Solution of the Eliashberg equations for a very strong electron-phonon coupling with a low-energy cutoff

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Abstract. We solve the Eliashberg equations for the case of an explicit \(k\) dependence of the interactions, and of the resulting self-energies \(\Sigma_1(k, \omega), \Sigma_2(k, \omega)\). We consider a strong energy-dependence of the electron-electron scattering-rate \(\tau_{ee}^{-1}\), which is associated with a strong energy-dependence of the electron-phonon matrix element \(g(k, k')\). We characterize this energy-dependence by a cutoff \(\xi_1\), which is of the order of the phonon frequency \(\omega_{ph}\). We find that we can account for a large number of unexpected features of the superconductivity of the cuprates by the BCS electron-phonon theory, if we consider very large values of the McMillian coupling constant \(\lambda_{ph}\), and small values of the cutoff \(\xi_1\). Specifically, the Coulomb interaction is found not to depress \(T_c\); the isotope effect is strongly reduced when \(\xi_1 < \omega_{ph}\). We find solutions in which the gap function \(\Delta(k, \omega)\) has extended s-wave symmetry but is very anisotropic. These large anisotropies are in good agreement with various experiments. We suggest that the underlying cause of the strong energy-dependence is a very small electronic screening parameter at the Fermi surface; the electron-phonon matrix element \(g\) is abnormally large, and this accounts for the high transition temperatures of the cuprates. An order of magnitude estimate suggests that the electron-phonon mechanism can account for transition temperatures up to about 200 K. We thus propose a very-strong-coupling theory, in which the renormalization functions, in particular the energy-renormalization \(X\), depend very strongly on the superconducting gap \(\Delta\), and thus display a very strong temperature-dependence between \(T_c\) and \(T = 0\). An experimental manifestation of the very strong coupling with a small cutoff is a zero bias anomaly sometimes observed in tunneling experiments.

Keywords: Superconductivity; Eliashberg equations; High-\(T_c\), cuprates; Organic superconductors.

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1 Introduction

High-\(T_c\) cuprates, as well as several other systems, are characterized by a very large ionic polarizability of the background non-metallic BaO, \(Y_2O_3\) layers. The ionic dielectric constant at low frequencies is in the range \(\varepsilon_{ion}(\omega) \approx 30-60\) [1]. This dielectric constant is obtained after subtracting the Lindhard-like dielectric polarizability of the conduction electrons. We believe that this huge ionic polarizability plays a key role in the superconducting process, and is the primary factor responsible for the high superconducting transition temperature. The conventional pairing theory of superconductivity is based on the Eliashberg Eqs. [2]. These are based on the Migdal scenario, in which
the interaction depends only on the frequency and not on the electronic momentum $|\vec{k}|$. This is a special case of the more general Nambu formalism [3], in which the interaction, and consequently the self-energies $\Sigma_1(\vec{k},\omega)$ and $\Sigma_2(\vec{k},\omega)$ depend on both the frequency $\omega$ and the energy $\xi(\vec{k})$. In the present work, we consider details of the Eliashberg equations that must be modified in order to take into account the effect of this ionic polarizability, through a strong explicit energy-dependence of the interaction, and show how this gives rise to the high value of $T_c$.

1.1 Reduction of the Thomas-Fermi screening parameter by the ionic polarizability

In “normal” metals, the ionic polarizability is screened-out by the conduction electrons, whose dielectric function is given by $\varepsilon_{el} = 1 + \kappa_T^2/q^2$, with $\kappa_T^2 = 4\pi e^2 n(E_F)$. For values of $q$ of order of $k_F$, $\varepsilon_{el} = 3 - 4$ [4]. This value is larger than $\varepsilon_{ion}$. In the cuprates and several other “exotic” systems, this situation is reversed and $\varepsilon_{ion} \gg \varepsilon_{el}$. This requires us to employ the “dressed” electronic dielectric function. The charge density $\rho$ is given by $\rho = \rho_{ext}/(1 + \chi_{ion})$, where $\chi_{ion} = \chi_{ion} + \chi_{el}/(1 + \chi_{ion})$.

\[
\rho = \frac{\rho_{ext}}{1 + \chi_{ion}}.
\]

Denoting $\rho_{bare} = \rho_{ext}/(1 + \chi_{ion})$, we obtain $\rho = \rho_{bare}/\varepsilon_{el}^{(dressed)}$, and $\varepsilon_{el}^{(dressed)} - 1 = (\varepsilon_{el}^{(bare)} - 1)/\rho_{ion}$. $\rho_{bare}$ is the (ionic) charge density without the screening of the conduction electrons, and division by $\varepsilon_{el}^{(dressed)}$ gives the effect of the screening by the conduction electrons. We describe $\varepsilon_{ion}$ by the standard expression $\varepsilon_{ion}(\omega) = \varepsilon_\infty + (\varepsilon_0 - \varepsilon_\infty) \frac{\omega_i^2}{\omega_i^2 - \omega^2 - i\omega \Gamma}$, where $\omega_i$ is the frequency of the low-frequency transverse phonons, which in the cuprates is about $10 - 20$ meV [5], and $\Gamma$ is the damping.

We illustrate $\varepsilon_{ion}(\omega)$ and $\varepsilon_{el}^{(dressed)}$ in Fig. 1a. At very low frequencies ($\omega < \omega_i$), $\varepsilon_{el}^{(dressed)} = 1 + \kappa_T^2/q^2$, with $\kappa_T^2/\varepsilon_0 = 4\pi e^2 n(E_F) = \kappa_T^2/\varepsilon_0$. This expression is used in conventional semiconductor theory, with $\varepsilon_0$ being the dielectric constant of the background (not necessarily ionic). For the cuprates, where $\varepsilon_0 = 30 - 60$, the dressed Thomas-Fermi screening parameter is $\kappa_T = 0.2 - 0.3 k_F$, i.e. a very small value. This weak screening was pointed out by Eliashberg [6]. In contrast, at higher frequencies

![Fig. 1](image)

(a) Illustration of the behaviour of the dielectric function of the ionic background $\varepsilon_{ion}(\omega)$ and of the dressed electronic dielectric function $\varepsilon_{el}^{(dressed)}$ (and the bare one $\varepsilon_{el}^{(bare)}$ that is shown by a dashed line). (b) Schematic dispersion curves of the “polaritons”. (c) Behaviour of the electron-electron scattering rate $\tau_{ee}^{-1}$ that is parabolic near $\omega_i$ [11] and becomes linear above $\omega_{ph}$ [12].
\[ (\omega > \omega_i, \varepsilon_{\text{el}}^{(\text{dressed})} = \varepsilon_{\text{el}}^{(\text{bare})} = 1 + \kappa_T^2/k_F^2, \text{with } \kappa_T = 1.5 - 2k_F. \] 
Thus we have a drastic reduction of the Thomas-Fermi screening parameter at low energies.

1.2 Effect of the screening on the electron-phonon matrix element

The effect of the screening by the conduction electrons on the electron-phonon matrix element \( I(\mathcal{I} = \langle \psi | \nabla \psi \rangle \psi \) for the free electrons), was first investigated by Bardeen in 1937 [7]. His result can be summarized as \( I^{(\text{screened})} = I^{(\text{bare})}/\varepsilon_{\text{el}}(q) \) with \( q = k_F \). \( I^{(\text{bare})} \) is the matrix element calculated assuming that the conduction electron gas is rigid, and \( I^{(\text{screened})} \) includes the effect of screening by the conduction electrons. Thus, \( I^{(\text{screened})} \approx I^{(\text{bare})}/(1 + \kappa_T^2/k_F^2) \approx (1/3)I^{(\text{bare})} \). The McMillan coupling constant \( \lambda \) is proportional to \( I^2 \), thus, \( \lambda^{(\text{screened}}) \approx (1/10)\lambda^{(\text{bare})} \). This calculation was carried out for monovalent metals, alkalies and noble metals, and the agreement with experiment was found to be excellent.

In our case, we must use the dressed electronic dielectric function. We assume here that the frequency \( \omega \) can be replaced by the energy-transfer \( \tilde{\xi}(\tilde{k}) - \tilde{\xi}(\tilde{k}^\prime) \). Thus for very small energy transfers, \( \tilde{\kappa}_{TF}/k_F^2 \ll 1 \) and therefore \( I^{(\text{screened})} \approx I^{(\text{bare})} \), which is very large; about 3 - 4 times larger than the value that we get assuming the conventional, "bare" electronic dielectric constant. At large energy transfers, \( \varepsilon_{\text{el}}^{(\text{dressed})} \) is large, and consequently \( I^{(\text{screened})} \) is small. In the present work, we assume for simplicity that \( I^{(\text{screened})} = 0 \) for high energy transfers. This assumption is not essential, and our results do not change significantly if we take \( I^{(\text{screened})} \approx (1/3)I^{(\text{bare})} \) for large energy transfers. The crossover is at an energy transfer \( \tilde{\xi}(\tilde{k}) - \tilde{\xi}(\tilde{k}^\prime) = \xi_i \) which is of order \( \omega_i \), the frequency characterizing the dispersion of the background dielectric constant, i.e. \( 10 - 20 \text{ meV} \) in the cuprates.

The assumption that the frequency \( \omega \) can be replaced by the energy \( \tilde{\xi}(\tilde{k}) \) is far from obvious. Along the physical line \( \omega = \xi(\tilde{k}) + \Sigma(\tilde{k}, \omega) \) the difference between \( \omega \) and \( \xi(\tilde{k}) \) is not very large, but the Green's function formalism requires a description of the functional dependence of \( I \) in the whole \( \omega, \xi(\tilde{k}) \) domain. There are some indications supporting this assumption [8, 9]. Abrikosov also considers a situation of weak electronic screening, with an electron-phonon coupling that depends on the electronic momentum, rather than on the frequency [10]. At the present stage, we make this assumption without a rigorous proof.

1.3 Energy dependence of the electron-electron scattering rate

In a highly-polarizable crystal, we illustrate the conventional ("polariton") dispersion curves in Fig. 1b. For low values of \( \omega \) and \( q = k - k^\prime \) the dispersion is given by \( \omega = cq/\varepsilon_0 \), while at high energies it is given by \( \omega = cq/\varepsilon_\infty \). In the cuprates, the ratio \( \varepsilon_0/\varepsilon_\infty \) is enormously large. Therefore the electron-electron interaction for states close to the FS \( e_\infty^2/\varepsilon_0 r \) is extremely weak, while for states removed from the FS by about \( \omega_i \) (\( \approx 60 - 80 \text{ meV} \)) or more, it is given by \( e_\infty^2/\varepsilon_\infty r \), which is very strong.

In the Fermi liquid theory, the electron-electron scattering rate is given by \( \tau_{ee}^{-1} = (\pi^2/3/128)\rho_0[\xi(\tilde{k})/E_F]^2 \) [11]. As described there, this expression is derived for the case when \( r_s < 1 \). Therefore application of this estimate for the cuprates requires extreme caution. Ruvalds and Virosztek [12] estimated the value of \( \tau_{ee}^{-1} \) expected from Fermi liquid theory in the cuprates, and their estimate is \( \tau_{ee}^{-1} \approx 10 \text{ meV} \) at
\( \xi (k) = 150 \text{ meV} \). Such an estimate is close to what the above expression yields for parameters characteristic of the cuprates. Empirically, \( \tau_{ee}^{-1} \approx 0.7 \xi (k) \) for \( \xi (k) \gtrsim 50 \text{ meV} \). Ruvalds and Virosztek account for the discrepancy between this value and the value derived from Fermi liquid theory by the nesting of the Fermi surface. However, we should note that the discrepancy is not very large, considering the uncertainties and particularly the large value of \( r_s = 2e^2/\epsilon_0 \hbar v_F \approx 8-10 \) at this energy range. At still higher energies, the Fermi-liquid relationship \( \tau_{ee}^{-1} \propto \xi (k)^2 \) cannot be expected to apply when the value of \( \tau_{ee}^{-1} \) that it predicts exceeds the value of \( \xi (k) \). Thus, for values of \( \xi (k) \gtrsim 50 \text{ meV} \), we adopt the empirical expression \( \tau_{ee}^{-1} \approx 0.7 \xi (k) \) without being concerned by its theoretical justification.

At very low energies, namely \( \xi (k) \lesssim 10 \text{ meV} \), the situation is entirely different. There the electron-electron interaction is weak, being screened-out by the large value of \( \epsilon_0 \) (Fig. 1 b). The large value of \( \epsilon_0 \) also makes the values of \( r_s = 2e^2/\epsilon_0 \hbar v_F \) extremely small (much less than 1), thus providing much more validity to the Fermi-liquid expression. Incorporating the value of \( \epsilon_0 \), the value of \( \tau_{ee}^{-1} \) is extremely small (less than 0.1 meV); therefore we can assume that \( \tau_{ee}^{-1} = 0 \) in the low-energy region. The behaviour of \( \tau_{ee}^{-1} (\xi_k) \) is illustrated in Fig. 1 c.

In the Eliashberg equations, the contributions to the gap \( \Delta \) come mainly from the regions where the electron-phonon coupling is strong (regions of low energies). We just saw that \( \tau_{ee}^{-1} \) is very small in such regions, therefore we shall neglect it.

Fig. 1 c also illustrates the relationship with the Landau Fermi liquid theory. Anderson [13] describes FLT as a situation of renormalizing-away interactions and states down to a very low, but finite, energy, below which the quasiparticles can be described by an effective mass, an inverse lifetime smaller than the excitation energy, and other parameters that no longer depend on energy. We here associate this low energy with \( \omega_f \). Thus at energies above about 10 meV, it is no longer possible to use FLT with fixed parameters \( F_0^s, F_0^q, F_s^s, F_s^q \), etc. And, since the superconducting gap \( 2 \Delta \) is about 40 meV, the theory of the superconductivity must also be modified. We suggest that most of the contribution to the superconducting condensation energy comes from the low-energy region (i.e. up to about 20 meV), where FLT is in principle valid.

1.4 Approximations applicable to the low-energy domain

The phonon spectrum of the cuprates is very broad. At the low end, are the optical modes with \( \omega_i \approx 10-20 \text{ meV} \), which dominate the dispersion of the dielectric constant of the background, and are responsible for the very large value of \( \epsilon_0 \). In the middle of the range, \( \omega_{ph} \approx 35-50 \text{ meV} \), are the Cu-O breathing modes that may provide most of superconducting pairing; Vedeneev et al. [14] propose from tunneling measurements on YBCO an \( \alpha^2(\omega)F(\omega) \) curve peaking in this range. In BiSCCO, a strong structure is seen by tunneling around 50 meV [15, 16] but the authors of the measurements do not claim that this structure is a McMillan-Rowell structure due to phonons, although no alternative is proposed. In the high end, \( \omega_i \approx 80 \text{ meV} \), there are phonons that possess a large density of states \( F(\omega) \), but there is no indication from tunneling measurements that their coupling with the conduction electrons possesses a large value of \( \alpha^2(\omega) \). The large ratio \( \omega_i/\omega_i \) makes it possible to have the large value of \( \epsilon_0 \), since by the Lyddane-Sachs-Teller relation, \( \epsilon_0/\epsilon_\omega < (\omega_i/\omega_i)^2 \approx 16 - 64 \).

In this work, we treat the low-frequency phonons \( \omega_i \) in a different way from the medium-frequency ones \( \omega_{ph} \). The low-frequency phonons are considered through
their effect on the dielectric constant, giving rise to the very large value of $\varepsilon_0$ and a strong dispersion at frequency $\omega_r$. Their contribution to the superconducting pairing does not appear to be very important, possibly because of their low frequency. The medium-frequency phonons that are mostly responsible for the pairing are treated by the Nambu-Eliashberg formalism.

Here, we are concerned with the value of the transition temperature $T_c$ and with the behaviour of the gap function $\Delta$, renormalization functions $Z$ and $X$, excitation energy $E$ and density-of-states $n_{qp}$ of the quasiparticles at low energies, i.e. energies less than $\omega_{ph} (\approx 35 - 50 \text{ meV})$ and in particular, near and below $\omega_i \approx 10 - 20 \text{ meV}$. Our approximations depend on this low-energy restriction. The electron-phonon coupling constant $g = \sqrt{\hbar/M \omega_{ph}}$ drops at energy transfers in excess of $\omega_i (\approx 10 - 20 \text{ meV})$ and is thus not very large at high energies. To simplify the calculation, we set it at zero at these energies. This does not have a large effect on the low-energy behaviour. This approximation causes the electron-phonon scattering rate (due to the medium-frequency phonons that possess the large electron-phonon coupling) to vanish as well. Furthermore, as we already said above, we can neglect the electron-electron scattering rate at these low energies. Therefore $E$ is real. The explicit $\omega$-dependence of $\Phi = Z \Delta$, $Z$ and $X$ is very weak for $\omega \ll \omega_{ph}$, therefore we approximate $\omega$ by the lowest Matsubara frequency $\omega_n = 0$. Since the scattering rate of the quasiparticles at these low energies is negligible, their density-of-states is given by the inverse of the dispersion relation of the quasiparticle energy $n_{qp} \propto |dE/d\xi|^\lambda$. When $\xi_i \ll \omega_{ph}$, the $\omega$-dependence can be integrated-out and we obtain a gap equation depending only on the energy $\xi_k$ [17] with a real gap $\Delta(\xi_k)$ and renormalization $X(\xi_k)$.

These approximations are no longer justified at higher energies (i.e. in excess of $\omega_{ph}$). The solution of the generalized Eliashberg equations in the high-energy region will be dealt with in a subsequent publication.

2 Model

We consider an electron-phonon coupling $g(\kappa, \kappa')$ that depends only on two components of the electronic momentum $\kappa = (k, q)$ where $k$ is the component perpendicular to the FS and $q$ is the one parallel to the FS (see Fig. 4a). Like in Ref. [18], we omit the dependence of $g$ on the phononic momentum. We use two types of simplified dependence:

$$g(\kappa, \kappa') = \begin{cases} g_0(q, q') & \text{if } |\xi_k|, |\xi_{k'}| < \xi_1(q, q') \\ 0 & \text{otherwise} \end{cases}$$  \hspace{1cm} (1)

(“Cooper” form) and

$$g(\kappa, \kappa') = \begin{cases} g_0(q, q') & \text{if } |\xi_k - \xi_{k'}| < \xi_1(q, q') \\ 0 & \text{otherwise} \end{cases}$$  \hspace{1cm} (2)

(“strip” form).
We solve the Eliashberg equations on a discrete mesh [19, 2]:

\[
(X(\kappa, \omega_n) - 1) \xi_k = T \sum_{n'} \int d^2 \kappa' \frac{N(\kappa') (V(\kappa, \kappa') - D(\kappa, \kappa', \omega_n - \omega_{n'})) X(\kappa', \omega_{n'}) \xi_{k'}}{\Omega}
\]

\[
(Z(\kappa, \omega_n) - 1) \omega_n = -T \sum_{n'} \int d^2 \kappa' \frac{N(\kappa') (V(\kappa, \kappa') - D(\kappa, \kappa', \omega_n - \omega_{n'})) Z(\kappa', \omega_{n'}) \omega_{n'}}{\Omega}
\]

\[
\Phi(\kappa, \omega_n) = -T \sum_{n'} \int d^2 \kappa' \frac{N(\kappa') (V(\kappa, \kappa') - D(\kappa, \kappa', \omega_n - \omega_{n'})) \Phi(\kappa', \omega_{n'})}{\Omega}
\]

\[
\Omega = (Z(\kappa', \omega_{n'}) \omega_{n'})^2 + (X(\kappa', \omega_{n'}) \xi_{k'})^2 + \Phi(\kappa', \omega_{n'})^2
\] (3)

where:

\[
\omega_n = \pi (2n + 1) T
\]

\[
D(\kappa, \kappa', \omega_n - \omega_{n'}) = g(\kappa, \kappa')^2 \frac{2\omega_{ph}}{(\omega_n - \omega_{n'})^2 + \omega_{ph}^2}
\] (4)

(i.e. we consider for simplicity an Einstein spectrum)

\[
V(\kappa, \kappa') N(0) = \begin{cases} 
\mu(q, q') & \text{if } |\xi_k - \xi_{k'}| < \xi_2(q, q') \\
0 & \text{otherwise}
\end{cases}
\] (5)

We consider a constant density-of-states (DOS) \( N(\xi) = N(0) \), \( \mu = N(0) V_0 \), \( \lambda_{ph} = 2 g_0^2 N(0)/\omega_{ph} \). The renormalization functions are defined by:

\[
(X(\kappa, \omega) - 1) \xi_k = \frac{1}{2} (\Sigma_1(\kappa, \omega) + \Sigma_1(\kappa, -\omega))
\] (6)

\[
(Z(\kappa, \omega) - 1) \omega = -\frac{1}{2} (\Sigma_1(\kappa, \omega) - \Sigma_1(\kappa, -\omega))
\] (7)

where \( \Sigma_1 \) is the normal self-energy of the electrons. (Because of the strong \( k \)-dependence at low energies, it is necessary to employ a strong-coupling scenario for the renormalization function \( X \) [17]). The superconducting gap-function is given by:

\[
\Delta(\kappa, \omega) = \frac{\Phi(\kappa, \omega)}{Z(\kappa, \omega)}
\] (8)

We choose a low, yet non vanishing temperature.

In order to calculate the excitation energy, we have to find the poles of the electronic Green function, i.e. we have to solve the equation \( \Omega(\omega, \kappa) = 0 \) for \( \omega \), where \( \omega \) is extended analytically in the complex plane; \( \omega \) turns out the be near the real axis. This equation has to be solved self-consistently. Since we consider energies small compared with \( \omega_{ph} \), we approximate:

\[
\omega \approx E \equiv \sqrt{\Phi(\kappa, \omega_{n=0})^2 + (X(\kappa, \omega_{n=0}) \xi_k)^2/Z(\kappa, \omega_{n=0})}
\] (9)
for small $\xi, \omega$. This approximation is not generally employed in conventional strong-coupling theory [20] since it ignores the finite lifetime of the quasiparticles (i.e. the imaginary components of $Z$ and $\Phi$ for $\omega$ along the real axis), and since, for strong coupling, $\Phi$ and $Z$ change with $\omega$ even for $\omega < \omega_{ph}$. Nevertheless, in the present case, this approximation is justified for the following reasons. First, at very low energies, the electron-electron scattering rate $\tau_{ee}^{-1}$ is very weak. Furthermore, the electron-phonon scattering rate that gives rise to the imaginary components of $Z$ and $\Phi$ (for $\omega$ along the real axis) is also very weak, in spite of the large value of $\lambda$, because the cutoff prevents the real processes for which $\xi(k) - \xi(k') = \omega_{ph}$. Secondly, the variation of Re($Z$) and Re($\Phi$) at low frequencies ($\omega < \omega_{ph}/2$) is not very large, even for strong coupling. In Pb, where $\omega_{ph} \approx 4$ meV, at frequencies up to 2 meV, Re($Z$) changes by about 12%, and Re($\Phi$) by about 25%, thus the change in Re($\Delta$) is only of about 12% [20]. While these changes are very large in comparison with the results of the weak-coupling theory (where $\Phi$ and $Z$ do not change at all), they are within the accuracy expected for our simple model. The value of $Z(\xi_k = 0, \omega_n = 0)$ which is a measure of the effective strength of the coupling, is not very different in our solutions from that of Pb ($Z(\xi_k = 0, \omega_n = 0) \approx 2.5 - 3$).

3 Results

3.1 Isotropic case

We first turn out attention towards the simpler case of isotropic solutions where we only consider one FS piece (i.e. $\kappa = k$).

In Fig. 2, we present the solutions for several values of the parameters. (The number of frequencies $\omega_n$ over which the sums in Eq. (3) run is chosen such that the maximum frequency $\omega_n$ is approximately 6 $\omega_{ph}$; the number of $k$-points used to perform the integration over $\xi_k$ is 101 throughout this paper.) Strip form, $\lambda_{ph} = 5$, $\mu = 2$, $\xi_1 = \omega_{ph}$, $\xi_2 = 6 \omega_{ph}$ (Fig. 2a). Strip form, $\lambda_{ph} = 10$, $\mu = 3$, $\xi_1 = 0.4 \omega_{ph}$, $\xi_2 = 2 \omega_{ph}$ (Fig. 2b). Note the large value of the gap at the FS; $\Delta(0) = 0.56 \omega_{ph}$ (Fig. 2b). The zero of the gap function is very close to the FS. The minimum excitation energy is 0.18 $\omega_{ph}$, i.e. 3 times smaller than $\Delta(0)$. The value of $Z(0) \approx 2$ is surprisingly small for this value of $\lambda_{ph}$. Note also the complex form of the renormalization function $X$. Cooper form, $\lambda_{ph} = 10$, $\mu = 1$, $\xi_1 = 0.2 \omega_{ph}$, $\xi_2 = E_F$ (Fig. 2c). Cooper form, $\lambda_{ph} = 15$, $\mu = 2$, $\xi_1 = 0.2 \omega_{ph}$, $\xi_2 = 1.2 \omega_{ph}$ (Fig. 2d). The values of $\Delta(0)$ are comparable to the values found for the strip form, but the minimum away from the FS is not so deep (Fig. 2c) or absent altogether (Fig. 2d).

In Fig. 3, we plot the quasiparticle DOS for the parameters of Fig. 2b (Fig. 3a) and Fig. 2c (Fig. 3b). Because of the smallness of the inverse lifetimes $\tau_{ee}^{-1}$ and $\tau_{e-ph}^{-1}$ at low energies, the DOS is given by the inverse dispersion $|dE/d\xi|^2$. At energies of about $\omega_{ph}$ or higher, this approximation is no longer applicable, but we see that the quasiparticle DOS does not have a structure there, thus we do not have to be concerned about broadening of peaks by the inverse lifetime of the high-energy region. We clearly see the very large, sharp maximum corresponding to the local maximum of $\Delta(0)$ at the FS, and the cutoff at the lower energy that we denote $\delta(0)$. $\delta(0)$ is the true thermodynamic gap; $\Delta(0)$ is a maximum of the tunneling conductivity but not a true thermodynamic gap. If we (loosely) call $\Delta(0)$ a "gap", then there are states in the "gap" down to quite low energies. We call $\delta(0)$ the zero bias anomaly (ZBA).
Fig. 2  Solutions of the Eliashberg equations for (a) Strip form, $\lambda_{ph} = 5$, $\mu = 2$, $\xi_1 = 0.4 \omega_{ph}$, $\xi_2 = 6 \omega_{ph}$, (b) Strip form, $\lambda_{ph} = 10$, $\mu = 3$, $\xi_1 = 0.4 \omega_{ph}$, $\xi_2 = 2 \omega_{ph}$, (c) Cooper form, $\lambda_{ph} = 10$, $\mu = 1$, $\xi_1 = 0.2 \omega_{ph}$, $\xi_2 = \infty$. (d) Cooper form, $\lambda_{ph} = 15$, $\mu = 2$, $\xi_1 = 0.2 \omega_{ph}$, $\xi_2 = 1.2 \omega_{ph}$. The energies are in units of $\omega_{ph}$. These functions are taken at $\omega_n = 0$ (e.g. $\Phi(\xi,\omega_n)|_{\omega_n = 0}$ is plotted).

The ZBA corresponds to a very small value of $\delta k = k - k_F$, $\delta k/k_F = \delta^{(0)}/E_F \approx 10^{-4} \omega_{ph}/E_F$, i.e. less than 1%. The ZBA is a clear manifestation of the very small cutoff $\xi_1$, associated with the very large value of $\lambda_{ph}$.

3.2 Anisotropic case

In this work, and the preceding one [18], we considered an isotropic Fermi surface for simplicity. We consider in this section an anisotropic model that may bear some relevance to the FS of the (CuO$_2$)$_n$ planes in YBCO. We consider a square with circular corners (Fig. 4a). On the planar sections, the x-y component of the Fermi velocity $v_F$ (plane) is high (the band velocity is about $4 \cdot 10^7$ cm/s), while on the circular corners, $v_F$ (corner) is considerably lower, because of the proximity of the Van Hove singularity [21]. The low $v_F$ (corner) causes the elastic scattering rate $\tau_{el}^{-1}$ to be large there, while on the planar sections it is much smaller. This assumes that due to the weak screening ($\kappa_{T_F} \approx 5$ Å), the scattering by defects, such as oxygen vacancies and interstitials, etc., is predominantly forward with only a small $q$-change. A large $\tau_{el}^{-1}$ smears out the momentum somewhat, and the cutoff $\xi_1$ cannot be smaller than $\tau_{el}^{-1}$. Thus, $\xi_1$ on the corners must be much larger than on the planar sections. In order to illustrate this, we modelize the FS shown in Fig. 4a with 2 FS pieces, the first ($q = 1$) standing for the “plane” and the second ($q = 2$) for the “corner”. Since we only have two FS pieces, we use a matrix notation to represent functions of $(q,q')$. The diagonal terms, representing the coupling in each FS piece, are chosen such that the parameters for the
Fig. 3. The quasiparticle DOS (calculated as $|\delta E/\delta \xi_k|^{-1}$) for the parameters of (a) Fig. 2b and (b) Fig. 2c (energies are in units of $\omega_{ph}$).

"plane" are the same as those of Fig. 2b and the parameters for the "corner" only differ from the latter by $\lambda_{ph} (2,2) = 5$ and $\xi (2,2) = 2\omega_{ph}$. The non-diagonal terms, that represent the coupling between the 2 pieces, are chosen small (the parameters are given in detail with Fig. 4b). Fig. 4b shows the solution of Eliashberg equations for the set of parameters described above, and Fig. 4c shows the DOS and the energy of the quasiparticles. We see that the gap parameter $\Phi$ is not so peaked for $q = 2$ and that the minimum of the quasiparticles energy occurs at the FS.

Some support for this model comes from the ARPES data of Shen et al. and Dessau et al. [21]; for the planes, since only a very small number of $k$-states in the immediate neighborhood of the FS have a large gap $\Delta (k, \omega)$, the overall shift of the ARPES spectrum is small, as observed. This explanation accounts also for the results of Chaudhari and Lin [22], who find a nearly isotropic gap from Josephson tunneling; the maximum Josephson current being proportional to $\Delta(0)$. Admittedly, many alternative explanations for this experimental behaviour are possible. Note that for a value of $k$ somewhat removed from the FS, the gap function changes sign between the corner and plane (i.e. there are 8 nodes), but the symmetry of the structure is not broken (hence it is not a $d$-wave). Such a model requires that the electron-phonon scattering is also pre-
Fig. 4 (a) Fermi surface model. (b) The solution of the Eliashberg equations for a potential coupling 2 FS pieces with strip form in $k, k'$. The parameters are (the matrix elements refer to the $(q, q')$ part of function of type $f(k, k')$, the $(k, k')$ part being defined through Eq. 1, 2, and 5):

$$
\lambda_{ph} = \begin{pmatrix} 10 & 5 \\ 0.5 & 5 \end{pmatrix}, \quad \xi_1 = \begin{pmatrix} 0.4 & \infty \\ \infty & 2 \end{pmatrix}, \quad \mu = \begin{pmatrix} 3 & 0.5 \\ 0.5 & 3 \end{pmatrix}, \quad \xi_2 = \begin{pmatrix} 2 \\ 2 \end{pmatrix}.
$$

(c) Energy (solid line for $q = 1$, dashed line for $q = 2$), and DOS of the quasiparticles (the DOS is calculated as $1/|\nabla_x E|$). The energies are in units of $\omega_{ph}$. 
dominantly forward (i.e. not from plane to corner), which is to be expected for a long-range electron-phonon coupling. Such a long-range interaction is expected to give rise to a very large value of $\lambda_{ph}$; thus this model is (at least) self consistent.

The coupling between the planes and chains further complicated the situation. If we assume for simplicity that the gap function of the chains does not change sign and is coupled to the gap function (of the planes) portrayed in Fig. 2b, then its sign may be either positive or negative, depending on the parameters involved. Thus, $\Delta(0)$ on the chains may have an opposite sign to $\Delta(0)$ on the planes. This may be one way to account for the SQUID experiment of Wollman et al. [23], where the sign of $\Delta(0)$ on $ac$ and $bc$ faces of YBCO seems to be opposite; one type of faces may be dominated by the chains, and the second by the planes, as suggested by Kresin [24]. Obviously, this is not the simplest way to account for this experiment. This section illustrates the richness of solutions of the Eliashberg equations when a $|k|$-dependent electron-phonon coupling is allowed. A study of the possibilities of anisotropic gap functions, and in particular of solutions with $d$-wave pairing, is published separately [25].

4 Discussion

4.1 Experimental manifestations of the ZBA

We find very sharp peaks in the quasiparticle DOS at low energies ($E = \Delta(0,0) < \frac{1}{2} \omega_{ph}$). These peaks are not expected to be sharp in “conventional” strong coupling theory, and the sharpness is a result of our small cutoff in $g$. Experimentally, sharp peaks in the tunneling conductivity are usually observed [15, 16, 26]. In order to account for the sharpness of the peaks with conventional theory, one sometimes postulates very sharp van Hove peaks [27]. We suggest here an alternative interpretation.

Another very sharp feature of our solutions is the sharp peak in the quasiparticle DOS at very low energies (Fig. 3), which we denote “Zero Bias Anomaly” (ZBA). A very strong ZBA in YBCO at an energy of 4 meV was reported by Gurvitch et al. [28], and its magnetic field behaviour studied by Lesueur et al. [29]. Point-contact spectroscopy (PCS) data of Srikanth & Raychaudhuri [30] also indicate a structure at 5 meV for an YBCO-Au contact. Indications of such a structure were also seen by Hass et al. [31]. A strong ZBA in the organic superconductor ET was also reported [26] and its magnetic field dependence studied [32]. In many other systems ZBA’s were reported, however they seem to be regarded as spurious phenomena, and attempts are made to change the experimental conditions so that they disappear. This usually works, and the ZBA can be eliminated. In particular, no ZBA has been reported (to our knowledge) for measurements carried out by tunneling with an STM; for example in YBCO by Edwards et al. [33], in ET by Bando et al. [34], and in BiSCO by Renner et al. [16, 27]. Therefore the first question is whether the ZBA is genuine, or just a spurious effect. The present work shows that observation of the ZBA (assuming that it is due to the mechanism presented here) requires a momentum resolution of better than 1% (of $k_F$), thus a junction of large dimensions. Therefore, the failure to observe the ZBA by STM is not surprising. Also, the PCS contacts of Srikanth & Raychaudhuri [30] possess a very low resistance ($\sim 7 \Omega$), indicating a large contact area; the PCS contacts of Hass et al. [31] possess a much higher resistance ($\sim 100 \Omega$).
and thus a much smaller contact area. The PCS contacts of ET have an extremely low resistance (less than 1 Ω) [26], and therefore the contact area is undoubtedly large.

Also, the discussion of section 3.2 shows that the ZBA should be washed out when the elastic mean-free-path becomes small. This can also occur in many "good" junctions. For an experimentalist, observation of a tunneling structure corresponding to Fig. 4b (q = 2) may appear "clean", while a structure corresponding to Fig. 2b may appear "dirty", i.e. essentially like a zero-gap structure that occurs when magnetic impurities smear-out the gap. Therefore, experimentalists may look for conditions in which the ZBA does not show up, and as we show here, such conditions are easy to fulfil.

Therefore, we believe at the present stage that the ZBA observed in YBCO and ET is a genuine property.

When a ZBA is present, it should manifest itself in "non BCS" behaviour of various properties, namely the temperature dependences of the London penetration depth $\lambda_L(T)$, the NMR relaxation rate $T_1^{-1}$, the microwave surface impedance $Z_{es}$, etc. At temperatures not significantly below $\delta^{(0)}$, the temperature dependence of these quantities should follow a power law, rather than the BCS exponential dependence $\exp(-\Delta/T)$. Only at very low temperatures should the exponential dependence $\exp(-\delta^{(0)}/T)$ show up. Such power-law dependences are indeed frequently observed in the cuprates [35] as well as in organic [36] superconductors. However, other experimentalists observe a BCS behaviour in the same materials [37, 38]. Since it is easy to establish conditions in which the ZBA is eliminated (without a significant change in $T_c$), for example by slightly reducing the elastic mean-free-path, it is possible that both sets of experiments are correct. This is not the case for the $s$-wave vs. $d$-wave pairing controversy.

4.2 Electron-phonon coupling, screening and $T_c$

The transition temperature of the cuprates is nearly an order-of-magnitude higher than that of normal superconductors. This suggests that a simple, transparent, physical reason is the cause of the high $T_c$. We suggest that within the standard, BCS electron-phonon mechanism, this simple reason is the fact that the screening close to the FS is ionic rather than electronic, and consequently the electron-phonon matrix element is much larger [40, 39].

In conventional metals, where the screening is electronic, we can make a rough estimate of the maximum $T_c$ as follows: Under conditions of strong coupling, $T_c = 0.18 \omega_{ph} \sqrt{\lambda_{ph}}$, with $\lambda_{ph} = \frac{I^2 n(E_F)/M}{\omega_{ph}^2}$, thus $(T_c)_{max} \approx 0.18 I \sqrt{n(E_F)/M}$. We then see that $\omega_{ph}$ drops out of the expression for $T_c$. The density-of-states is given roughly by: $n(E_F) \approx \rho/E_F$, where $\rho$ is the degeneracy, i.e. 5 for $d$-electrons. The matrix element $I$ is given approximately by: $I = I^{(\text{bare})}/[1 + (\kappa_{TF}/k_F)^2]$, where $I^{(\text{bare})}$ is the rigid-ion (i.e. unscreened) matrix element, and $\kappa_{TF}$ is the Thomas-Fermi screening parameter. Normally, $\kappa_{TF}/k_F > 1$, and $I^{(\text{bare})} = r_s k_F E_F$, where $r_s$ is the average distance between electrons in units of the Bohr radius $a_0$; $r_s = 2/k_F a_0$. Thus, since $(\kappa_{TF}/k_F)^2 \approx r_s$, the matrix element is given by $I \approx k_F E_F$. Explicit calculations by Bardeen on monovalent metals in 1937 [7] show that this estimate is indeed very good. Thus, $(T_c)_{max} \approx 0.18 k_F E_F \sqrt{\rho/E_F M}$. We define an effective electronic mass $m^*$ by: $E_F = k_F^2/2m^*$. Thus, we have $(T_c)_{max} \approx 0.25 E_F \sqrt{\rho m^*/M}$.
For niobium compounds, if we take $E_F = 2 \text{ eV}$, $m^* \approx 2m_0$, $\rho = 5$, we obtain $(T_c)_{\text{max}} \approx 30 \text{ K}$. Note that for Nb$_2$Ge, $T_c \approx 22 \text{ K}$ and McMillan [41] also estimated $(T_c)_{\text{max}} \approx 30 \text{ K}$ for niobium compounds.

Note that Van-Hove peaks of the density-of-states near $E_F$ [42], as well as a strongly anisotropic gap [19], increase the value of $T_c$ above this estimate, while the Coulomb repulsion $\mu^*$ decreases it. Thus these two factors partially compensate each other, and therefore this crude estimate is somewhat better than one may expect. Still, it apparently overestimates $(T_c)_{\text{max}}$ of conventional superconductors somewhat, probably because of the large effect of the Coulomb, and possibly spin-fluctuation interactions.

For the cuprates, taking $p = 1$ (only $p\sigma$ orbitals), and similar values of $E_F$ and $m^*$, we obtain $(T_c)_{\text{max}} \approx 40 \text{ K}$. This is close to the result obtained by Weber [43].

The ionic dielectric function $\varepsilon_{\text{ionic}}(\omega)$ is big for small frequencies $\omega$ and small for big $\omega$ [1]. The crossover is given approximately by $\omega_{\text{ph}}$. Since $\kappa^2_{TF} = 4\pi e^2 n(E_F)/\varepsilon_{\text{ionic}}(\omega)$ and the electronic dielectric function $\varepsilon_{\text{el}}(q) = 1 + \kappa^2_{TF}/q^2$, we immediately see that $\varepsilon_{\text{el}}$ is small for small $\omega$ and vice versa. As we saw above, the electron-phonon matrix element $I$ can be approximated by $I = I_{\text{screened}} \approx I_{(\text{bare})}/[1 + (\kappa_{TF}/k_F)^2]$. We see that $I_{\text{screened}}$ is big for small $\omega$ and small for big $\omega$. Furthermore, we can link the frequency $\omega$ to the electronic momentum. The cutoff $\xi_1$ is thus of order $\omega_{\text{ph}}$. We now see that in the vicinity of the FS, $I \approx I_{(\text{bare})} \approx r_s k_F E_F$. For reasonable values of $\xi_1$ (i.e., $\xi_1 \approx \omega_{\text{ph}}/2$), $\Delta(0)$, and thus $T_c$, are reduced by about a factor of 2 (Fig. 1 of [18]). Thus,

$$(T_c)_{\text{max}} \approx 0.25 E_F \sqrt{p m^*/M}(r_s/2), \quad (10a)$$

where $r_s$ is given by: $r_s = 1.92 \frac{e^2}{\varepsilon_{\infty} \hbar \nu_F}$. For YBCO, the isotropic band-structure velocity is given approximately by: $\nu_F \approx 2.7 \cdot 10^7 \text{ cm/s}$ [44]. $\varepsilon_{\infty}$ is the dielectric constant of the background at a frequency somewhat higher than the phonon frequency (i.e., at about 0.1 eV). At a frequency of $3 - 4 \text{ eV}$, $\varepsilon_{\infty} \approx 4$ [45]; but at this high frequency, internal electronic oscillations increase the dielectric constant (the midband structure). At lower energies (i.e., a few tenths of an eV), the proximity of the plasma frequency of the conduction electrons obscures the background dielectric constant. In insulating cuprates, $\varepsilon_{\infty} \approx 1.5 - 2$ [1] in this frequency range; thus $r_s \approx 8 - 10$, and $(T_c)_{\text{max}}$ is 4 - 5 times larger than for "conventional" metals, i.e., about 160 - 200 K. We can rewrite Eq. (10a) as:

$$(T_c)_{\text{max}} \approx 0.12 \left( \frac{e^2}{\varepsilon_{\infty}} \right) k_F \sqrt{p m^*/M} \quad (10b)$$

More recently, the electron-phonon matrix element $I$ is calculated from Local Density Approximation (LDA) theory [40]. When screening is complete as in self-consistent calculations one obtains moderately high values for $n(E_F) I^2$ for phonon modes involving displacements in the $x$-direction. For instance, in YBCO $\lambda_{ph}$ is about 1 for movements of apical oxygens and about 3 for movements of Ba ($\lambda_{ph}$ is the contribution to $\lambda_{ph}$ from the $i$th phonon mode). This applies for an assumed value of the force constant $M\omega_{ph}^2$ of 5 eV/Å$^2$. The reason for these rather large $\lambda_{ph}$-values is the large ionicity in combination with geometrical details of movements perpendicular to the
layers, which together induce large shifts to the Madelung potential. It leads to a strong monopole coupling, in contrast to the weaker dipole coupling of the Rigid Muffin-Tin Approximation (RMTA) in these materials. Screened calculations by another group also yield rather small values for $I$ when several phonon modes are considered [46].

However, YBCO is an unusual member of the high-$T_c$ family, since it has a CuO chain structure in addition to the CuO-planes. This gives an additional Fermi-Surface piece, the “ridge”, which contributes to the DOS at $E_F$ so $n(E_F)$ is high, about 6 states/cell/eV. Here we calculate $n(E_F)I^2$ for the HgBa$_2$CuO$_4$ compound, which is more typical since it has no chains and no FS-ridge, and therefore $n(E_F)$ is lower, 0.9 states/cell/eV (both spins) [47]. We consider two displacements; one of the O(2)-sites (the oxygens between Hg and Cu) and one of the Ba-sites, both in the $z$-direction. Fully screened calculations give $n(E_F)I^2 = 0.6$ eV/$\AA^2$ for O(2) and $\approx 5.5$ eV/$\AA^2$ for Ba. For $M\omega^2 \approx 3$ eV/$\AA^2$ this gives $\lambda_{ph} = 0.2$ and 1.8, respectively for the two phonon movements. These values tend to increase when the atoms (O(2) or Ba) are approaching the CuO planes. The decreased values compared to YBCO are to a large extent explained by the decrease of $n(E_F)$ in HgBa$_2$CuO$_4$. As for YBCO we also calculate $\lambda_{ph}$ in the extreme case of no screening. This is done by calculating $I^2$ directly from the Madelung shifts that are induced when the atoms move to new positions [40]. This gives $n(E_F)I^2 \approx 7$ and $\approx 60$ eV/$\AA^2$ for O(2) and Ba, respectively. This is seen to be an order of magnitude larger than for the screened case. As discussed earlier for YBCO, it is high frequency phonons involving light atoms as oxygens, that are likely to be weakly screened, but it is worth noting that $\lambda_{ph}$ for low frequency Ba movements is high even when the screening is complete.

Another way to estimate the screening is to relate the screening parameter $\kappa_{TF}$ to the dielectric constant: $\kappa_{TF}^2 = 4\pi e^2n(E_F)/\varepsilon_0$ is found to be very small, because of the very large value of $\varepsilon_0$ (about 26–50 in YBCO [1]). In HgBa$_2$CuO$_4$, $n(E_F) = 0.9$ states/eV-cell (for both spins), leading to $\kappa_{TF} = 0.2$ $\AA^{-1}$, and $\kappa_{TF}/k_F \approx 0.3$. In YBCO, $n(E_F)$ is larger, mainly because of the contribution of the chains (ridge structure of the FS [48]). Since we are concerned with the (CuO$_2$)$_n$ planes (barrel structure of the FS), and the chains are removed from the planes by about 4 $\AA$, screening by the chains should not reduce the screening length in the planes to less than $\kappa_{TF}^{-1} = 4$ $\AA$.

Because of the long range of the interaction, the scattering is predominantly forward, with a scattering angle of order $\kappa_{TF}/k_F \approx 0.3$. This makes it possible to have a very large anisotropy even for extended s-wave pairing.

This estimate is obviously very crude, and its main purpose is to provide a qualitative explanation why $T_c$ is high.

There are some questions raised by the present model.

(a) The large matrix element $I$ implies a large value of $\lambda_{ph}$. A large value of $\lambda_{ph}$ may be expected to cause a lattice instability especially for soft phonons. Fortunately, the ionic-screening involves a small cutoff $\xi$ for the electron-phonon interaction, and this stabilizes the lattice, as described in Ref. [18]. Another argument is that the ionic contribution to the total energy and the phase stability is large in these oxides, and therefore a large $\lambda_{ph}$ due to states at the FS is not necessarily sufficient to cause a lattice instability. Moreover, the value of $\lambda_{ph}$ is usually estimated from strong-coupling effects such as the enhancement of the electronic specific heat, or the jump in the specific heat at $T_c$. Such estimates seem to indicate a smaller value of $\lambda_{ph}$. Note that some recent electronic specific heat measurements by Reeves et al. [49] suggest a rather large value of $\lambda_{ph}$; they suggest $2.5 < \lambda_{ph} < 7$. However, these measurements actually give the value of the renormalization function $Z$; the connection $Z = 1 + \lambda_{ph}$ between
it and the coupling constant is broken when there is a cutoff $\xi_1$ (Ref. [18]). Thus a finite cutoff $\xi_1$ increases the value of $\lambda_{ph}$ (determined from the specific heat) to well above this value. Therefore, a larger value of $\lambda_{ph}$, in line with the large value of $2\Delta(0)/T_c$, is plausible.

(b) The small value of the Bohr radius $a_0 = (\hbar^2\epsilon_\infty/m^*e^2)$ normally implies a small overlap and therefore a very narrow band (very small $E_F$). Fortunately, here the copper $d$-band is degenerate with the oxygen $p\sigma$-band, and therefore there is strong indirect hopping between oxygens via the copper. Therefore we have a large value of $E_F$ (small value of $m^*$), together with a very small value of $a_0$.

(c) Normally, for a value of $r_c \approx 8 - 10$, we would expect a Mott insulator. Here, the ionic screening, (in conjunction with the ordered lattice), inhibits the Mott transition. That is a subtle effect, that we describe in some length elsewhere [8].

Some other questions regarding the elimination of the effects of the Coulomb interaction, the isotope effect, phonon damping and pulling (expected when $\lambda_{ph}$ is large), the Hebel-Slichter peak, and the McMillan-Rowell structure, are discussed in Ref. [18].

4.3 Very strong coupling features of the solutions

A salient feature of conventional strong-coupling theory of superconductivity, is the gap-dependence of the renormalization function $Z$; in Pb, $Z$ decreases by about 5% as $T$ changes from $T_c$ to zero, due to the buildup of the gap $\Delta$ [20]. Because of this interdependence of $Z$ and $\Delta$, the equations for these two parameters must be solved self-consistently. This effect manifests itself, for example, in a temperature-dependence of the enhancement of the critical field $H_{c2}(T)$ over the weak-coupling value. However, this effect is weak in conventional superconductors, about 10% in "extreme" strong coupling superconductors [50].

For the solutions that we propose here, we find that the gap-dependence of the renormalization function $Z$ is somewhat stronger, because of the large value of $\lambda_{ph}$, but still in the range of about 20% (Fig. 5, Ref. [18]). However, the gap-dependence of the momentum renormalization function $X$ is very large. In Fig. 5, we plot the temperature-dependence of $Z$ and $X$ for two sets of parameters, one (a) without a Coulomb interaction, and one (b) with a Coulomb interaction with a cutoff $\xi_2$. We consider the "strip" form of the electron-phonon coupling constant. We believe that the parameters of Fig. 5(b) are representative of YBCO.

We see that $X$ changes from about $2$ at $T_c$ to about $1$ at low temperatures. This very large change represents a very-strong-coupling scenario.

Physical manifestations of this enormous change in $X$, are the following:

(a) The Pippard coherence length $\xi_0$ is extremely small. Since $\xi_0 = \hbar v_F/\pi \Delta$, and $v_F = v_{\text{band}} X/Z$, the decrease in $X$ decreases $\xi_0$ below the "expected" value. $\xi_0$ in YBCO is indeed abnormally small, $\xi_0 \approx 12 - 15$ Å. In Pr$_{0.4}$Y$_{0.6}$Ba$_2$Cu$_3$O$_7$, $\xi_0 \approx 60$ Å, $T_c \approx 40$ K [51]. Scaling this value by the $T_c$ of YBCO ($\approx 90$ K), we would expect a value of $25 - 30$ Å in YBCO. Thus, $\xi_0$ is a factor of 2 smaller than expected. This is just what the variation in $X$ suggests. (In PYBCO, the small elastic mean-free-path $l_{el}$ prevents the cutoff $\xi_1$ from being very small, and as a result $X \approx 2 - 2.5$, independent of temperature below $T_c$).

(b) The London penetration depth is given by: $\lambda_L^{-2} = (4\pi ne^2/\hbar kp)^2 v_F f(T)$, $f(T) = \sqrt{T_c/(T_c - T)}$, $v_F = v_{\text{band}} X/Z$. Thus, the decrease in $X$ below $T_c$, should in-
increase $\lambda_L$ by about a factor of $\sqrt{2}$. Preliminary measurements [52] suggested that the value of $\lambda_L$, (corrected by the $f(T)$ factor) increases from 850 Å at $T_c$ to about 1400 Å as $T \to 0$. However, more recent experiments indicate a smaller increase (from about 1200 Å to 1400 Å [53]). We should note that the "strong coupling effect" on $Z$ is much smaller, and in the opposite direction, i.e. it would decrease $\lambda_L(0)$ below the value extrapolated from the $T \approx T_c$ region. Lifetime effects also decrease $\lambda_L(0)$ below the extrapolated value. Thus, an observed increase in $\lambda_L(0)$ is a clear signature of the decrease in $X(T)$ with decreasing $T$ below $T_c$.

(c) The decrease in $X$ at very low temperatures ($T \ll T_c$) increases $H_{c2}$ above the value predicted by "conventional" strong coupling theory [50]. Such effects were indeed seen in the cuprates [54].
4.4 Physical relevance of our model

(a) We saw that a large value of \( \lambda_{\text{ph}} \), coupled with a small cutoff \( \xi_1 \), gives rise to a ZBA. With the “strip” form of \( g(k,k') \), \( \delta^{(0)} \) is considerably smaller than with the “Copper” form. Also the small coherence length \( \xi_0 \) in YBCO can easily be accounted by the “strip” form. The question arises whether the strip form has a physical justification. We attribute the cutoff to electron-electron scattering, which relaxes the charge-fluctuation term \( \langle c_k^\dagger (t) c_{k+q}(t) \rangle \) \( (q \) is the phonon wavevector). The relaxation of such non-diagonal elements of the density matrix is discussed by Slichter [55]. It is analogous to a \( T_2 \) process in NMR. The characteristic frequency of this term is given by: \( \omega = \xi_{k+q} - \xi_k \). Coulomb interactions are reduced by the dielectric background by a factor \( \varepsilon(\omega)^{-1} \), the inverse dielectric function of the background. At small values of \( \omega, \varepsilon(\omega)^{-1} \) is very small and the Coulomb interactions that relax the charge fluctuation are very weak, therefore the relaxation rate is small, probably smaller than the phonon frequency \( \omega_{\text{ph}} \) and the electron-phonon coupling is not significantly affected. At high frequencies, \( \varepsilon(\omega)^{-1} \approx \varepsilon_{\infty}^{-1} \) which is large, and the relaxation rate may exceed the phonon frequency. The relaxation rate of the non-diagonal element of the density matrix is not identical with the electron-electron scattering rate \( \tau_{ee}^{-1} \), and probably exceeds it (just as \( 1/T_2 \) frequently exceeds \( 1/T_1 \)), thus exceeds \( \xi_k \) for energies from about 30 meV and up. Therefore, we believe that the strip form, with a cutoff even somewhat lower than the phonon frequency, has a physical justification.

(b) Even if we believe that the ZBA observed in various tunneling and PCS experiments is a “genuine” physical phenomenon, the question arises whether there are alternative physical mechanisms accounting for it. Initially, a ZBA in normal metals was attributed to the Appelbaum effect [56], i.e. a Kondo-like effect. Recently, van Wees et al. [57] attributed the ZBA to multiple Andreev reflections. Alternatively, in YBCO a gap of 4 meV can be attributed to the chains [58]. Recently, Chakravarty et al. [59] proposed a ZBA with \( \delta^{(0)} \) due to the phonon mechanism, and the maximum in the quasiparticle DOS, at a considerably higher energy, attributed to Josephson tunneling between planes. Still, the number of theories that are consistent with the ZBA is considerably smaller than the number of theories proposed to account for high-temperature superconductivity; thus a presence of the ZBA is highly discriminatory. We believe that the observation of the ZBA in ET, where there is a single, cylindrical FS, eliminates the two band possibility; the magnetic-field independence [32] eliminates the Appelbaum effect interpretation. The same applies to the recently reported ZBA in Nb-Ag, Nb-Al contacts [60]. Thus, the definitive experimental establishment of the ZBA, together with a detailed investigation of its properties, may prove to be a decisive tool for the elucidation of the microscopic origin of high-\( T_c \) superconductivity.

5 Conclusion

We propose an extension of Eliashberg theory for very-strong coupling. Such an extension is warranted by the large value of the gap parameter in the cuprates, namely \( \Delta(0) \approx 20-30 \) meV, in conjunction with a phonon frequency of about \( \omega_{\text{ph}} \approx 30-40 \) meV for the phonons that interact strongly with the electrons [14]. Tunneling data somewhat similar to those of [14] were obtained by Mandrus et al. [15] and
Renner et al. [16, 27]. They also see the structure at 30—50 meV above the gap that Vedeneev et al. interpret as a McMillan-Rowell structure due to phonons, but do not provide an interpretation to this structure. It is conceivable that this structure is of an electronic origin. Note that in Pb, $\Delta(0) \approx 1.2$ meV while $\omega_{ph} \approx 4$ meV for the transverse and $\approx 8$ meV for the longitudinal modes; thus $\Delta(0)/\omega_{ph}$ in the cuprates is about a factor of 3 larger than in Pb, and assuming that the superconductivity is caused by the phonon-mediated interaction, this implies very-strong coupling.

We point-out that a physical reason for this very strong coupling is the very small electronic screening, characterized by a value of $\kappa_{TF}$ considerably smaller than $k_F$, in contrast with the situation in normal metals, where $\kappa_{TF} > k_F$. This weak electronic screening is due to the large ionic polarizability, which is present only at very low frequencies. As a result, the very large value of $\lambda_{ph}$ is present only at very low energies, and there is a cutoff $\xi_1$ which may be lower than the frequency of the phonons that are responsible for the pairing. We solve the Eliashberg equations for this situation, namely a $|k|$-dependent interaction with a low energy cutoff, and show that they possess a very rich variety of solutions. The solutions apparently can account for all observations on high-$T_c$ superconductors. $\xi_1$ is the only new parameter that has to be added to the well-known Eliashberg equations. Moreover, the small value of $\xi_1$ accounts naturally for the stability of the lattice in spite of the very strong electron-phonon coupling $\lambda_{ph}$.

Since we work with imaginary (Matsubara) frequencies, we have rather roughly estimated the energy of the quasiparticles. In order to solve the problem properly, an analytical continuation of the Green function should be done. The question then arises concerning the relevance of our estimate. We have therefore solved the Eliashberg equations with real frequencies (Poisson sum-formula and change of path of integration as indicated by Schrieffer [61]), and we found that the above conclusion can be verified in this way. These calculations, and an extension to a gap with angular dependence, will be treated in a later paper.

This very-strong coupling scenario causes the renormalization function $Z$, and in particular the momentum-renormalization $X$, to be strongly temperature-dependent below $T_c$, in contrast with the conventional strong-coupling scenario, where this dependence is not very strong. The very large value of $\Delta(0)$, together with the small value of the cutoff $\xi_1$, may give rise to a minimum of the excitation energy in the superconducting state not quite on the Fermi surface. In conjunction with the large momentum-renormalization, this minimum can be considerably smaller than the gap at the Fermi surface, giving rise to a "Zero Bias Anomaly", which is sometimes observed in tunneling and point-contact spectroscopy. In spite of the very strong coupling, the excitation spectrum at very low energies ($E<\frac{1}{2}\omega_{ph}$) displays sharp structures that are normally associated with a weak-coupling scenario. This follows from the small cutoff on $g$, that suppresses real processes that are responsible for short lifetimes.

A simple order-of-magnitude estimate accounts for transition temperatures up to about 200 K in the cuprates.
References

[24] V. Z. Kresin (private communication)
[38] G. Gruner (private communication)
[41] W. L. McMillan, Phys. Rev. 167 (1968) 331
[53] Dong Wu, Jian Mao, private communication