The pairing glue in cuprate superconductors from the self-energy revealed via machine learning

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Recently, machine learning was applied to extract both the normal and the anomalous components of the self-energy from photoemission data at the antinodal points in Bi-based cuprate high-temperature superconductors [Y. Yamaji et al., arXiv:1903.08060]. It was argued that both components do show prominent peaks near 50 meV, which hold information about the pairing glue, but the peaks are hidden in the actual data, which measure only the total self-energy. We analyze the self-energy within an effective fermion-boson theory. We show that soft thermal fluctuations give rise to peaks in both components of the self-energy at a frequency comparable to superconducting gap, while they cancel in the total self-energy; all irrespective of the nature of the pairing boson. However, in the quantum limit $T → 0$ prominent peaks survive only for a very restricted subclass of pairing interactions. We argue that the way to potentially nail down the pairing boson is to determine the thermal evolution of the peaks.

Introduction: The analysis of fine structures in the single-particle excitation spectrum is one of most reliable approaches to identify the interaction responsible for the pairing in superconductors. The prime example is the identification of phonons as pairing bosons in lead via their fingerprints in the single-particle tunneling density of states (TDOS)$^{1-3}$. There have been several attempts to extend this logic to cuprate superconductors, analyzing tunneling, angle-resolved photoemission (ARPES), optical, or inelastic neutron scattering spectra$^{4,5,8-14}$. Such approaches are particularly challenging for the cuprates because i) the d-wave pairing interaction depends on both momentum and frequency and ii) the pairing interaction likely changes due to feedback from superconductivity.

In a superconducting state two distinct self-energies emerge due to mixing of electrons and holes$^{15-18}$. This gives rise to a matrix $2 × 2$ structure of the fermionic Green’s function. To determine the pairing glue it is highly desirable to have information about both, the normal self-energy $\Sigma_k(\omega)$ and the anomalous self-energy $\Phi_k(\omega)$. In a situation when the exchange of the same boson accounts for the pairing and for fermionic incoherence, the two self-energies are related. If both are extracted from the data, one can either verify - with a higher precision - the applicability of a given boson-mediated interaction, or put strong constraints on the pairing glue without assuming a particular scenario. However, single-particle probes, like TDOS and ARPES, provide information solely about the normal component of the Green’s function $G_k(\omega)$, which depends only on the combination $\Sigma_k^{(\text{tot})}(\omega) = \Sigma_k(\omega) + W_k(\omega)$, where

$$W_k(\omega) = \frac{\Phi_k^*(\omega)}{\omega + \epsilon_k + \Sigma_k(-\omega)}$$

contains the information about $\Phi_k(\omega)$. To deduce two complex functions $\Sigma$ and $\Phi$ from only one observable seems hopeless at first glance. Recently, however, Yamaji et al.$^{21}$ argued that this can be achieved using a Boltzmann machine-learning approach. They analyzed ARPES spectra$^{22,23}$ for optimally doped Bi2212 with $T_c ≈ 90$ K and underdoped Bi2201 with $T_c ≈ 29$ K, both at antinodal momenta $k_{\alpha,n} ≈ (0, \pi)$. In both cases they found sharp structures in $\Sigma_k^{(\text{an})}(\omega)$ and $\Phi_k^{(\text{an})}(\omega)$ at a frequency near 50 meV, which is close to the value of the antinodal gap $\Delta_{\alpha,n}$ (panels (c) and (d) of Fig.1). They further argued that these structures do not appear in the total self-energy $\Sigma_k^{(\text{tot})}(\omega)$ (black data in the panels).

In this communication we compare the results of Ref.21 with the forms of $\Sigma_k^{(\text{an})}(\omega)$ and $\Phi_k^{(\text{an})}(\omega)$ obtained in various quantum-critical models of d-wave pairing due to a dynamic interaction $V_q(\Omega)$, mediated by a soft boson. We show that thermal fluctuations give rise to peaks in both $\Sigma_k^{(\text{an})}(\omega)$ and $\Phi_k^{(\text{an})}(\omega)$ at a frequency slightly above $\Delta_{\alpha,n}$, and these peaks do cancel in the total self-energy. The peaks are present for any form of $V_q(\Omega)$, as long as a boson is soft and $V_q(0)$ is large, and in this respect do not place constraints on a pairing interaction. They do, nevertheless, strongly support the view that in optimally doped and underdoped cuprates the pairing boson is soft. Our results for the self-energies due to thermal fluctuations are shown in Fig.1 (a). We can draw much stronger conclusions if singular structures in the self-energies survive in the quantum limit $T → 0$. In this case it must hold that the momentum-averaged pairing interaction

$$\bar{V}(\Omega) = N_F \int V_q(\Omega) \sim 1/|\Omega|^\gamma$$

is governed by an exponent $\gamma > 1$. This would exclude Landau-overdamped spin or charge fluctuations with Ornstein-Zernike form of the static $V_q$, or pairing due to nematic fluctuations, as for these theories $\gamma \leq 1$, etc.
FIG. 1: Imaginary parts of the normal (red), total (black), and pairing (green) self-energies $\Sigma(\omega)$, $\Sigma_{\text{tot}}(\omega)$, and $W(\omega)$, respectively, obtained for a pairing interaction with thermal fluctuations (a), quantum fluctuations and $\gamma = 2$ (b) and from ARPES experiments using the machine-learning analysis of Ref.21 for Bi2212 (c) and Bi2201 (d).

even when we include the feedback from superconductivity on a pairing boson. On the other hand this condition is satisfied for the pairing by nearly dispersionless boson, in which case $\gamma = 2$ and $V_q(\Omega) = V(q)/(\Omega_{\text{bos}}^2 - \Omega^2)$, where $\Omega_{\text{bos}}$ is small and $V(q)$ has an attractive $d$-wave component. This is the case for pairing by a soft optical phonon40–42 and the strong coupling limit in a model of dispersionless fermions randomly coupled to optical phonons37,38. In Fig.1 (b) we show the self-energies for $\gamma = 2$ in the quantum regime.

The frequency dependence of all self-energies in panels (a) and (b) is in good agreement with the behavior obtained via machine learning, panels (c) and (d). The self-energies in Bi2212 and Bi2201, extracted in Ref.21, were obtained at $T = 11 K$ and $T = 12 K$, respectively22,23, which are significantly below $T_c$. This indicates that the sharp features may be due to quantum fluctuations and thus do impose the restriction on the pairing mechanism.

Our scenario differs from the one presented in Refs.6,7. In their approach, peaks in $\Sigma_{\text{a.n.}}(\omega)$ and $\Phi_{\text{a.n.}}(\omega)$ originate from Mott physics, and the pole in $\Sigma_{\text{a.n.}}(\omega)$ exists already in the normal state. In our scenario, the peak position is associated with the pairing gap and exists in the superconducting and pseudogap states, as long as pseudogap can be viewed as precursor to superconductivity.

The model: We use the Nambu-Gor’kov formalism with spinor $\psi(x) = \begin{pmatrix} \psi_1(x), \psi_2(x) \end{pmatrix}^T$, where $x = (x, t)$ combines coordinates and time. The Green’s function $G(x, x’) = -i\theta(t - t’) \begin{bmatrix} \psi_1(x, t), \psi_2(x, t’) \end{bmatrix}$ is a $(2 \times 2)$ matrix. Fourier transformation to the momentum and frequency representation yields

$$G_k^{-1}(\omega) = \begin{pmatrix} \omega -\epsilon_k - \Sigma_{k}(\omega) & \Phi_k(\omega) \\ \Phi_k(\omega)^* & \omega + \epsilon_k + \Sigma_k^*(\omega) \end{pmatrix} ,$$

with bare dispersion $\epsilon_k$ and two self-energies, $\Sigma_k(\omega)$ and $\Phi_k(\omega)$. The total self-energy $\Sigma_k^{\text{tot}}$ is defined via

$$G_k^{-1}(\omega) = \omega - \epsilon_k - \Sigma_k^{\text{tot}}(\omega) ,$$

where $G_k(\omega)$ is the upper-left element of $G_k(\omega)$ and $\Sigma_k^{\text{tot}}(\omega)$, is given by Eq. (1). In what follows we assume particle-hole symmetry $\Sigma_k(-\omega) = -\Sigma_k(\omega)$. This assumption breaks down near an antinodal point at energies above a few hundred meV, but holds at energies $\omega \sim \Delta_{\text{a.n.}}$.

To obtain the coupled equations for $\Sigma_k(\omega)$ and $\Phi_k(\omega)$ in closed form we further assume, following earlier works8, that corrections to side vertices in the diagrams for $\Sigma$ and $\Phi$ can be neglected. This allows one to obtain a set of self-consistent equations for the two self-energies. The coupled equations are expressed most naturally in the Matsubara formalism, where we have

$$\Sigma_k(i\omega_m) = -\int_{k'} V_{k-k'} (i\omega_m - i\omega_m') \frac{i\omega_m' - \Sigma_{k'}(i\omega_m')}{\mathcal{N}_{k'}(i\omega_m')} ,$$

$$\Phi_k(i\omega_m) = \pm \int_{k'} V_{k-k'} (i\omega_m - i\omega_m') \frac{\Phi_{k'}(i\omega_m')}{\mathcal{N}_{k'}(i\omega_m')} .$$

We defined $\mathcal{N}_{k'}(i\omega_m) = \epsilon_k^2 + (\omega_m + i\Sigma_k(i\omega_m))^2 + \Phi_k(i\omega_m)^2$ and $\int_{k'} \cdots = T \sum_{\omega_m} \int \frac{d^2k}{(2\pi)^2} \cdots$. The upper (the lower) sign refers to the charge (spin) channel. Finally, we assume that the pairing interaction is attractive in the $d$-wave channel and that self-energies for antinodal fermions at $k = k_{\text{a.n.}}$, $\Sigma_{k_{\text{a.n.}}}(i\omega_m) = \Sigma(i\omega_m)$ and $\Phi_{k_{\text{a.n.}}}(i\omega_m) = \Phi(i\omega_m)$, are primarily determined by internal fermions with momenta $k'$ that are also near one of antinodal points.

At this stage we are agnostic about the nature of the pairing interaction. It might come from spin or charge fluctuations (or the combination of the two)8,24–27, from nematic fluctuations28–33, from fluctuations of a current order parameter34, or from soft phonons35–38. The exponent $\gamma$ of Eq.2 depends on the mechanism under consideration; see above. In all cases, $V_q(\Omega)$ gives rise to a strong attraction in the pairing channel, and, simultaneously, to a large fermionic self-energy $\Sigma_k(\omega)$, which
makes fermions incoherent. The incoherence and the pairing originate from the same $V_g(\Omega)$ and compete with each other. The competition gives rise to structures in both, $\Sigma(\omega)$ and $\Phi(\omega)$ that must be simultaneously understood.

We consider two complementary limits with regards to the electronic dispersion $\epsilon_k$. One is the case of a strong dispersion, where the momentum integration can be performed similar to the usual Eliashberg theory. In the opposite limit the dispersion near the antinodes is so flat that it can be ignored all-together (Ref. 37). This second case has been extensively studied recently in the context of Sachdev-Ye-Kitaev-type models$^{37,38}$. Interestingly we find quantitatively the same behavior in both limits. Below we first present the results for a strong and then for a flat dispersion.

**Thermal fluctuations:** The thermal contributions to $\Sigma$ and $\Phi$ come from the terms with $\omega_m = \omega_m'$ in (4). These terms contain the static interaction $V_{k-k'}(0)$, which is large when the pairing boson is soft (e.g., $V_{q}(0) = V(\mathbf{q})/\Omega_{\text{boson}}^2$ for $\gamma = 2$). Introducing, as usual, $\Sigma(\omega_m) = \omega_m(1 - Z(\omega_m))$ and $\Phi(\omega_m) = Z(\omega_m)\Delta(\omega_m)$ and singling out the thermal piece, we obtain from (4)

$$Z(i\omega_m) \approx \pi T \frac{V(0)}{\sqrt{\omega_m^2 + (\Delta(\omega_m))^2}},$$

$$\Delta(i\omega_m) = \pi T \sum_{\omega_m'} \frac{\bar{V}(i\omega_m - i\omega_m')}{\sqrt{\omega_m'^2 + (\Delta(\omega_m'))^2}} \left( \Delta(i\omega_m') - \Delta(i\omega_m) \frac{\omega_m'}{\omega_m} \right).$$

(5)

We see from Eq.(5) that the thermal contribution $\bar{V}(0)$ determines the value of $Z(i\omega_m)$ but cancels out in the r.h.s. of the equation for $\Delta(i\omega_m)$. As the result, $\Delta(i\omega_m)$ is determined by non-thermal terms and remains non-singular even when $V(0)$ diverges. The cancellation holds for the same reason as the Anderson theorem, because thermal fluctuations scatter with zero frequency transfer and a finite momentum transfer act as non-magnetic impurities. Because of this cancellation, $\Delta(i\omega_m)$ remains non-singular even at criticality and at small $|\omega_m|$ can be approximated by a frequency-independent constant $\Delta$. This approximation holds for $|\omega_m| \leq \Delta$. Performing the analytical continuation to the real axis we then obtain normal and anomalous self-energies in the form

$$\Phi(\omega)/\Delta = -\Sigma(\omega)/\omega \approx \pi TV(0) \frac{1}{\sqrt{\omega^2 - (\omega + i\delta)^2}},$$

$$\Sigma^{(\text{tot})}(\omega) \approx \pi TV(0) \frac{\omega}{\sqrt{\omega^2 - (\omega + i\delta)^2}} \left( 1 - \frac{\Delta^2}{\omega^2} \right).$$

(6)

We see that both $\Sigma(\omega)$ and $\Phi(\omega)$ in Eq.(6) are singular at $\omega \approx \Delta$, but the singularities cancel out in the total self-energy because of the factor $\omega^2 - \Delta^2$. More detailed calculations, in which sub-leading terms in $Z(i\omega_m)$ are kept$^{39}$, give a very similar result, only the damping $\delta$ becomes finite and the singularity shifts to somewhat larger $\omega$. We plot the real and imaginary parts of $\Sigma(\omega)$ and $\Phi(\omega)$ in panels a,b in Fig. (2) and in panel (a) of Fig.1. We see that Im$\Sigma(\omega)$ and Im$\Phi(\omega)$ have peaks at $\omega$ slightly above $\Delta$. At larger $\omega$, Im$\Sigma(\omega)$ saturates, while Im$\Phi(\omega)$ rapidly drops. Re$\Sigma(\omega)$ is linear in $\omega$ at small frequencies and Re$\Phi(\omega)$ is finite. Both pass through maximum at $\omega \approx \Delta$ and then rapidly drop and are already small at a frequency where Im$\Sigma(\omega)$ has a maximum. All these features are also present in the normal and anomalous self-energies extracted in Ref.21.
\[ T = 0 \text{ due to quantum fluctuations as at } T > 0 \text{ due to classical, thermal fluctuations.} \]

The analysis at \( T = 0 \) can be further advanced for \( \gamma = 2 \) as in this case the solution for \( \Delta(\omega) \) in real frequencies is highly unconventional \(^{39-42} \). Namely, it does saturate at a finite \( \Delta \) at frequencies \( \omega \leq \Delta \), but at larger \( \omega \) behaves as \( \Delta(\omega) \propto \Delta(\omega / \sin \psi(\omega + i\delta)) \), where \( \psi(\omega + i\delta) \) is an increasing function of \( \omega \), approximately linear in \( \omega \) (Ref. 42). In this situation, the self-energies behave as

\[ \Sigma(\omega) \approx -V* \tan \psi(\omega + i\delta) + \ldots, \]
\[ \Phi(\omega) \approx \frac{V*}{\cos \psi(\omega + i\delta)} + \ldots, \]
\[ \Sigma^{(\text{tot})}(\omega) \approx -V* \cot \psi(\omega + i\delta) + \ldots \]

where dots stand for non-singular terms. For infinitesimally small \( \delta \), \( \text{Im} \Sigma(\omega) \) and \( \text{Im} \Phi(\omega) \) have strong peaks at \( \omega \) where \( \psi(\omega) = \pi/2 + n\pi \). At these frequencies, the singular part of \( \Sigma^{(\text{tot})}(\omega) \) vanishes. Conversely, when \( \psi(\omega) = m\pi, m \neq 0 \), \( \text{Im} \Sigma^{(\text{tot})}(\omega) \) has a peak, while the singular parts of \( \Sigma(\omega) \) and \( \Phi(\omega) \) vanish. For a finite \( \delta \), the peaks get broadened and only the peak at \( \omega \approx \Delta \) remains. In panels c,d in Fig. 2 and in panel (b) of Fig. 1 we show the self-energies using \( \psi(\omega + i\delta) = \omega + i\delta \) and \( \delta = \delta(\omega) = 0.1\omega^2/\Delta \). We see that the behavior is qualitatively similar to that in Fig. 2, the only difference is that \( \text{Re} \Sigma(\omega) \) and \( \text{Re} \Phi(\omega) \) change sign at \( \omega \geq \Delta \). Interestingly, \( \text{Re} \Sigma(\omega) \) and \( \text{Re} \Phi(\omega) \), extracted by in Ref. 21, also change sign at \( \omega \geq \Delta \).

The same set of results is obtained if one completely ignores the electronic dispersion. In this limit the equations for \( Z(\omega_m) \) and \( \Delta(\omega_m) \) become, at \( T = 0 \),

\[
Z(\omega_m) = 1 + \frac{g}{\omega_m} \int \frac{d\omega'_m}{|\omega_m - \omega'_m|} \frac{\omega'_m}{\sqrt{(\omega'_m)^2 + (\Delta(\omega'_m))^2}}
\]
\[
\Delta(\omega_m) = g \int \frac{d\omega'_m}{|\omega_m - \omega'_m|} \frac{\Delta(\omega'_m) - \Delta(\omega_m)\omega'_m}{\sqrt{(\omega'_m)^2 + (\Delta(\omega'_m))^2}}
\]

where \( g_{\text{eff}} = g/(V*)^{1/2} \). This equation is exactly the same as the gap equation (7) for strong dispersion. Hence, the functional forms of normal and anomalous self-energies are the same as in Fig. 2.

**Conclusions:** The simultaneous extraction of the normal and anomalous self-energy from photoemission data, enabled by recent machine-learning approaches\(^ {21} \), allows for significantly deeper insight into the nature of the dynamic pair formation. We argue that it implies that pairing is mediated by a soft, near-critical bosonic mode. Furthermore, if sharp peaks in both self-energies survive down to the lowest temperatures (i.e., they are due to quantum excitations), their presence alone imposes strong restrictions on the energy dependence of a soft pairing boson. We call for a systematic analysis of the peaks as function of temperature.
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