Supplementary Information for “Strength of the Spin-Fluctuation-Mediated Pairing Interaction in a High-Temperature Superconductor”

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Fit to INS data

The INS results were fitted by simple analytic forms which could then be numerically integrated in the self-energy and $T_c$ calculations. In constructing these fits, the energy range was divided into upper ($u$) and lower ($\ell$) branches corresponding to energies above and below the resonance energy $\omega_r$.

$$\text{Im} \chi(\vec{Q},\Omega) = \text{Im} \chi_{\ell}(\vec{Q},\Omega) + \text{Im} \chi_u(\vec{Q},\Omega)$$

(1)

The data in the superconducting state at $T = 5$ K were fitted as follows. On the lower branch

$$\text{Im} \chi_{\ell}(\vec{Q},\Omega) = N_0 N_\ell(\Omega) N_L(\Omega) \frac{2(2\Omega_r - \Omega)\gamma_Q}{((2\Omega_r - \Omega)^2 - \Omega_Q^2)^2 + (2(2\Omega_r - \Omega)\gamma_Q)^2}$$

(2)

Here the frequency $\Omega$ is measured in meV with the resonance frequency $\Omega_r = 38.5$ meV. The prefactors are given by

$$N_\ell(\Omega) = 1 - \frac{1}{1 + \exp[(\Omega - 24)/3]}$$

(3)

and

$$N_L(\Omega) = \frac{1}{1 + \exp[\Omega - 42]}$$

(4)

These factors essentially cut off the lower branch at frequencies above 42 meV and below 24 meV (spin gap). The momentum dispersion of the resonance mode is given by

$$\Omega_Q = \Omega_r + s_a(Q_a - Q_{0a})^2 + s_b(Q_b - Q_{0b})^2$$

(5)

with $\mathbf{Q}_0 = (Q_{0a}, Q_{0b})$ the antiferromagnetic wave vector, $s_a = 280$ meV Å$^2$ and $s_b = 455$ meV Å$^2$. The damping width $\gamma_Q$ has an angular dependence of the form

$$\gamma_Q = \gamma_a + \Delta \gamma \frac{(Q_a - Q_{0a})^2}{|\mathbf{Q} - \mathbf{Q}_0|^2}$$

(6)

where the index $a$ denotes the $a$-axis direction in the Brillouin zone and $b$ the $b$-axis direction, respectively. The parameter values are $\gamma_a = 1.5$ meV and $\Delta \gamma = 6.5$ meV.

For the upper branch we have

$$\text{Im} \chi_u(\vec{Q},\Omega) = N_0 N_{0u} N_u(\Omega) N_{dip}(\Omega) N_{rot}(\vec{Q}) \frac{2\Omega \Gamma}{(\Omega^2 - \Omega_Q^2)^2 + (2\Omega \Gamma)^2}$$

(7)
Here, $\Gamma = 11$ meV and

$$\Omega_Q = \Omega_c + \left[ S_a^{2/p} (Q_a - Q_{0a})^2 + S_b^{2/p} (Q_b - Q_{0b})^2 \right]^{p/2}$$

(8)

where $p = 4$ is the power of the dispersion of the upper branch (somewhat steeper than quadratic) with $S_a = 4830$ meV Å$^p$ and $S_b = 10065$ meV Å$^p$. The prefactor $N_{0u}$ is 1.35 and

$$N_u(\Omega) = 1 - \frac{1}{1 + \exp[(\Omega - 36)/1.5]}$$

(9)

provides a cut-off of the upper branch for energies below 36 meV. The prefactor $N_{dip}(\Omega) = 1 - 0.2 \exp \left[ - (\Omega - \Omega_{dip})^2 / (2\sigma_{dip}^2) \right]$ with $\Omega_{dip} = 47$ meV and $\sigma_{dip} = 2$ meV accounts for the reduction in intensity just above the resonance. The prefactor $N_{rot}$ has a momentum dependence of the form

$$N_{rot}(\vec{Q}) = 1 - 0.3 \left( \frac{(Q_a - Q_{0a})^2 - (Q_b - Q_{0b})^2}{|Q - Q_0|^2} \right)^2$$

(11)

accounting for the 45 degree rotation of the signal above the resonance [S1, S2]. The overall normalization factor $N_0$ is chosen such that the momentum integrated $\text{Im} \chi(\vec{q}, \Omega)$ has a peak value of $16 \mu^2_B/\text{eV/f.u.}$ in the superconducting state at 5 K, which is known from previous work [S1, S3, S4]. In order to account for lattice symmetry, the function $\text{Im} \chi(\vec{q}, \Omega)$ is cut at the zone center and continued periodically.

Let us now discuss the fitting formula for the normal state data at 70 K. Again, the fitting formula is subdivided into an upper and lower branch. For the lower branch we have

$$\text{Im} \chi_\ell(\vec{Q}, \Omega) = N_0 N_{0\ell} N_{in}(\Omega) N_\ell(\Omega) N_L(\Omega)$$

(12)

$$\{ \exp[-4 \ln 2[((Q_a - Q_{1a})/\sigma_a)^2 + ((Q_b - Q_{1b})/\sigma_b)^2]] + \exp[-4 \ln 2[((Q_a - Q_{2a})/\sigma_a)^2 + ((Q_b - Q_{2b})/\sigma_b)^2]] \}$$

Here, the two Gaussians describe an energy-independent incommensurability with $\sigma_a = 0.125$ r.l.u., $\sigma_b = 0.17$ r.l.u., $Q_1 = (Q_{1a}, Q_{1b}) = (0.575, 0.5)$ r.l.u., and $Q_2 = (Q_{2a}, Q_{2b}) = (0.425, 0.5)$ r.l.u. The normalization factors are given by $N_{0\ell} = 0.001807$

$$N_\ell(\Omega) = 1 - \frac{0.5}{1 + \exp[(\Omega - 29.5)/2]}$$

(13)
and
\[ N_L(\Omega) = \frac{1}{1 + \exp[(\Omega - 37)/2]} . \] (14)

These factors essentially cut off the lower branch at frequencies above 37 meV and partially below 29.5 meV. The factor
\[ N_{lin}(\Omega) = \begin{cases} 1 & \text{for } \Omega \geq 27 \text{ meV} \\ \Omega/27 & \text{for } \Omega < 27 \text{ meV} \end{cases} \] (15)

represents a simple linear decrease below 27 meV consistent with previous work [S5]. For the upper branch we have the same expression as in the superconducting state at 5 K except that
\[ N_{dip}(\Omega) = 1 \] (16)

and
\[ N_u(\Omega) = 1 - \frac{1.02}{1 + \exp[(\Omega - 37)/2]} . \] (17)

Figure S1 shows the momentum integrated \( \text{Im} \chi(\vec{q}, \Omega) \) in absolute units obtained from the two formulae. The “sum-rule” integral
\[ S = \int_0^\infty \frac{d\Omega}{\pi} \left\{ \frac{\text{Im} \chi(Q, \Omega)}{g^2 \mu_B^2} \right\}_Q \] (18)
for the two fits gives \( S = 0.071 / \text{f.u.} \) for the normal phase (\( T = 70 \) K) and \( 0.070 / \text{f.u.} \) for the superconducting phase (\( T = 5 \) K). These numbers are in reasonable agreement with each other.

Figure S2 shows typical measured scans compared with our fit formula convoluted with the instrumental resolution function and demonstrates the good agreement.

In order to check the sensitivity of our results, reported in the main manuscript, to the high energy part of the magnetic excitation spectrum, we have repeated our calculations with a spectrum cut off at 200 meV. As a result we found that the coupling constant \( \bar{U} \) had to be increased by 3 percent. \( T_c \) was found to decrease by 1 Kelvin, showing that the details of the high energy part of the spectrum do not affect \( T_c \) very much.

Further on, we have phenomenologically added a normal state \( d \)-wave pseudogap of 30 meV into our calculation and found that \( T_c \) increases by 20 percent, due to the suppression of pairbreaking low-energy magnetic excitations. We conclude that the influence of the pseudogap does not alter our two major findings: the high value of \( T_c \) and the nodal kink generated by the upper branch of the hourglass.
In order to assess the possible influence of electron-phonon interaction onto our results we have made an additional calculation in which we assume that phonons having a coupling strength of $\lambda_{ph} = 0.3$ [S8] are contributing to the nodal mass renormalization without contributing to the d-wave pairing channel. In this case we find that the nodal kink can still be fitted reasonably well, while $T_c$ is reduced by 10 percent.

**Fit to fermionic band dispersions**

As a starting point for our theoretical calculation we also need the unrenormalized dispersions $\epsilon_k^{A,B}$ for the bonding (B) and antibonding (A) bands of the two-layer system. In contrast to previous calculations, here we keep the renormalized Fermi surface fixed during the iterative solution of Eqs. (1–3) of the main manuscript, because the Fermi surface is known from the ARPES data. In order to achieve this, we keep the renormalized quantity $\tilde{\epsilon}_k^{A,B} = \epsilon_k^{A,B} + \text{Re} \xi_{A,B}(k; \omega = 0)$ fixed during the calculation and obtain it from tight-binding fits to the ARPES data of the form

$$\tilde{\epsilon}_k^{A,B} = \mu_{A,B} - 2t_{A,B}(\cos k_x + \cos k_y) + 4t'_{A,B} \cos k_x \cos k_y - 2t''_{A,B}(\cos 2k_x + \cos 2k_y)$$

with the parameters

$$\begin{align*}
\mu_A &= 556 \text{ meV} \quad t_A = 409 \text{ meV} \quad t_A' = 150 \text{ meV} \quad t_A'' = 40 \text{ meV} \\
\mu_B &= 417 \text{ meV} \quad t_B = 550 \text{ meV} \quad t_B' = 231 \text{ meV} \quad t_B'' = 67 \text{ meV}
\end{align*}$$

which yield excellent descriptions of the ARPES Fermi surfaces (Fig. 2). These parameters are scaled such that the unrenormalized Fermi velocity at the nodal point in the antibonding band equals 5 eVÅ, as found in *ab-initio* bandstructure calculations [S6].

In order to test the sensitivity of the numerical results to the assumed unrenormalized Fermi velocity, we have repeated the calculations with an unrenormalized Fermi velocity of 4 eVÅ, a value that deviates from the *ab-initio* predictions for YBa$_2$Cu$_3$O$_{6+x}$ but is close to the one found in Bi$_2$Sr$_2$Ca$_1$Cu$_2$O$_{8+\delta}$ [S7]. In order to reproduce the renormalized Fermi velocity, the coupling constant $\bar{U}$ has to be reduced from 1.59 to 1.23 eV, and the nodal mass renormalization drops from 3.7 to 3.0. As shown in Fig. S3, the agreement of the numerical and ARPES data for the nodal dispersion at higher energies is worse than that obtained with the more realistic parameters in the main text. Nonetheless, the estimate of
the critical temperature for $d$-wave superconductivity remains high. For the INS spectrum at 70 K, we obtain a $\lambda_d = 1.28$, corresponding to $T_c = 140$ K.

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References


FIG. 1: Momentum-integrated spin excitation spectra at $T = 5$ K and $T = 70$ K according to the fitting formulae.

FIG. 2: Comparison of typical constant-energy scans at $T = 5$ K (black squares) with our fit formula convoluted with the instrumental resolution function (open circles). The black lines are guides to the eye for the measured data points. High- and low-energy scans were measured at different $k_f$, thus the intensities are not comparable.
FIG. 3: Comparison of the nodal dispersion measured by ARPES (crosses) and evaluated theoretically for unrenormalized Fermi velocities of 4 eVÅ (solid line) and 5 eVÅ (dashed line).