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I. Vekhter
Los Alamos National Laboratory Theoretical Division

C. M. Varma
Nokia Bell Labs

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A proposal to determine the spectrum of pairing-glue in high-temperature superconductors

I. Vekhter[1] and C. M. Varma[2]

[1] *Theoretical Division, MS B262, Los Alamos National Laboratory, Los Alamos, NM 87545*
[2] *Bell Laboratories, Lucent Technologies, Murray Hill, NJ 07974*

We propose a method for an analysis of the angle-resolved photoemission data in two-dimensional anisotropic superconductors which directly yields the spectral function of the bosons mediating Cooper pairing. The method includes a self-consistency check for the validity of the approximations made in the analysis. We explicitly describe the experimental data needed for implementing the proposed procedure.

Introduction. Understanding the mechanism of superconductivity in the high temperature superconducting cuprates requires knowledge of the spectral function of the bosons mediating the pairing as well as their coupling to the fermions. For conventional superconductors, such as Pb or Al, the phonon mechanism of superconductivity was firmly established through development of a procedure to invert the tunneling spectra (conductance as a function of voltage) and obtain the phonon spectral density [1, 2]. Here we propose a generalization of this procedure for anisotropic superconductors, which in general may have pairing mediated by the electron-electron interactions, using the angle resolved photoemission (ARPES) data as an input.

Recall that in conventional superconductors the dependence of the normalized tunneling conductance, $G_s(V)/G_n(V)$, where s and n refer to the superconducting and the normal state respectively, on the energy dependent gap function, $\Delta(\omega)$, is known. In turn, $\Delta(\omega)$ is related to the spectrum of pairing bosons through the Eliashberg theory [3]. This makes the inversion of the tunneling spectra possible.

Several important differences arise in the case of unconventional superconductors. First, since for an anisotropic gap function the tunneling current strongly depends on direction, and since the tunneling spectra are integrals over all the directions (often with a varying weight due to the spatial structure of the matrix element), such spectra in general neither provide sufficient information to resolve the anisotropy of the boson-fermion coupling nor allow its frequency dependence to be determined quantitatively. Second, in contrast to the case of phonons, in superconductors where the pairing is mediated by electron-electron interaction, the pairing spectra change and are temperature dependent below the transition temperature, T_c, when the single particle spectra are gapped. Also, since the typical energy of interaction between electrons is high, any inversion procedure must determine whether Eliashberg theory is suitable for the analysis.

We propose an inversion procedure using the ARPES data, which is applicable to anisotropic superconductors, uses the Eliashberg theory and contains a consistency check [4]. Below, we first summarize the procedure and the experimental input required to implement it, and then describe the technical details.

Outline of the procedure. As input the following experimental information for an optimally doped or overdoped sample is required: *(i) For Normalization.* Just above T_c, for several points at the Fermi surface, we require the integrated area under the momentum distribution curve (MDC) for momentum perpendicular to the Fermi surface, as defined in Eq.(5) below. This step gives the anisotropic equivalent of normal state conductance in the McMillan-Rowell procedure and provides the necessary normalization for the second step. *(ii) For Inversion.* With the same polarization and incoming photon energy, and at the same set of points at the Fermi surface, we need, at several temperatures below T_c, the difference in the intensity of the MDCs between the normal state above T_c and the superconducting state, for energies up to several times the superconducting gap. These data may be either a function of momentum or (better still) integrated during measurement over the momentum normal to the Fermi surface as in *(i)*. This step allows the extraction of the spectral density of the boson and the form of the coupling function. The data are used to extract the superconducting gap function, according to Eq.(10). The gap function is then inverted by using Eliashberg theory to obtain the boson spectrum and its coupling to fermions in different angular channels according to Eq.(18). The self-consistency check on the Eliashberg theory is obtained by comparing the energy range of the bosons with the input ARPES spectra and with the estimates of the bandwidth.

ARPES spectra. The intensity of the ARPES signal, $I(\mathbf{k},\omega)$, for a fixed momentum and binding energy of the emitted electron, is [5]

$$I(\mathbf{k},\omega) = \mathcal{M}(\mathbf{k}) f(\omega/T) A(\mathbf{k},\omega). \tag{1}$$

Here f is the Fermi function, and $\mathcal{M}$ is a prefactor, which depends on the square of the dipole matrix element between the initial and the final states, and on the kinematical factors. The information about the fermion spectrum is contained in the spectral function

$$A(\mathbf{k},\omega) = -\frac{1}{\pi} Im\ G^R(\mathbf{k},\omega), \tag{2}$$

where G^R is a retarded Green's function. It is the $\mathbf{k}$-dependent prefactor, $\mathcal{M}$, that obscures the true momentum dependence of the spectral function, and prevents direct inversion of the ARPES intensity.

In disentangling the momentum dependence of the spectral density, $A(\mathbf{k},\omega)$, from the signal intensity measured in ARPES, we rely on several properties of the prefactor. First, while $\mathcal{M}$ depends on the momentum, $\mathbf{k}$, it does not contain a significant dependence on the temperature, T, or the electron binding energy, ω [5]. Second, since the momentum dependence of $\mathcal{M}(\mathbf{k})$ is determined by the spatial structure of the electron wave functions, the energy and momentum range over which it varies are of the order of the Fermi energy and the Brillouin Zone respectively. Consequently, if, for fixed ω, the spectral density, A, is sharply peaked in the momentum space, the dependence of the prefactor on $|\mathbf{k}|$ may be ignored.

Step (i): MDCs and normalization. We write the momentum $\mathbf{k} = (k_f + k_\perp, s)$, where $k_f(s)$ is the Fermi momentum and s is the tangential component of $\mathbf{k}$ at a point on the Fermi surface. The normal state Green's function at Matsubara frequencies, $\omega_n = 2\pi T(n+1/2)$, is

$$G_N(\omega_n,\mathbf{k}) = \left[i\omega_n \mathcal{Z}(\mathbf{k},\omega_n) - \xi(\mathbf{k})\right]^{-1}, \tag{3}$$

where $\mathcal{Z}$ contains the effects of the interactions, $\xi(\mathbf{k}) \approx v_f(s)k_\perp$, and v_f is the bare, unrenormalized, Fermi velocity. Therefore the spectral function is

$$A_N(\mathbf{k},\omega) = \frac{1}{\pi}\frac{\omega Z''(\mathbf{k},\omega)}{(\omega Z'(\mathbf{k},\omega) - v_f k_\perp)^2 + (\omega Z''(\mathbf{k},\omega))^2}, \tag{4}$$

where $Z = Z' + iZ''$ is the analytic continuation of $\mathcal{Z}(\mathbf{k},\omega_n)$ to real frequencies.

Our subsequent analysis assumes that Migdal's theorem is valid for high-T_c superconductors, and checks for the validity of this assumption at the end. The essential statement of the theorem is that, when the energy range of the interaction is small compared to the electron bandwidth but the momentum ranges of the electrons and the boson are comparable, (a) the electronic self-energy is momentum-independent, (b) the vertex corrections to the interactions are negligible [6]. Under such conditions, we can approximate $Z(\mathbf{k},\omega_n) \approx Z(s,\omega_n;k_f)$ in Eq.(4) to a high degree of accuracy. We believe that this assumption will be borne out by the self-consistency check since both the neutron scattering data [7] and the analysis of the ARPES data in the normal state [8, 9] indicate the range of the interactions to be 0.2-0.4 eV, only a fraction of the bandwidth.

In contrast to the usual Eliashberg theory, we must consider the change in the spectrum of the boson in the superconducting state. We show below that the inversion of the ARPES data at different temperatures below T_c explicitly gives the evolution of the pairing interaction as the superconducting order develops. This point is very important because the value of T_c is determined by the spectrum just above T_c, while all the properties below T_c (for example the temperature dependence of the superconducting gap) are determined by the self-consistent change of the pairing spectrum as a function of temperature.

The momentum distribution curves (MDC), are obtained by plotting the intensity of the ARPES spectra, $I(\mathbf{k},\omega)$ at a fixed electron energy ω as a function of $\mathbf{k}$ [8]. The MDCs needed here are those taken along the lines normal to the Fermi surface for several direction. These curves have Lorentzian shape as a function of $k_\perp$ [8], which confirms (by inspection of Eq.(4)) that both the renormalization function, Z, and the prefactor $\mathcal{M}$ depend only weakly on $k_\perp$ in the neighborhood of the peak of the MDC, $\mathcal{M}(s,k_f+k_\perp) \approx \mathcal{M}(s,k_f) \equiv M(s)$. [10]

Divide the ARPES intensity by the Fermi function to remove the temperature dependence, and consider the area under thus rescaled MDC,

$$\mathcal{J}(s,\omega) = \int dk_\perp \frac{I(\mathbf{k},\omega)}{f(\omega/T)} \approx M(s)\int dk_\perp A(\mathbf{k},\omega). \tag{5}$$

It follows from the Lorentzian shape of the spectral function in the normal state that

$$\mathcal{J}_N(s,\omega) \approx \frac{M(s)}{v_f(s)} \tag{6}$$

is independent of the binding energy, and only depends on the position on the Fermi surface via the prefactor and the bare Fermi velocity. Therefore it serves to normalize the MDCs. It also follows that the energy and temperature dependence of the area under the MDC is simply given by the Fermi function. Note that to recover most of the area under the MDCs in the experiment it is sufficient to carry out the integration over the range of $k_\perp$ of only a fraction of the Brillouin Zone.[8]

Step (ii): Extraction of the gap function. Next consider the difference between the electron Green's functions in the normal and the superconducting state, and employ the spectral representation to write this difference as

$$\begin{aligned} &G_N(\mathbf{k},\omega_n) - G_s(\mathbf{k},\omega_n) \\ &\quad = \int_{-\infty}^{+\infty} \frac{dx}{i\omega_n - x}\Big(A_N(\mathbf{k},x) - A_s(\mathbf{k},x)\Big). \end{aligned} \tag{7}$$

Here G_s is the '11' component of the matrix (Nambu-Gorkov) Green's function of a superconductor

$$\widehat{G}(\mathbf{k},\omega_n) = -\frac{i\omega_n \mathcal{Z}(\mathbf{k},\omega_n) + \xi(\mathbf{k})\tau_3 + \Phi(\mathbf{k},\omega_n)(i\tau_2)}{\mathcal{Z}^2(\mathbf{k},\omega_n)\omega_n^2 + \Phi^2(\mathbf{k},\omega_n) + \xi^2}, \tag{8}$$

and Φ is the anomalous part of the self-energy. We now integrate both parts of Eq.(7) over the momentum normal to the Fermi surface at a given point s. Using

Migdal's theorem, we replace both Φ and $\mathcal{Z}$ in the integrand by their values at the Fermi surface, and introduce the gap function $\Delta(s,\omega_n) \equiv \Phi(s,\omega_n)/Z(s,\omega_n)$ to find

$$-\frac{i\pi}{v_f(s)}\left(\mathrm{sgn}(\omega_n) - \frac{\omega_n}{\sqrt{\omega_n^2+\Delta^2(s,\omega_n)}}\right) = \int_{-\infty}^{+\infty}\frac{dx}{i\omega_n - x}\int dk_\perp\Big(A_N(\mathbf{k},x) - A_s(\mathbf{k},x)\Big). \quad (9)$$

Assuming particle-hole symmetry, $A(-k_\perp,s,-x) = A(k_\perp,s,x)$, and the existence of the center of inversion for the Fermi surface, $\mathcal{M}(\mathbf{k}) = \mathcal{M}(-\mathbf{k})$, we rewrite the integral over the energy, x, via an integral over only the occupied states, $x<0$ (cf.[11]). Using the normal state result, Eq.(6), to eliminate $M(s)/v_f(s)$, we find ($\omega_n>0$)

$$\Delta(s,\omega_n) = \omega_n\left[\big[1-\omega_n\mathcal{K}(\omega_n,s)\big]^{-2}-1\right]^{1/2} \quad (10)$$

$$\mathcal{K}(\omega_n,s) = \frac{2}{\pi}\big[\mathcal{J}_N(s)\big]^{-1} \times\int_{-\infty}^{0}\frac{dx}{\omega_n^2+x^2}\big[\mathcal{J}_N(s,x)-\mathcal{J}_s(s,x)\big] \quad (11)$$

At each $\omega_n = \pi T(2n+1)$ and for given direction s at the Fermi surface, the function $\mathcal{K}(\omega_n,s)$ depends solely on experimentally measured intensities. Therefore using Eqs.(10)-(11) the gap function $\Delta(s,\omega_n)$ can be determined directly from the ARPES spectra.

Inversion of the gap equation. We assume a pairing function of the form $|\mathrm{g}(\mathbf{k},\mathbf{k}')|^2 B(\mathbf{k}-\mathbf{k}',\omega_n-\omega_{n'})$, where $|\mathrm{g}(\mathbf{k},\mathbf{k}')|$ is the matrix element of the interaction, and $B(\mathbf{k},\omega_n)$ is the propagator of the boson. In the Eliashberg theory the equations for the normal and the anomalous part of the self-energy take the form

$$\Big[1-\mathcal{Z}(\mathbf{k},\omega_n)\Big]i\omega_n = -T\sum_{\omega_{n'}}\int d\mathbf{k}'|\mathrm{g}(\mathbf{k},\mathbf{k}')|^2\frac{i\omega_{n'}\mathcal{Z}(\mathbf{k}',\omega_{n'})B(\mathbf{k}-\mathbf{k}',\omega_n-\omega_{n'})}{\omega_{n'}^2\mathcal{Z}^2(\mathbf{k}',\omega_{n'})+\Phi^2(\mathbf{k}',\omega_{n'})+\xi^2(\mathbf{k}')} \quad (12)$$

$$\Phi(\mathbf{k},\omega_n) = \eta T\sum_{\omega_{n'}}\int d\mathbf{k}'|\mathrm{g}(\mathbf{k},\mathbf{k}')|^2\frac{\Phi(\mathbf{k}',\omega_{n'})B(\mathbf{k}-\mathbf{k}',\omega_n-\omega_n')}{\omega_{n'}^2\mathcal{Z}^2(\mathbf{k}',\omega_{n'})+\Phi^2(\mathbf{k}',\omega_{n'})+\xi^2(\mathbf{k}')}, \quad (13)$$

where $\eta=+1$ ($\eta=-1$) for coupling in the channel even (odd) under time-reversal [12]. Integrating over $k'_\perp$ in the right hand side, we arrive at an equation for the gap function

$$\omega_n\Delta(s,\omega_n) = -\pi T\sum_{\omega_{n'}}\int ds' g(s,s')B(s-s',\omega_n-\omega_{n'})\big[G(s,\omega_{n'})\Delta(s,\omega_n)-\eta\omega_n F(s,\omega_{n'})\big], \quad (14)$$

where $g(s,s') \equiv |\mathrm{g}(s,s')|^2/|v_f(s)|$ is the effective coupling at the Fermi surface, and G and F are the ξ-integrated diagonal and off-diagonal components of the Green's function respectively,

$$G(s,\omega_n) = \frac{\omega_n}{\sqrt{\omega_n^2+\Delta^2(s,\omega_n)}} \quad (15)$$

$$F(s,\omega_n) = \frac{\Delta(s,\omega_n)}{\sqrt{\omega_n^2+\Delta^2(s,\omega_n)}}. \quad (16)$$

We now make a simplifying assumption (to be verified) that the pairing function is separable and diagonal in the space of the Fermi surface harmonics, $\psi_i(s)$. These harmonics are the orthonormal eigenfunctions of the symmetry operators of the Fermi surface, and correspond to different angular channels for a cylindrical Fermi surface [13]. Therefore

$$g(s,s')B(s-s',\omega_n-\omega_{n'}) = \sum_i B_i(\omega_n-\omega_{n'})\psi_i(s)\psi_i(s'). \quad (17)$$

Expand in $\psi_i(s)$ all functions of s in Eq.(14), $\Delta(s,\omega_n) = \sum_i\Delta_i(\omega_n)\psi_i(s)$ and the same for functions G and F, to obtain a linear system for the coupling function

$$\sum_{k,\omega_{n'}}\beta_{ik}(\omega_n,\omega_n-\omega_{n'})B_k(\omega_{n'}) = \alpha_i(\omega_n). \quad (18)$$

All the coefficients in this equation are known from the form of the gap function and the Fermi surface,

$$\beta_{ik}(\omega_n,\omega_{n'}) = \pi T\Big[\eta\delta_{ik}\omega_n F_k(\omega_{n'}) - b_{ik}(\omega_n)G_k(\omega_{n'})\Big],$$

$$b_{ik}(\omega_n) = \sum_j a_{ijk}\Delta_j(\omega_n), \qquad \alpha_i(\omega_n) = \omega_n\Delta_i(\omega_n),$$

$$a_{ijk} = \int ds\psi_i(s)\psi_j(s)\psi_k(s).$$

Solution of Eq.(18) gives the pairing function at Matsubara frequencies and in particular angular channels. It can then be analytically continued to real frequencies using either the Pade approximation [14] or by solving

the integral equation obtained by analytic continuation of Eq.(18) in analogy to Ref.15. The full pairing function, $\sum_i B_i(\omega)\psi_i(s)\psi_i(s')$ can then also be used to obtain the self-energies, Z and Φ, using Eqs.(12)-(13).

Self-consistency. Two major assumptions have been made in our analysis, and have to be checked for self-consistency. First, we assumed that Migdal's theorem holds. If the energy range of the pairing function is significantly smaller than the bandwidth in all channels i, the procedure is self-consistent. Second, we assumed separable form of the pairing function, Eq.(17). In a realistic calculation we truncate the number of angular channels, i, in Eq.(18); if inclusion of an additional channel does not change appreciably the pairing functions in the other channels, the approximation is justified. Note that a minimum of two channels is required: the isotropic channel which alone determines the self-energy in the normal state if the Fermi-surface is circular, and the $d_{x^2-y^2}$ channel responsible for pairing; we expect additional channels to enter with smaller couplings. The change of spectral strength with temperatures in these channels, obtained via the outlined procedure, yields crucial information on the change of self-energies below T_c.

Experimental constraints. Most available ARPES spectra are taken on $Bi_2Sr_2CaCu_2O_{8+\delta}$ samples. Since our analysis includes only superconducting order and does not account for the pseudogap, the measurements should be done on an optimally doped or overdoped sample. In the normal state the width of the peak in MDCs is a fraction of the Brillouin Zone [8], and we expect that the data in the superconducting state have to be collected over the same window in momentum space. Since the area $\mathcal{J}_N$ in Eq.(6) does not depend on the energy ω, and since MDC is a Lorentzian with a flat ($k_\perp$-independent) background at $\omega = 0$, we suggest that $\mathcal{J}_N$ is most easily determined at the Fermi energy. Away from the Fermi energy the background becomes momentum-dependent; however, the difference between the signal in the normal and superconducting state, required in Eq.(11) is insensitive to the background. In that equation we expect the energy range over which the $k_\perp$-integrated difference in intensity is appreciable to be of the order of a few times the superconducting gap, so that the data should be taken up to $\omega \sim 0.1 - 0.2$eV.

Such data may be difficult to take near the $(\pi, 0)$ points because of the bilayer splitting, not accounted for in our one-band approach (generalization to a multi-band case is, however, straightforward). Also, near these points the MDCs corresponding to different Fermi arcs begin to overlap at energies away from $\omega = 0$ [8]. Consequently, it is more feasible to measure the spectra close to the nodal directions; we expect that spectra taken over half of the angular range between the node and the antinode would contain enough information to carry out the analysis suggested here. Since the analysis of the spectra is complicated by the superstructure in Bi-O layer, samples containing Pb, which suppresses Bi-O modulations, may be more suitable. Finally, the resolution function of the measurement apparatus has to be disentangled from the signal intensity; the separation can be done by an integral transform if the energy dependence of the resolution function is known. A numerical procedure for implementing the method has been developed and will be made available.

We have proposed a method to extract the spectrum of the pairing function from the ARPES measurements in high temperature superconductors which makes a minimum of theoretical assumptions, does not use any prejudicial form of the pairing fluctuation spectrum as an input, and contains a self-consistency test. In contrast to the analysis of optical conductivity [16], our approach uses single particle spectra which contains more information and explicitly gives the evolution of the pairing spectrum with temperature in the superconducting state. Implementation of this approach through appropriate experiments promises to yield the answer to one of the central questions in the high T_c problem.

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