Real-axis direct solution of the $d$-wave Eliashberg equations and the tunneling density of states in optimally doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$

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Abstract

In this work we calculate the direct solution of the equations for the retarded electron-boson interaction in the case of $d$-wave symmetry for the pair wave function and in the real axis formulation. We use a spectral function containing an isotropic part and an anisotropic one: $\alpha^2(\Omega, \phi, \phi')F(\Omega) = \alpha^2_s F(\Omega) + \alpha^2_d F(\Omega) \cdot \cos (2\phi) \cos (2\phi')$ and make the simple assumption: $\alpha^2_d F(\Omega) = g_d \alpha^2_s F(\Omega)$ where $g_d$ is a constant. For appropriate values of the isotropic electron-boson coupling constant $\lambda_s$ and the anisotropic one $\lambda_d$, solutions are obtained with only $d$-wave symmetry for the order parameter and only $s$-wave one for the renormalization function. We have employed the real axis formulation in order to compare the theoretical curves to the tunneling density of states of the optimally-doped high-$T_c$ superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$. The results of our numerical simulations are able to fit very well the value of the gap, the critical temperature and the shape of the density of states in all the energy range, as recently determined in our break-junction tunneling experiments. At $T > T_c$ the theoretical conductance still shows a broaden peak that disappears at $T^* \approx 140$ K.

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At the present moment, there are many experimental results that strongly suggest the presence of a dominant $d$-wave symmetry of the pair wave function in high-$T_c$ cuprates, at least the layered ones [1]. Recent tunneling measurements on the layered high-$T_c$ superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (Bi 2212) [2 8] yielded high or very high values of the low-temperature gap, gapless features and a small but finite value of the quasiparticle density of states (DOS) at zero bias. These facts could be explained, at least partially, by assuming a $d$-wave pair state which has nodes within the superconducting gap. On the other hand, in the last years, a few attempts have been made to fit some of the high-$T_c$ superconducting properties by using the Migdal-Eliashberg theory [9–11], but most of the works concerned only the solution in $s$-wave pair symmetry. In particular, we recently used the superconducting DOS of optimally-doped Bi 2212 single crystals with $T_c \simeq 93$ K, determined in break-junction tunnel experiments, in order to reproducibly determine the electron-boson spectral function of Bi 2212 by inversion of the $s$-wave Eliashberg equations [3 4].

In the present paper, we extend the real-axis direct solution of the Eliashberg equations for strong electron-boson coupling to the $d$-wave case and discuss the main features of the solution as function of temperature and boson coupling strength. In the framework of this model, we are able to obtain a very good agreement between our experimental break-junction tunneling data and the theoretical results with regard to both the DOS shape in all the energy range and the critical temperature.

Our numerical analysis starts from the well-known generalized Eliashberg equations for the order parameter $\Delta(\omega, \mathbf{k})$ and the renormalization function $Z(\omega, \mathbf{k})$. They have kernels that depend on the retarded interaction $\alpha^2(\Omega, \mathbf{k}, \mathbf{k'})F(\Omega)$, the coulomb interaction $\mu^*(\mathbf{k}, \mathbf{k'})$, and the effective band $\varepsilon_\mathbf{k}$ [12–15]. For simplicity we suppose that $\mathbf{k}$ and $\mathbf{k'}$ lie in the CuO$_2$ plane ($ab$ plane) and we neglect the relatively small band dispersion and the gap in $c$ direction. Therefore we use a single band approximation where the Fermi line is nearly a circle while $\phi$ and $\phi'$ are the azimuthal angles of $\mathbf{k}$ and $\mathbf{k'}$ in the $ab$ plane, respectively. We thus expand $\alpha^2(\Omega, \phi, \phi')F(\Omega)$ and $\mu^*(\phi, \phi')$ in terms of basis functions $\psi_i(\phi)$ where the first few functions of lowest order are:
ψ_0(φ) = 1; ψ_1(φ) = \sqrt{2} \cos(2φ); ψ_2(φ) = \sqrt{2} \sin(2φ);

In the present paper we study the simplest d-wave electron-boson model interaction expressed by the following separable expressions

\[ \alpha^2(Ω, φ, φ')F(Ω) = \alpha^2_{00}F(Ω) + \alpha^2_{11}F(Ω) \cdot ψ_1(φ) ψ_1(φ') \]  

(1)

\[ \mu^*(φ, φ') = \mu^*_{00} + \mu^*_{11} \cdot ψ_1(φ) ψ_1(φ') \]

(2)

and we search for a s + id solution given by

\[ \Delta(ω, φ) = \Delta_s(ω) + \Delta_d(ω) \cdot ψ_1(φ) \]

\[ Z(ω, φ) = Z_s(ω) + Z_d(ω) \cdot ψ_1(φ). \]

With these assumptions the Eliashberg equations in presence of impurities [16] become:

\[ \Delta_s(ω)Z_s(ω) = \int_0^{+∞} P_s(ω') \cdot [K_{00+}(ω, ω') - \mu^*_{00} \cdot Θ(ω_c - ω')] dω' + \]

\[ iπΓ \cdot P_s(ω) / [C^2 + P_s(ω) + N_s(ω)] \]

(3)

\[ \Delta_d(ω)Z_s(ω) = \int_0^{+∞} P_d(ω') \cdot [K_{11+}(ω, ω') - \mu^*_{11} \cdot Θ(ω_c - ω')] dω' \]

(4)

\[ [1 - Z_s(ω)] \cdot ω = \int_0^{+∞} N_s(ω') \cdot K_{00-}(ω, ω') dω' + \]

\[ iπΓ \cdot N_s(ω) / [C^2 + P_s(ω) + N_s(ω)] \]

(5)

where Γ = n_I/N(0)π², C = cotg(δ_0), n_I is the impurity concentration, N(0) is the value of the normal DOS at the Fermi energy and δ_0 is the scattering phase shift. We have not written the equation for Z_d(ω) that is homogeneous. In the weak-coupling case its only solution is Z_d(ω) ≡ 0, while in the strong-coupling one, in principle, there is a possibility that a nonzero solution exists above some coupling-strength threshold. In the present work, we assume that the stable solution corresponds to Z_d(ω) ≡ 0 for all the couplings and we do not consider the rather exotic possibility of Z_d(ω) ≠ 0 [13,14]. In eqs. (3)-(5), ω_c is a cut-off energy and we have
\[
K_{ii\pm}(\omega,\omega') = \int_0^{+\infty} d\Omega \alpha_{11}^2(\Omega) F(\Omega) \cdot \frac{f(-\omega') + n(\Omega)}{\Omega + \omega' + \omega + i \cdot \delta} \pm \frac{f(\omega') + n(\Omega)}{\Omega - \omega' + \omega + i \cdot \delta} \mp \frac{f(\omega') + n(\Omega)}{\Omega - \omega' - \omega - i \cdot \delta}
\]

where \( f(\omega') \) and \( n(\Omega) \) are the Fermi and Bose functions, respectively, and furthermore we know that

\[
P_s(\omega) = \frac{1}{2\pi} \int_0^{2\pi} \text{Real} \left( \Delta_s(\omega) / \sqrt{\omega^2 - \Delta_s^2(\omega)} - [\Delta_d(\omega) \cdot \psi_1(\phi)]^2 \right) d\phi
\]

\[
P_d(\omega) = \frac{1}{2\pi} \int_0^{2\pi} \text{Real} \left( \Delta_d(\omega) \cdot \psi_1(\phi) \psi_1(\phi) / \sqrt{\omega^2 - \Delta_d^2(\omega)} - [\Delta_d(\omega) \cdot \psi_1(\phi)]^2 \right) d\phi.
\]

The quasiparticle DOS that is compared to the experimental data is given by

\[
N_s(\omega) = \frac{1}{2\pi} \int_0^{2\pi} \text{Real} \left( \omega / \sqrt{\omega^2 - \Delta_s^2(\omega)} - [\Delta_d(\omega) \cdot \psi_1(\phi)]^2 \right) d\phi. \tag{6}
\]

In the case we want to obtain a \( s + d \) solution, we need only to replace the denominator of \( P_d(\omega), P_s(\omega) \) and \( N_s(\omega) \) with \( \sqrt{\omega^2 - [\Delta_s(\omega) + \Delta_d(\omega) \cdot \psi_1(\phi)]^2} \).

In our numerical analysis we have put, for simplicity, \( \alpha_{11}^2 F(\Omega) = g_d \alpha_{00}^2 F(\Omega) \) where \( g_d \) is a constant \( [17] \). As a consequence, the electron-boson coupling constants for the \( s \)-wave channel and the \( d \)-wave one are \( \lambda_s = 2 \int_0^{+\infty} d\Omega \alpha_{00}^2 F(\Omega) / \Omega \) and \( \lambda_d = (1/\pi) \int_0^{2\pi} d\phi \psi_1^2(\phi) \int_0^{+\infty} d\Omega \alpha_{11}^2 F(\Omega) / \Omega = g_d \cdot \lambda_s \), respectively.

We solved the generalized, real-axis, Eliashberg equations (3)-(5) in direct way by using an iterative procedure that continues until all the real and imaginary values of the functions \( \Delta_s(\omega), \Delta_d(\omega) \) and \( Z_s(\omega) \) at a new iteration show differences less than \( 1 \cdot 10^{-3} \) with respect to the values at the previous iteration. Usually the convergence occurs after a number of iterations between 10 and 15. By using this approach we found that \( \Delta(\omega, \phi) \) has either a pure \( s \)-wave or a pure \( d \)-wave symmetry depending on the values of the coupling constants \( \lambda_s \) and \( \lambda_d \). The values of the parameter \( g_d = \lambda_d / \lambda_s \) determine the stability of the two types of solution: if \( 1.5 < g_d < 5 \), there are no problems for an automatic convergence to the pure \( d \)-wave solution. When \( g_d < 1.5 \), the choice of the starting values of \( \Delta_s(\omega) \) and \( \Delta_d(\omega) \) determines the symmetry of the final solution to which the iteration procedure converges.
If \( g_d \gg 1 \) (i.e. roughly \( g_d > 7 \)) the iteration procedure converges only in the complex-axis formulation.

We can now check if exists a couple of \( \lambda_s \) and \( \lambda_d \) values that, together with a proper electron-boson spectral function \( \alpha^2(\Omega, \phi, \phi')F(\Omega) \), can reproduce our tunneling density of states \( N_{ex}(\omega) \) of Bi 2212 in the framework of a pure \( d \)-wave strong-coupling solution. For doing this we compare the \( N_{ex}(\omega) \) to the quantity \( N(\omega) = \int_{-\infty}^{+\infty} N_s(E+\omega) |f(E) - f(E + \omega)| \, dE \) where \( N_s(\omega) \) is calculated from eq.(6) by using \( \alpha_{00}^2F(\Omega) = (\lambda_s/\lambda) \alpha^2F(\Omega)_{Bi2212} \). As a first-order approach to the \( d \)-wave modeling of the tunneling curves, we used the electron-boson spectral function previously determined by the inverse solution of the \( s \)-wave Eliashberg equations applied to the same Bi 2212 data as \( \alpha^2F(\Omega)_{Bi2212} \) (see the inset of Fig. 1) \[3,4\]. Of course, \( \lambda \) is the corresponding coupling constant.

In Figure 1 our tunneling experimental data (open circles) and the best fit curve at 4 K (solid line) that is obtained for \( \lambda_s = 2, \mu_{11}^* = 0, g_d = 1.15 \) and yields almost the experimental \( T_c, T_{c^{calc}} = 99 \) K, are shown. We want to emphasize the impressive agreement of the theoretical curve to the experimental one in all the energy range, including the region at \( V < \Delta_M \) (peak of the conductance) where states inside the gap in all the experimental tunneling curves are present. Taking into account a small amount of impurities corresponding to \( \Gamma = 0.3 \) meV and \( C \approx 0 \), also the zero-bias conductance is reproduced and \( T_{c^{calc}} = 96 \) K. In the case of \( g_d = 1.12 \) and no impurities, \( T_{c^{calc}} = 93 \) K, that is exactly the experimental value, but the fit is a little less good. It is interesting to note that there are different pairs of \( \lambda_s \) and \( \lambda_d \) values with \( 2 \leq \lambda_s \leq 2.5 \) and \( 2 \leq \lambda_d \leq 2.25 \), all giving \( T_{c^{calc}} = 93 \) K and producing a good fit of the experimental data, the best remaining that one shown in Fig.1. When the \( d \)-wave component of the Coulomb pseudopotential is different from zero (the \( s \)-wave component does not affect the results in pure \( d \)-wave symmetry) the above mentioned best-fit parameters give the experimental \( T_c \) value for \( \mu_{11}^* = 0.0125 \). The short dash line of Fig. 1 shows the normalized \( dI/dV \) curve obtained at 4 K in this case. It is practically indistinguishable from the curve at \( \mu_{11}^* = 0 \). In general, the main consequence of a \( \mu_{11}^* \neq 0 \) is the reduction of the values of \( T_{c^{calc}} \) and \( \Delta_M \). In Fig. 1 we also show the
theoretical normalized conductances, obtained by using the parameters of the best-fit curve, at different temperatures between 60 K (long dash line) and 140 K (tiny short dash one). We can see that the normalized conductance is practically flat only at $T^* \simeq 140$ K $\geq T_c$: this is a strong-coupling effect that occurs at $\lambda \geq 2$ and has been briefly discussed in s-wave symmetry [18–22]. Here we demonstrate that it also exists in d-wave symmetry, is enhanced by the particular characteristics of Bi 2212 and could be related to the pseudogap observed in underdoped and overdoped Bi 2212 [3].

In this d-wave strong-coupling regime we have observed other unusual facts already partially predicted in s-wave symmetry [18–22], but here enhanced by the specific properties of Bi 2212. Some of them can be discussed with reference to Fig. 2 where the real and imaginary parts of the renormalization function $Z_s(\omega)$ (Fig. 2a) and of the gap function $\overline{\Delta}_d(\omega) = \sqrt{2}\Delta_d(\omega)$ (Fig. 2b) are shown for $T = 4.2, 99$ and $140$ K. In particular, one can observe that the function $\text{Real}(\overline{\Delta}_d(\omega)) = \overline{\Delta}_{d1}(\omega)$ goes to zero very abruptly for $\omega \to 0$ and $T \simeq T_c$ (see the short dash curve of Fig. 2b), but, in general, at that temperature it is considerably different from zero at higher energies, whereas in the weak and intermediate coupling regime the whole curve goes to zero in uniform way at the increase of temperature.

In addition, Fig. 1 shows that the normalized conductance is practically flat at $T > T^*$ but, at the same temperature, $\overline{\Delta}_d(\omega)$ is still different from zero, as it is suggested by dot and short dot curves of Fig. 2b that are calculated at $T = 140$ K.

In the best fit case represented by the continuous line of Fig. 1 and at $T = 4$ K, our theoretical model produces $\overline{\Delta}_0 = \sqrt{2}\Delta (\omega = 0) = 21.22$ meV that gives a ratio $2\overline{\Delta}_0/k_BT_{c,\text{calc}} = 4.98$, but the values of the gap edge $\overline{\Delta}_g = \sqrt{2}\Delta_g = \sqrt{2}\text{real}[\Delta (\omega = \Delta_g(T))]$ and the peak $\Delta_M$ are rather different: $\overline{\Delta}_g = 24.5$ meV and $\Delta_M = 25$ meV. In Fig. 3a we can see the plot of $\overline{\Delta}_0$, $\overline{\Delta}_g$ and $\Delta_M$ as function of temperature: the last one (solid triangles) does not go to zero at $T_c$ and, in addition, it grows considerably at larger $T$, being thus present also at $T \geq T_c$. Particularly at $T > T_c/2$ this peak is very different from the gap edge $\overline{\Delta}_g$ (solid squares). On the other hand, it can be seen in Fig. 3a that both $\overline{\Delta}_g$ and $\overline{\Delta}_0$ have a BCS-like temperature dependency, but with a different $T_c$ of the order of 115 K and
99 K, respectively. This effect is typical of a very strong-coupling regime while in the weak and intermediate coupling $\Delta_g$ and $\Delta_0$ always coincide.

Another very interesting and unusual phenomenon related to $\Delta_g$ occurs for high values of $\lambda_s$ \cite{22}. When $\lambda_s \geq 2$, a $T^{**}$ exists for which at $T \geq T^{**}$ (in our case $T^{**} = 65$ K) there is an energy value $\omega^*(T)$ that verifies the expression: $\text{real}(Z_s(\omega^*(T))) = \text{imag}(Z_s(\omega^*(T)))$. In this case the quasiparticle approximation is no more valid and it is possible to have more than one solution of the equation $\Delta_g(T) = \text{real} \left[ \Delta (\omega = \Delta_g(T), T) \right]$. In Fig. 3b we show the temperature dependencies of the two solutions $\Delta_{g1}, \Delta_{g2}$ of the previous equation, obtained for the spectral function of Fig. 1 and the parameters of the solid line curve of the same figure, together with the $\omega^*(T)$ curve and its approximate value $\omega_{th}^*(T)$ given by

$$\omega_{th}^*(T) \simeq \frac{2\pi}{(1 + \lambda_s)} \int_0^{+\infty} \alpha_0^2 F(\Omega) \cdot [f(\Omega) + n(\Omega)] d\Omega.$$ \hspace{1cm} (7)

This effect is also present in pure $s$-wave symmetry and is strongly enhanced by the particular shape of the spectral function of Bi 2212. In conventional strong-coupling superconductors the range of temperature where two solutions of the gap equation are present is of the order of $10^{-2}$ K \cite{22}, while here it is of the order of 50 K. Particularly in the present situation, this fact suggests that the gap edge is no more the most relevant physical quantity. As a consequence, the gap, experimentally determined from different measurements, is not the gap edge $\Delta_g$ but an average over the frequency of the function $\Delta (\omega, T)$ with a weight factor depending on the property being measured \cite{22}. This fact could have important consequences in the interpretation of the experimental data in Bi 2212.

In summary, we have shown that the simplest approach to the pure $d$-wave solution of the equations for the retarded strong electron-boson interaction reproduces very well and in the whole energy range the normalized conductance of optimally-doped Bi 2212, recently determined in our break-junction tunneling experiments \cite{3,4}. The addition of a small amount of impurity scattering in the unitary limit accounts also for the small but finite value of the normalized conductance at zero bias \cite{23}. In the best-fit cases, the calculated critical temperatures differ no more than 6% from the experimental ones. The temperature dependency of
the normalized conductance, calculated for the best-fit values of the electron-boson coupling constants, shows non-flat curves at $T > T_c$ up to $T^* \approx 140$ K. This numerical result seems to suggest the presence of a strong-coupling ”pseudogap” even in the DOS of optimally-doped Bi 2212 samples where, up to now, it has never been clearly observed. The evolution of the present work will be its extension to the non half-filling case, in order to compare the $d$-wave solution of the Eliashberg equations to the DOS of underdoped and overdoped Bi 2212, and the comparison with other experimental data. Nevertheless, we believe the generality of the Eliashberg formalism and its independence of a specific assumption for the microscopic coupling mechanism gives the present results a hardly questionable validity.
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FIGURE CAPTIONS

Fig. 1 The theoretical normalized conductances for $\mu_{11}^{*} = 0$ at various temperature values: $T = 4, 60, 100, 120, 140$ K and for $\mu_{11}^{*} = 0.0125$ at $T = 4$ K, calculated with $\lambda_{s} = 2$ and $\lambda_{d} = 2.3$. The optimally-doped Bi 2212 break-junction experimental data at $T = 4.2$ K are shown as open circles. In the inset, the $\alpha^{2}F(\Omega)_{B2212}$ used in the fit of experimental data is shown.

Fig. 2 (a) The calculated values of $\text{Re}Z_{s}(\omega) = Z_{s1}(\omega)$ and $\text{Im}Z_{s}(\omega) = Z_{s2}(\omega)$ at three different temperatures $T = 4.2, 99, 140$ K; (b) the same as in (a) but for $\text{Re}\Delta_{d}(\omega) = \Delta_{d1}(\omega)$ and $\text{Im}\Delta_{d}(\omega) = \Delta_{d2}(\omega)$.

Fig. 3 (a) Calculated values of $\Delta_{M}(T)$ (peak of the DOS), $\Delta(\omega = 0, T)$ and $\Delta_{g}(T)$ (gap edge) as function of temperature. The solid and dash lines represent the BCS dependence of the gap for $T_{c} = 115$ K and $T_{c} = 99$ K, respectively; (b) the two solutions of the gap equation $\Delta_{g1}$ and $\Delta_{g2}$, together with $\omega^{*}(T)$ and its approximate analytical expression (short dash line) as function of temperature.


Fig. 1

G.A. Ummarino and R.S. Gonnelli, "Real-axis direct solution of..."
G.A. Ummarino and R.S. Gonnelli, "Real-axis direct solution of..." Fig. 2
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Fig. 3