, which are estimated self-consistently through dynamic spin susceptibility.

The parameters were taken as:  $t = 0.2$  eV,  $t' = -0.4t$ ,  $t'' = 0.1t$ ,  $\mu = -0.4t$ . The exchange integral between the nearest neighbors is  $J_1 = 0.11$  eV. Projective parameters are  $F_1^J = F_1^T = 0.7$ . The spin-spin correlation function for the nearest neighbors is  $K_1 = -0.22$