Anisotropic Strong Coupling Calculation of the Local Electromagnetic Response of High-\(T_c\) Superconductors

A. Bille and K. Scharnberg

Fachbereich Physik, Universität Hamburg, Jungiusstraße 11, D-20355 Hamburg, Germany

The fundamental information required to perform strong coupling calculations for conventional superconductors is the Eliashberg function which incorporates both the phonon spectrum and the electron-phonon interaction. These properties can be determined in the normal state and they are not expected to be affected significantly by the onset of superconductivity. Since much evidence for a highly anisotropic pair state in the high-\(T_c\) materials has accumulated in the recent past, the momentum dependence of the Eliashberg function needs to be taken into account. Upon the assumption that the underlying interaction is an exchange of spin-fluctuations, such an Eliashberg function has been modelled quite successfully to explain normal state properties. There is still some controversy about the best possible model but we feel that the function suggested by Monthoux and Pines, which contains the momentum dependence in a nonseparable form, is a reasonable starting point. Since this Eliashberg function is supposed to arise from electron-electron interactions, we expect it to change when superconductivity sets in. One way this change could manifest itself is a lower frequency cut-off approximately of the size and temperature dependence of the superconducting order parameter amplitude.

In this paper we have not included such strongly temperature dependent modifications of the Eliashberg function. Instead, we focus on the momentum and frequency dependence of the various self-energies, in particular the scattering rate, which in conjunction with the anisotropy of the Fermi velocity could have a marked effect on the conductivity. For an energy dispersion of the form

\[ \varepsilon(k) = \frac{\mu}{4} \left[ \cos(k_\mu \pi) + 2 \cos(k_\nu \pi) \cos(k_\rho \pi) \right], \]

with \(k_{\mu,\nu}\) given in units of \(\pi/a\), we have plotted in Fig. 1 the Fermi lines (inset) and the Fermi velocities in the first quadrant of the Brillouin zone. For each choice of the parameter \(B\) the band filling parameter \(\mu\) is chosen such that the Fermi line meets the zone boundary at the same point \((1,0,1)\). For a simple tight binding band \(B = 0\), quasiparticles with momenta in \((1,1,1)\) direction have indeed the highest Fermi velocities and thus contribute most strongly to the conductivity. For the modified tight binding band with \(B = 0.45\) there is very little variation of the Fermi velocity, which may be an artefact of this particular model band structure, as the comparison with the dot-dot-dashed curves show.

![Fermi velocities](image)

**FIG. 1.** Fermi velocities \(|\nabla \varepsilon(k)| = v_F (\hbar \pi/a)^2\) as calculated from Eq. (1) for a band width \(8t = 1.44\) eV. The inset shows the corresponding Fermi lines. The dot-dot-dashed lines are for the 8 parameter tight binding approximation to the odd band of the CuO\(_2\)-double layers in YBCO scaled to the same band width.

It has been noted before that a pairing interaction, which is attractive at small momentum transfers, can contribute to the formation of a \(d\)-wave state in addition to the spin fluctuation induced pairing interaction.

\[ \alpha^2 F_{SF}(\mathbf{q}, \Omega) = \left[ \pi \Omega \frac{\mu Q}{\omega_{SF}} \right] \frac{\lambda Q \Omega}{\omega_{SF}} \left[ 1 + \pi^2 \xi^2 (\mathbf{q} - \mathbf{Q})^2 \right]^2 + \frac{\Omega^2}{\omega_{ph}^2} \]  

we have, therefore incorporated into our strong coupling calculations a phonon contribution of the form

\[ \alpha^2 F_{ph}(\mathbf{q}, \Omega) = g_{ph} \left[ \pi \frac{1}{G(\mathbf{q})} \sum_{\sigma = \pm} \pi \xi \frac{\Gamma^2 \Omega}{(\Omega + \sigma^2 \Omega_0)^2 + \Gamma^2} \right] \]
Numerical results are for \( \Omega_\alpha = 41 \) meV and \( \Gamma = 8 \) meV. A very similar frequency dependence for \( \alpha^2 F_{ph} \) has been suggested by Golubov. Note that at low frequencies both functions vary linearly with frequency but for a typical value \( \omega_{SF} = 7.1 \) meV, which is much smaller than the value 30 meV used in Ref. [3], \( \alpha^2 F_{SF} \) dominates.

We have antisymmetrized \( \alpha^2 F_{ph}(q, \Omega) \) with respect to \( \Omega \), which has little effect on the physical meaning of this function but ensures that the coupling constant

\[
\lambda_{ph} = 2 \int_0^1 dq_x \int_0^1 dq_y \int_\Omega^{\infty} d\Omega \alpha^2 F_{ph}(q, \Omega) = g_{ph}
\]

is independent of both \( \Omega_0 \) and \( \Gamma \). The normalized \( q \)-dependent form factor

\[
G(q) = 36.9 e^{-25q_x^2} \frac{1-q_x q_y}{1+(2q_y)^2} q_x > q_z
\]

reflects nesting properties of the Fermi surface. The expression Eq. [3] represents a good fit to the numerical results shown in Fig. 3 of Ref. [8]. In all our calculations the coupling constant \( g_{SF}^2 \) was adjusted such that \( T_c = 92 \) K was kept constant.

Details of the calculation of the self-energies \( Z(k, \omega) \), which renormalizes the frequency to \( \tilde{\omega} = \omega Z(k, \omega) \), \( \chi(k, \omega) \), which is added to the band energy Eq. [1], and of the anomalous self-energy \( \Phi(k, \omega) \) have to be given elsewhere. To calculate these quantities we used the Eliashberg equations in the form given by Marsiglio et al. [Ref. 10].

For the energy dispersion Eq. [1] with \( B = 0.45 \) we show in Fig. 2 \( \text{Re} Z(k, \omega) \), which is related to the mass renormalization, as function of \( \omega \) for three different temperatures and two points on the Fermi line, one on the zone boundary, the other one at the position of the order parameter node. In Fig. 3 the corresponding results are shown for \( \text{Im} \omega Z(k, \omega) \), which is often identified with the quasiparticle scattering rate [1].

These figures show that there is considerable anisotropy already in the normal state, indicating much stronger interactions where the Fermi line meets the zone boundary than on the zone diagonal. This is due to the fact that for the particular band considered the nesting condition \( q = (\pm 1, \pm 1) \) which maximizes the interaction Eq. [3], is fulfilled to a much higher degree for points \( k_F = (1.0, 0.12) \) than for \( k_F = (0.37, 0.37) \). Large values of \( Z \) are found on the image of the Fermi line under a translation by \( Q \), i.e. near \( k = (1 - 0.37, 1 - 0.37) \). The anisotropy of \( Z \) on the Fermi line is not altered when phonons are included because these scatter most strongly between Fermi lines near \( k_F = (1.0, \pm 0.12) \). An interaction peaked at zero momentum transfer, however, would reduce the anisotropy.

Both mass renormalization and scattering rates are smaller at low frequencies when phonons are included because the coupling parameter \( \lambda_{SF} \), defined in analogy to \( \lambda_{ph} \) Eq. [1], has to be taken as \( \lambda_{SF} = 2.545 \) eV to obtain \( T_c = 92 \) K which is larger than \( \lambda_{SF} + \lambda_{ph} = 1.979 \) eV + 0.25 eV which gives the same \( T_c \). The source of this discrepancy is the contribution to the phonon spectrum at high frequencies which is absent in \( \alpha^2 F_{SF} \).

When the temperature is lowered below \( T_c \), the scattering rate drops much faster at the zone boundary where it was largest. The effect that this behaviour will have on the conductivity depends very much on the variation of the Fermi velocity (see Fig. 1). At \( T \approx 0.1 T_c \), the scattering rate for \( \omega < 15 \) meV has dropped well below typical disorder induced scattering rates [2].

FIG. 2. Mass renormalization function versus frequency for reduced temperatures \( T/T_c = 1.0, 0.9, 0.1 \). At \( \omega = 60 \) meV, \( \text{Re} Z \) increases monotonically with decreasing temperature. Dashed curves are for \( g_{ph} = 0 \) in Eq. [1], solid curves are for \( g_{ph} = 0.25 \) eV. Note the different ordinate scales.

FIG. 3. Scattering rates versus frequency for \( T/T_c = 1.0, 0.9, 0.1 \). At around \( \omega = 30 \) meV, \( \text{Im} Z \) increases monotonically with increasing temperature. Dashed curves: \( g_{ph} = 0 \), solid curves: \( g_{ph} = 0.25 \) eV.

In Fig. 4 we show the order parameter \( \Delta(k, \omega) = \Phi(k, \omega) / Z(k, \omega) \), on the Fermi line at the zone boundary. The ratio \( \text{Re} \Delta(\omega=0, T=0.1 T_c) / T_c = 2.79 \) without phonons and 3.42 with phonons is larger than the weak coupling value 2.14 but is still at the lower end of the
range of values required to fit experiments within weak-coupling theories.\textsuperscript{4}

Fig. 4. Real and imaginary parts of the order parameter versus frequency for $T/T_c = 0.99, 0.9, 0.1$ and $g_{ph} = 0$ (dashed) and $g_{ph} = 0.25$ eV (solid).

The surface impedance is calculated in the local limit which is well justified for all high-$T_c$ materials. The conductivity is obtained without taking vertex corrections into account. Since the interactions are momentum dependent, this is an approximation.\textsuperscript{12}

Fig. 5. Real part of the conductivity versus reduced temperature at fixed microwave frequency.

Fig. 5 shows the real part $\sigma_1$ of the conductivity at 87 GHz as function of temperature for different energy dispersions and different interactions. The only parameter adjusted in this figure is $g_{SF}$ and this is chosen to fit $T_c$, not $\sigma_1$. For $B = 0.45$ in Eq. (4) the agreement with a typical experiment (Ref. [11], Sample B) is good, because the scattering rates near the nodes are much smaller than the average value. At low temperatures, $\sigma_1$ drops too fast because the inelastic scattering rate falls below the experimental frequency. For these temperatures it is essential to take disorder induced elastic scattering into account. This would also reduce the peak height so that the conclusion seems to be inescapable that the interactions must become smaller below $T_c$. How large a reduction one would infer from experiment depends crucially on the energy dispersion. With $B = 0$ we have nearly perfect nesting and hence a large scattering rate on the Fermi line where the order parameter vanishes and where the Fermi velocity is maximal. For this case we find that the peak in $\sigma_1$ is far too small to be anywhere near the data.

Fig. 6. Imaginary part of the conductivity

Fig. 6 compares the superfluid density in the form $\sigma_2(\omega, T)$ with data taken at 87 GHz. Since $\text{Re} Z$ renormalizes the bare London penetration depth, which is determined by the band structure, we obtain $\lambda(0) = 123$ nm when phonon-exchange is included instead of $\lambda(0) = 155$ nm. The data are scaled to fit these different values of $\lambda(0)$. Including phonons gives a much improved fit because of the fast rise in $\text{Re} \Delta(k_F, \omega)$ at high frequencies (see Fig. 4). As in the case of $\sigma_1$, reaching agreement with experiment seems to require scattering rates which drop more rapidly in the superconducting state than our temperature-independent Eliashberg functions predict.

\begin{thebibliography}{12}
\bibitem{1} P. Monthoux and D. Pines, Phys. Rev. B \textbf{47}, 6069 (1993).
\bibitem{2} E. Schachinger, J. P. Carbotte, and F. Marsiglio, Phys. Rev. B \textbf{56}, (1997).
\bibitem{3} T. Schneider, H. de Raedt, and M. Frick, Z. Phys. B \textbf{76}, 3 (1989).
\bibitem{4} O. K. Andersen, O. Jepsen, A. I. Liechtenstein, and I. I. Mazin, Phys. Rev. B \textbf{49}, 4145 (1994).
\bibitem{5} T. Dahm, J. Erdmenger, K. Scharnberg, and C. T. Rieck, Phys. Rev. B \textbf{48}, 3896 (1993).
\bibitem{6} A. A. Golubov, Physica C \textbf{156}, 286 (1688).
\bibitem{7} T. Dahm, D. Manske, D. Fay, and L. Tewordt, Phys. Rev. B \textbf{54}, 12006 (1996).
\bibitem{8} S. Y. Savrasov and O. K. Andersen, Phys. Rev. Lett. \textbf{77}, 4430 (1996).
\bibitem{9} A. Bille, Diplomarbeit, Universit"at Hamburg, 1996.
\bibitem{10} F. Marsiglio, M. Schoosmann, and J. P. Carbotte, Phys. Rev. B \textbf{37}, 4965 (1988).
\bibitem{11} S. Hensen, G. M"uller, C. T. Rieck, and K. Scharnberg, Phys. Rev. B \textbf{56}, (1997).
\bibitem{12} P. Monthoux and D. Pines, Phys. Rev. B \textbf{49}, 4261 (1994).
\end{thebibliography}