Eliashberg Analysis of Temperature Dependent Pairing Mechanism in d-wave Superconductors: Application to High Temperature Superconductivity.

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Results are presented for the temperature and frequency dependence of the real and imaginary parts of the diagonal self energy for a d-wave superconductor. An Eliashberg analysis, which has been successful in recent fitting of superconductor-insulator-superconductor (SIS) tunnel junction conductances for Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi-2212), is extended to finite temperatures. The superconducting pairing mechanism is assumed to originate in the spin fluctuations of the copper-oxide planes, and is modelled by a function incorporating the spin resonance mode measured at an energy of approximately 40 meV for optimally doped Bi-2212. The effect of the temperature dependence of the spin resonance mode, measured in inelastic neutron scattering (INS), on the finite temperature self energies is investigated.

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Recently, self consistent Eliashberg theory has been quite successful in fitting zero temperature superconductor-insulator-superconductor (SIS) point contact tunnel (PCT) junction characteristics in the high temperature superconducting cuprate Bi-2212.\(^1\)

The success of that work indicates that the superconducting state of the cuprates may be understood to originate from a low frequency spectrum of spin fluctuations. This interpretation is sometimes referred to as the pairing glue scenario\(^2\), and is most likely to be appropriate for the optimal to overdoped regime of the cuprates. For an explanation of the origin of high temperature superconductivity in the underdoped regime, and in proximity to the insulating antiferromagnetic phase of the cuprates, the RVB singlet picture\(^3,4\), involving the exchange constant \(J\) in the t-J model Hamiltonian, provides an explanation for the emergence of the high temperature superconducting phase.

A strong coupling analysis has also been used to interpret both angle resolved photoemission spectroscopy (ARPES)\(^5–7\), and optical conductivity\(^8,9\). The former yields results for the single quasiparticle self energy \(\Sigma(\omega, T)\). In the latter case, a memory function analysis of the optical conductivity results in a frequency dependent optical self energy \(\Sigma_{opt}(\omega, T)\)\(^10\).

The origin of structure in the electronic spectra of the cuprates, measured in such experiments as ARPES and optical conductivity, is a topic of much debate. In some analyses of ARPES\(^11\), dispersion anomalies observed along the nodal line in the copper-oxide plane Brillouin Zone, have been interpreted in terms of quasiparticle scattering involving phonons, rather than spin fluctuations. The energy scales of importance in the spin fluctuation spectrum, namely the so-called spin resonance mode (at approximately 40 meV), and certain phonon modes in optimally doped Bi-2212 make them potential candidates for understanding structure seen in ARPES. Higher energy spin fluctuations at 80meV have been proposed for the observed dispersion anomaly in YBaCuO using an Eliashberg analysis\(^12\). As will be discussed later, the absence of a temperature dependence in the measured low frequency slope of the real part of \(\Sigma(\omega, T)\) (Re \(\Sigma(\omega, T)\)) in the case of nodal ARPES measurements on Bi-2212, suggests that the spin resonance mode is not involved in nodal quasiparticle interactions in Bi-2212, similar to the situation proposed for YBaCuO\(^12\).

One motivation for applying a strong coupling, Eliashberg-like approach to the cuprates is the success of the same approach in conventional superconductors. In conventional superconductors, such as Pb, a self consistent Eliashberg theory, based on the use of a single self energy diagram, with no vertex corrections, can be justified by Migdal’s theorem since the characteristic energy scale of phonons relative to the Fermi energy is very small\(^13\).

Another important point is that in the case of conventional superconductors, there exists a detailed, and quantitative description of the phonon spectral function, denoted by \(\alpha^2F(\omega)\), describing the superconducting pairing mechanism. The analog of \(\alpha^2F(\omega)\) for the spin fluctuation spectrum in the cuprates, denoted by \(I^2\chi(\omega)\) in some work, is not as well understood. The spectral function, describing the pairing glue due to spin fluctuations is modelled phenomenologically in the present work by a prominent peak at the energy of the spin resonance mode \(\Omega_{Res}\) accompanied by a broad background continuum extending up to higher energies\(^14\). The value of \(\Omega_{Res}\) has been measured in inelastic neutron scattering (INS) experiments\(^15\), and is about 40meV for optimally doped Bi-2212, which is the focus of the present work. The ubiquitous dip feature seen in spectroscopies such as tunneling\(^16\) and ARPES\(^17\) is taken as evidence of the key role of the spin resonance mode peak in the superconducting state of the cuprates.

Furthermore, support for the partly phenomenological approach of the present work comes from extensive, ab initio, Quantum Monte Carlo numerical studies\(^2,18–20\) on the Hubbard and t-J models which indicate a key role is played by a low frequency spin fluctuation spectrum in determining the properties of the superconducting state of these models.

One of the most unusual aspects of the spin fluctuation physics in the cuprates is the decrease in intensity with increasing temperature of the spin resonance peak at \(\Omega_{Res}\), along with its disappearance at the superconduct-
ing transition temperature $T_C$. This was first directly measured in INS measurements on Bi-2212.\textsuperscript{15} Similar behavior has also been extracted from analysis of optical conductivity, although in that case the mode appears to survive, albeit significantly diminished in intensity, above $T_C$.\textsuperscript{9} The emergence of such a peak in the spin fluctuation spectrum at the superconducting transition may be the result of a feedback effect into the electronic spin susceptibility due to the onset of the superconducting gap\textsuperscript{21}.

In the pairing glue scenario, the disappearance of the resonance mode peak would imply that the superconducting pairing mechanism weakens with increasing temperature, very unlike conventional, phonon mediated, superconductors. The effect of a temperature dependent pairing glue on the temperature dependence of important quantities such as the superconducting gap, and the value of the transition temperature $T_C$, is one of the subjects of the present work. It also results in significant temperature dependent effects in the real and imaginary parts of $\Sigma(\omega, T)$ such as a change in slope of the Re$\Sigma(\omega, T)$ at low frequencies. Comparison between finite temperature model calculations and measurements of the temperature dependence of the self energy from ARPES and optical conductivity, may serve as an important test of the validity of the spin fluctuation pairing glue hypothesis for the cuprates.

**Theoretical Formalism**

In the present work, a modified version of the standard finite temperature ($T \neq 0$) Eliashberg equations\textsuperscript{13} are solved self consistently. The zero temperature ($T = 0$) case of these equations was used in\textsuperscript{1,16}. The coupled equations to be solved are given by

\begin{equation}
\Delta(\omega, T) = \frac{1}{Z(\omega, T)} \int_0^{\omega_i} d\nu \int_0^{2\pi} \frac{d\phi}{2\pi} \Delta \text{Re} \left\{ \frac{1}{\nu^2 - \Delta^2(\nu, T) \cos^2(2\phi)} \right\} \int_0^{\omega_j} d\omega' F(\omega', T) \times \left\{ [n(\omega') + f(-\nu)] \left[ \frac{1}{\omega + \omega' + \nu + i\delta} - \frac{1}{\omega - \omega' - \nu + i\delta} \right] - [n(\omega') + f(\nu)] \left[ \frac{1}{\omega + \omega' - \nu + i\delta} - \frac{1}{\omega - \omega' + \nu + i\delta} \right] \right\}
\end{equation}

and

\begin{equation}
[1 - Z(\omega, T)] = \int_0^{2\pi} \frac{d\phi}{2\pi} c_Z \text{Re} \left\{ \frac{\nu}{\nu^2 - \Delta^2(\nu, T) \cos^2(2\phi)} \right\} \int_0^{\omega_{\text{max}}} d\omega' F(\omega', T) \times \left\{ [n(\omega') + f(-\nu)] \left[ \frac{1}{\omega + \omega' + \nu + i\delta} + \frac{1}{\omega - \omega' - \nu + i\delta} \right] + [n(\omega') + f(\nu)] \left[ \frac{1}{\omega + \omega' - \nu + i\delta} + \frac{1}{\omega - \omega' + \nu + i\delta} \right] \right\}
\end{equation}

In the present work

\begin{equation}
\Delta(p, \omega) = \Delta(\omega, T) \cos(2\phi)
\end{equation}

$\phi$ denotes the angular position on the Fermi surface, with the $\cos(2\phi)$ dependence incorporating a d-wave symmetry superconducting state.

In place of the conventional phonon spectral function $\alpha^2 F(\omega)$ in the Eliashberg equation formalism, the spin fluctuation pairing glue is described by\textsuperscript{22}

\begin{equation}
[c_Z + c_\Delta \cos(2(\phi - \phi_0))] F(\omega, T)
\end{equation}

The spin fluctuation spectral function $F(\omega, T)$ will be discussed in detail in the next section.

**Results**

The results presented here are for optimally doped Bi-2212, and are an extension of our successful fitting of the SIS tunneling conductance for this material at $T = 0$.\textsuperscript{1} The superconducting transition temperature is chosen to be 90K in the present work. The values of $c_Z = 0.2$ and $c_\Delta = 0.83$ were used in reference (1) to fit the optimally doped SIS PCT experimental conductance. The coupled Eliashberg equations for $Z(\omega, T)$ and $\Delta(\omega, T)$ are solved self consistently Results for the diagonal self energy $\Sigma(\omega, T)$ are presented and discussed later, where $\Sigma(\omega, T)$ is defined by

\begin{equation}
\Sigma(\omega, T) = (1 - Z(\omega, T)) \omega
\end{equation}

The Re$\Sigma(\omega, T)$ is usually called the mass enhancement.
factor, and $-2 \text{Im}\Sigma(\omega, T)$ is the quasiparticle scattering rate ($1/\tau$). These two quantities can be measured in APRES\textsuperscript{5,6}. Optical conductivity experiments\textsuperscript{8} yield a related optical self energy function as well. The temperature dependent superconducting gap, usually denoted by $\Delta(T)$, is defined as the frequency $\omega$ at which $\omega = \text{Re}\Delta(\omega, T)$.

The spectral function $F(\omega, T)$ describing the pairing glue in this work is shown in Figure 1. The intensity of the main peak, at the resonance mode frequency $\Omega_{\text{Res}}$, decreases as the temperature is increased, eventually vanishing at $T_c$. The $F(\omega, T)$ curves shown in Figure 1 incorporate the temperature dependence of the resonance mode, seen in INS and optical conductivity experiments. The resonance mode rides on a weakly temperature dependent background which extends to higher frequencies.

Figure 1 is generated using a model for the spectral function of the form

$$F(\omega, T) = H(T)F(\omega)^{\text{Res}} + BG(T)F(\omega)^{BG}$$

The resonance mode is modelled by a Gaussian $F(\omega)^{\text{Res}}$ with peak magnitude given by $H(T) = H_0(1-T/90K)^{1/2}$, where $H_0$ is the initial peak height at $T=0K$. The temperature dependence of the peak height is similar to the BCS mean field $\Delta(T)$ behavior, and also consistent with the temperature dependent mode height seen in INS experiments.\textsuperscript{15}

The background continuum is modeled using a broad temperature independent Gaussian function of frequency $\omega$ denoted by $F(\omega)^{BG}$ multiplied by a temperature dependent factor $BG(T) = 1 + \alpha T/90K$, where $\alpha$ is adjusted to yield $\Delta(T) = 0$ at $T = 90K$ in the self consistent solution of the Eliashberg equations.

The consequences of a complete disappearance of the resonance mode peak are investigated in this work, but uncertainties in the frequency dependence of the pairing glue spectral function should be kept in mind.

In one analysis (see Fig (18) of reference (10)) of ARPES experimental data, the resonance mode peak sits on a relatively large, temperature independent, background continuum. In that case, the decrease in the peak height, as the temperature is increased up to $T_c$, results in a correspondingly smaller reduction in the pairing glue coupling strength compared to the current results presented here.

Finally, the issue of whether the area under the $F(\omega, T)$ curve should be conserved, as the temperature changes, is unclear. This would require that area lost from the main peak would be redistributed to higher frequencies. However, even if this requirement were imposed, there would still likely be a reduction in the strength of the pairing glue (see equation (7) ahead) with increasing temperature.

Table 1 lists values from reference (23) of measured $T_C$ and zero temperature gap values ($\Delta(0)$) and the corresponding $2\Delta(0)/k_B T_C$.

| $T_C$(K) | $\Delta(0)$ (meV) | $2\Delta(0)/k_B T_C$ |
|---------|------------------|-----------------------|
| 51      | 10.5             | 4.78                  |
| 62      | 17.5             | 6.56                  |
| 92      | 31               | 7.83                  |
| 95      | 38               | 9.3                   |

The disappearance of the resonance mode at the measured $T_C$ may be an important contribution to the large $2\Delta(0)/k_B T_C$ ratios in Table 1.

To illustrate the effect of assuming a temperature independent pairing glue, Figure 2 shows the resulting $\Delta(T)$ from using the $T = 0K$ $F(\omega, T)$ from Figure 1 for all finite temperatures in the Eliashberg equations. The calculated $T_C$ for this case is 153K as seen in Figure 2, much higher than the measured 90K value for optimally doped Bi-2212. The value of the ratio $2\Delta(0)/k_B T_C$ is 5.7, much less than the observed value of 9.3. This same discrepancy will occur in the case of the other Bi-2212 doping levels previously analysed\textsuperscript{3}. This observation implies that a temperature dependent weakening of the strength of the pairing glue, and a consequent re-
duction in the transition temperature $T_C$, may be at the origin of the large ratio values shown in Table 1. Furthermore, the trend seen in Table 1 for the $2\Delta(0)/k_BT_C$ ratio to decrease with overdoping is also consistent with the decreasing prominence of the resonance mode in the pairing glue spectrum with overdoping.

Figures (3) and (4) show the Re$\Sigma(\omega,T)$ and Im$\Sigma(\omega,T)$ for the case where $F(\omega,T)$ is kept at its $T = 0$ shape for all temperatures up to the transition temperature of 153K. As temperature increases, the peak structures in the self energy functions are smeared out due to the Fermi and Bose functions in the Eliashberg equations. It is worth noting that, in the d-wave superconductor, the main peak in the Re$\Sigma(\omega,T = 0)$ is located at approximately 75 meV, slightly below the value $\Delta(0) + \Omega_{Res} = 82$ meV (using $\Delta(0) = 38$meV and $\Omega_{Res} = 44$ meV$^1$), which would be expected for an s-wave superconductor.

A measure of the pairing glue coupling constant involved in determining $\Sigma(\omega,T)$, which is denoted by $\lambda$ in the present work, can be extracted in two ways. One is by analogy with the electron-phonon coupling constant in conventional superconductors, by use of

$$\lambda = 2\alpha^2 \int_0^\infty \frac{F(\omega,T)}{\omega} d\omega$$

(7)

A second measure of $\lambda$ is from the slope, at low $\omega$, of Re$\Sigma(\omega,T)$. Results for $\lambda$ from both of these procedures are tabulated in Table II for the case of a temperature dependent pairing glue, which will be discussed later. For the current situation where the $F(\omega,T)$ is assumed to stay constant at its $T = 0$K shape, the slope of Re$\Sigma(\omega,T)$ in Figure (3) is constant at low $\omega$, and consequently $\lambda$ does not change with temperature.

It is interesting to compare the temperature evolution seen in Figures (3) and (4) with that of Pb for which the Re$\Sigma(\omega,T)$ and Im$\Sigma(\omega,T)$ are shown in Figures (5) and (6). The lead gap $\Delta(0) = 1.35$meV is almost a factor of 3 less than the first phonon peak of approximately 4.4meV in the lead phonon $x_2^2F(\omega)$ spectral weight, which itself is temperature independent. The result is a relatively undramatic temperature evolution in the Pb Re$\Sigma(\omega,T)$ and Im$\Sigma(\omega,T)$ compared with that seen in Figures (3) and (4) where the value of $\Delta(0)$ and $\Omega_{Res}$ are comparable.

Figures (7), (8) and (9) show results for $\Delta(T)$, Re$\Sigma(\omega,T)$ and Im$\Sigma(\omega,T)$ for the case of the temperature dependent $F(\omega,T)$ shown in Figure (1). The superconducting gap $\Delta(T)$ now goes to zero at 90K, due to the choice of $\alpha = 0.6$ in the background continuum BG$(T)$ function. The $T = 0$ value for $\Delta(0) = 38$meV is in agreement with measured value from SIS PCT measurements$^{23}$, and so the correct $2\Delta(0)/k_BT_C$ of 9.3 is reproduced. The overall temperature dependence of $\Delta(T)$ in Figure (4) resembles that of the resonance mode peak height temperature dependence used for $H(T)$.

Figures (8) and (9) show the corresponding temperature dependent real and imaginary parts of $\Sigma(\omega,T)$. There are significant differences between these results and those shown in Figures (3) and (4). The Re$\Sigma(\omega,T)$ of Figure (8) show a much more rapid decrease in the main peak at approximately $\Omega_{Res} + \Delta(T)$ which reflects the decrease in the intensity of the resonance mode with in-
creasing temperature. The dip feature also fills in more rapidly compared to the temperature evolution of Figure (3). Furthermore, there is now a noticeable decrease in the slope of ReΣ(ω, T) at low frequencies, reflecting the decrease in the effective coupling constant (λ) as the resonance mode disappears. This is illustrated in the accompanying Table II.

In Figure (9), the disappearance of the spin resonance mode peak with increasing temperature results in a significant reduction in ImΣ(ω, T) in the energy range 50 meV to 100 meV. This energy range brackets the energy Ω_{Res} + Δ(T) where the mode shows up in such quantities as the self energy in Eliashberg theory. A significant reduction in the measured width of the MDC peak in the same frequency range, measured by ARPES, could search for this effect.

A limited amount of experimental measurements of the real and imaginary single particle Σ(ω, T), have been extracted from ARPES MDC curves on Bi-2212\(^5,6\). Optical conductivity experiments on Bi-2212\(^8\) have also yielded an optical self energy Σ_{opt}(ω, T), along with a temperature dependent spectral function for the underlying modes interacting with the quasiparticles. These analyses appear to reveal several different contributions to the extracted self energies. Separating out different contributions to the real and imaginary components of the quasiparticle self energy has been the subject of recent work (see Figure (10) of reference (10)) and reference (24).

In reference(8), a contribution is present in \(1/\tau = -2\text{Im}\Sigma_{opt}(ω, T)\) which increases linearly with energy, and is temperature dependent. The linear behavior with energy in \(1/\tau\) has been interpreted as evidence for the Marginal Fermi Liquid hypothesis\(^25\). Furthermore, a large energy and temperature dependent background is measured in the ReΣ(ω, T) in reference (6) which is subtracted off to yield the temperature dependent contribution to ReΣ(ω, T). These contributions complicate interpretation of the ARPES and optical conductivity data, and their comparison with the present model. In the analyses of ARPES and optical conductivity experiments, a background continuum extending up to 400 meV is present in the \(I^2\chi(ω)\) curves (see Figures (18) and (31) of reference (10)), in contrast to the pairing glue spectral curves shown in Figure (1) of this work where the high energy continuum extends up to 175 meV approximately.

The linear increase in \(1/\tau\) with increasing energy in ref-

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**Table II**: Coupling strength of optimally doped Bi2212 for various temperatures up to \(T_c\) (from Figure (8)) \(\lambda\) (see text)

| T(K) | \(\partial\Sigma(ω)\)  | \(\partialω\) | \(\lambda\) |
|------|-------------------------|--------------|------------|
| 0.01 | 0.46                    | 0.59         |            |
| 36   | 0.45                    | 0.57         |            |
| 54   | 0.44                    | 0.54         |            |
| 72   | 0.41                    | 0.49         |            |
| 85.5 | 0.36                    | 0.41         |            |
| 90   | 0.23                    | 0.29         |            |
FIG. 8: Temperature dependence of ReΣ(ω) for the temperature dependent F(ω, T) spectra shown in Figure (1).

FIG. 9: ImΣ(ω) for same conditions as in Figure (8).

In conclusion, results have been presented for an finite temperature Eliashberg calculation of a d-wave superconducting case with temperature dependent pairing glue. The calculated real and imaginary diagonal self energies may prove a useful probe of the pairing glue description of high temperature superconductors when compared with ARPES and optical conductivity experiments.

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