Breakdown of Migdal’s theorem and intensity of electron-phonon coupling in high-$T_c$ superconductors

G.A. Ummarino and R.S. Gonnelli

*INFN – Dipartimento di Fisica, Politecnico di Torino, 10129 Torino, Italy*

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Abstract

In this article we quantify the possible effects of the breakdown of Migdal’s theorem on the electron-phonon coupling constant $\lambda$, on the critical temperature $T_c$ and on the superconducting gap $\Delta$ by examining different kinds of superconducting materials either with low and high critical temperature. We use the theoretical approach developed by Grimaldi, Pietronero and Strässler [PRB 52, 10516 & 10530, 1995] on experimental data taken both from literature and from our recent break-junction tunneling experiments in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$. The results show that a large violation of the Migdal’s theorem (as in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$) yields to a large increase of $\lambda$ and, in a first approximation, to a large but different increase of $T_c$ and $\Delta$. The same theory gives no modifications when applied to low-$T_c$ conventional superconductors.

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The high-$T_c$ superconductors (HTS), included the fullerenes, are all characterized by a very low Fermi energy, here $E_F$, that is comparable with the Debye phonon frequency: this involves the breakdown of the Migdal’s theorem for the electron-phonon (e-p) interaction, and requires a generalization of the many-body theory of superconductivity.

Recently this generalization has been made by using an extremely simplified model, isotropous, tridimensional, mono-band and with the spectral function for the e-p interaction represented by an appropriate Dirac function: $\alpha^2 F(\omega) = 0.5 \cdot \lambda \cdot \omega_0 \cdot \delta (\omega - \omega_0)$ where $\omega_0 = \omega_{\log} = \exp \left( \frac{2}{\lambda} \int_0^{+\infty} d\omega \frac{\alpha^2 F(\omega) \ln \omega}{\omega} \right)$, $\lambda = 2 \int_0^{+\infty} d\omega \frac{\alpha^2 F(\omega) \ln \omega}{\omega}$ and $\alpha^2 F(\omega)^{ex}$ is the e-p spectral function experimentally determined by quasiparticle tunneling measurements. In addition, a perturbative scheme for what concerns the parameter $(\lambda \omega_0/E_F)$ and a not perturbative one for $\lambda$ has been used. The main result is that the vertex function shows a complex behaviour as function of the phonon wavevector $q$ and frequency $\omega$ and, in particular, it assumes positive values in correspondence of small $q$. The region where $q$ is low can be favorite by the presence of electronic correlations and by effects due to the electronic density of states. This fact makes it possible a strong increase of the $T_c$ value, in comparison with the results of conventional BCS theory. This approximate vertex-corrected Migdal-Eliashberg theory, required by the breakdown of Migdal’s theorem and performed up to now only in $s$ wave, at $T = T_c$ and with $\mu^* = 0$, gives rise to very interesting phenomena but, in order to examine them in detail, it is necessary to solve numerically the Eliashberg equations. This can be done by introducing a cutoff value for the wavevector $q_c$, also useful in order to obtain some analytic results such as the extension to this theory of the McMillan’s formula for the calculation of $T_c$. As we already pointed out, the main result is the strong $T_c$ increase which occurs together with a relatively low $q_c$ and almost ordinary values for the coupling constant ($\lambda \simeq 0.5 - 1$). A complex behaviour is present for the isotopic effect which can be very high in correspondence of some parameters’ regions, but can also cancel when $\omega_0 > E_F$. It is also interesting to note that intermediate coupling constant values ($\lambda \simeq 1$) can reproduce properties which, in the standard Eliashberg theory, correspond to very high values ($\lambda \simeq 3$). The theory produces also effects on the normal-state properties, which can
draw away from the usual Fermi liquid behaviour. At $T = T_c$, the new Eliashberg equations, that take into account the first-order vertex corrections, are [3,4]:

$$\Delta(\omega_n)Z(\omega_n) = \pi T_c \sum_{\omega_m} \frac{\omega_0^2}{(\omega_n - \omega_m)^2 + \omega_0^2 |\omega_m|} \Delta(\omega_n).$$

$$\lambda_\Delta(\omega_n, \omega_m, q_c, m, \lambda) \frac{2}{\pi} \arctan \left[ \frac{E_F}{Z(\omega_m) |\omega_m|} \right] (1)$$

$$[1 - Z(\omega_n)] = \frac{\pi T_c}{\omega_n} \sum_{\omega_m} \frac{\omega_0^2}{(\omega_n - \omega_m)^2 + \omega_0^2 |\omega_m|} \omega_m.$$

$$\lambda_Z(\omega_n, \omega_m, q_c, m, \lambda) \frac{2}{\pi} \arctan \left[ \frac{E_F}{Z(\omega_m) |\omega_m|} \right] (2)$$

where $\Delta(\omega_n)$ is the gap function, $Z(\omega_n)$ is the renormalization function, $\omega_n = (2n-1)\pi k_B T$ with $n = 0, \pm 1, \pm 2, ...$ are the Matsubara frequencies and $m = \omega_0 / E_F$ is a parameter that represents a sort of indicator for the breakdown of the Migdal’s theorem. The functions $\lambda_\Delta$ and $\lambda_Z$ are defined as:

$$\lambda_\Delta(\omega_n, \omega_m, q_c, m, \lambda) = \lambda [1 + \lambda P_c(\omega_n, \omega_m, q_c, m)]$$

$$+ 2\lambda^2 P_V(\omega_n, \omega_m, q_c, m)$$

(3)

$$\lambda_Z(\omega_n, \omega_m, q_c, m, \lambda) = \lambda [1 + \lambda P_V(\omega_n, \omega_m, q_c, m)]$$

(4)

where $P_c(\omega_n, \omega_m, q_c, m)$ and $P_V(\omega_n, \omega_m, q_c, m)$ are cumbersome functions defined in the original papers [3,4], while $\lambda$ is the bare e-p coupling factor not renormalized by the violation of the Migdal’s theorem.

Following the usual procedure [11,12], it is possible to simplify Eqs. 3 and 4 by calculating them at $\omega_n = 0$ and $\omega_m = \omega_0$ and then to obtain an approximate expression for $T_c$:

$$T_c(q_c, m, \lambda) = \frac{1.13 \omega_0}{k_B \sqrt{e(1 + m)}} \exp \left[ \frac{m}{2(1 + m)} \right] \exp \left[ -\frac{1 + \lambda Z(q_c, m, \lambda) / (1 + m)}{\lambda_\Delta(q_c, m, \lambda)} \right].$$

(5)

In the limit $m \to 0$, $\lambda_Z = \lambda_\Delta$ and this formula coincides with the exact result obtained by Combescot [11] in the weak coupling regime.
Our original approach consists in numerically solving the system made by Eqs. 4 and 5, with $T_c(q_c, m, \lambda) = T_c^{ex}$, and $\lambda_Z(q_c, m, \lambda) = \lambda^{ex}$, where $T_c^{ex}$ and $\lambda^{ex}$ are the experimental values for the critical temperature and for the e-p coupling constant. In this way we obtain approximate values for $q_c$ and the bare $\lambda$ value not renormalized by vertex corrections. We use the experimental e-p spectral function $\alpha^2 F(\omega)^{ex}$, determined from tunneling experiments, to calculate $\lambda^{ex}$, $\omega_0$ and the opportune Dirac’s function $\alpha^2 F(\omega) = 0.5 \cdot \lambda^{ex} \cdot \omega_0 \cdot \delta(\omega - \omega_0)$ that has the property to give the critical temperature closest to the experimental one in low-$T_c$ superconductors. Of course, the frequency $\omega_0$ also permits us to calculate the ratio $m$ which, as a consequence, is not a free parameter of the model.

We applied this procedure to four different superconducting materials both low-$T_c$ and high-$T_c$: Lanthanum, Bismuth, Ba$_{1-x}$K$_x$BiO$_3$ and Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$. The first two are conventional low-$T_c$ superconductors [11] characterized by a gap of the order of 0.9-1.3 meV and $T_c \approx 5 - 6$ K. The main difference among them is the value of the e-p coupling constant which is in the intermediate coupling regime for La ($\lambda = 0.98$) and in the very strong one for Bi ($\lambda = 2.46$). Ba$_{1-x}$K$_x$BiO$_3$ (BKBO) is a well known ceramic superconductor with an intermediate $T_c \approx 24.5$ K and a cubic crystallographic structure. Experiments have shown that the $\alpha^2 F(\omega)$ can be determined from phonon anomalies in the quasiparticle tunneling conductance at $eV > \Delta$ and an intermediate $\lambda = 1.23$ has been determined [12]. In the past years we have largely studied the high-$T_c$ superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (BSCCO) for the determination of the e-p spectral function [13]. Very recently we obtained reproducible tunneling results on optimally doped BSCCO single crystals with $T_c = 93$ K [14]. The Eliashberg function $\alpha^2 F(\omega)$ was determined from break-junction tunneling data and a good agreement was obtained at $eV > \Delta$ between the experimental density of states and the theoretical one calculated by a direct solution of the Eliashberg equations in presence of an energy-dependent normal density of states. The coupling constant was consistent with a very strong coupling regime ($\lambda = 3.34$). Similar results have been recently obtained by other groups [15]. The superconducting properties of the four materials are summarized in Table 1. It is important to notice that we selected only materials characterized by small or very
small values of the Coulomb pseudopotential $\mu^* \simeq 0$ (see Table 1), in order to be consistent with the approximate vertex-corrected theory [2–4] that has been written for $\mu^* = 0$.

Table 2 shows the logarithmic phonon energy $\omega_0$ calculated by the already mentioned equation, the maximum phonon energy of the spectrum $\omega_{\text{max}}$, the Fermi energy $E_F$, and the ratio $m = \omega_0/E_F$ for the selected superconductors. Actually, in Bi, due to its amorphous structure and the consequent particular shape of the spectral function at low energy (i.e. for $\omega \to 0 \alpha^2 F(\omega) \neq b\omega^2$ with $b = \text{const}$) [11], we have used $\omega_0 = 2A/\lambda$ where $A$ is the area of the spectral function. This $\omega_0$ value, unlike $\omega_{\log}$, gives the correct critical temperature in Bi. Due to the rather small value of $\omega_0$ (few meV) and the large value of $E_F$ (some eV), the breakdown of Migdal’s theorem is practically absent in La and Bi ($m \sim 10^{-3}$ or less). Quite different situation is present in BKBO and BSCCO where $\omega_0$ is of the order of 10-20 meV while $E_F$ of the order of 100 meV. As a consequence, the violation of Migdal’s theorem is moderate in BKBO ($m \simeq 0.14$) and strong in BSCCO ($m \simeq 0.26$).

Figures 1 and 2 show the e-p spectral functions $\alpha^2 F(\omega)$ of the selected superconducting materials taken from literature [11] or from recent tunneling experiments [12,14]. The tiny vertical line at abscissa $\omega_0$ in every graph indicates the position of the Dirac’s function which plays the role of $\alpha^2 F(\omega)$ in the approximate vertex-corrected theory.

As already mentioned, by numerically solving the system of Eqs. 4 and 5 with

$$\lambda^{ex} = \lambda_Z(q_c, \lambda)$$
$$T_c^{ex} = T_c(q_c, \lambda)$$

we can determine the cutoff value of the wavevector $q_c$ and the bare e-p coupling constant $\lambda$.

It is important to remark that:

1) For the comparison with experimental values $\lambda^{ex}$, we used $\lambda_Z(m, q_c, \lambda)$ and not $\lambda_\Delta(m, q_c, \lambda)$ because the renormalization effect on the coupling constant is present in the normal state too;

2) The bare $\lambda$ values, determined by the above mentioned procedure, are not the results
of an exact numerical solution of the system of Eqs. 4 and 5 because such a solution generally does not exist. As a matter of fact they are obtained by the average of the two values $\lambda_1$ and $\lambda_2$ that fulfil the following conditions: $T_c(q_c, \lambda_2) = T_{c\text{ex}}$, $\lambda_Z(q_c, \lambda_1) = \lambda^{\text{ex}}$ and $\Delta \lambda = |\lambda_1 - \lambda_2|$ is minimum ($\Delta \lambda_{BKBO} = 0.08$ and $\Delta \lambda_{BSCCO} = 0.3$). In practice we determine the smallest region in the space of the parameters $q_c$ and $\lambda$ that is consistent with an approximate numerical solution of the system. In the first three columns of Table 3 the results of this procedure are shown for the selected superconductors.

It is clear that for La and Bi, where the breakdown of Migdal’s theorem is absent, we obtain $\lambda = \lambda_Z = \lambda_{\Delta} = \lambda^{\text{ex}}$ and all the values of $q_c$ between 0.2-0.3 and 1 give an approximate solution of the system. On the contrary, in BKBO the bare $\lambda$ is reduced of the order of 20% with respect to the experimental one and the solution is possible only for an intermediate $q_c = 0.6$. The largest renormalization is present in BSCCO where the e-p coupling constant the superconductor would have had in absence of effects due to the Migdal’s theorem violation is $\lambda = 1.85$, about 45% less than the experimental value. In this case the solution is possible only for a very small value of the wavevector $q_c = 0.15$. The fourth column of Table 3 reports the values of the product $m \cdot \lambda$ which is the original parameter of the Migdal’s expansion and quantifies the amount of deviation from the standard Migdal-Eliashberg theory.

After having calculated the bare $\lambda$, we determine a proper scaling factor $\rho$ that, when applied to the $\alpha^2 F(\omega)^{\text{ex}}$, permits to obtain a scaled e-p spectral function which gives a coupling constant just equal to $\lambda$. The values of $\rho$ are shown in the fifth column of Table 3. This scaled $\alpha^2 F(\omega)$ is then inserted in a program for the direct solution of the standard Eliashberg equations at $T = 0$ [14] and with $\mu^* = 0$ to be consistent with the vertex-corrected theory. By using this approach we determine a first approximation for the values of the energy gap $\Delta_\lambda$ and the critical temperature $T_{c\lambda}$ the superconductor would have had in absence of the breakdown of Migdal’s theorem. These values together with the ratio $2\Delta_\lambda/k_B T_{c\lambda}$ are shown in the last three columns of Table 3. Of course, due to the practical absence of lowest-order vertex corrections, $\Delta_\lambda$ and $T_{c\lambda}$ of La and Bi are exactly the same as the experimental values. In BKBO and BSCCO the effects of these corrections on $\Delta$ and $T_c$ are very relevant. $\Delta_\lambda$
and $T_{c\lambda}$ of BKBO are about 33% and 28% lower than the corresponding experimental values (see Table 3) giving a ratio $2\Delta_\lambda/k_BT_{c\lambda} = 4$ that is consistent with an intermediate coupling regime very similar to the La case. In BSCCO the reductions of $\Delta_\lambda$ and $T_{c\lambda}$ with respect to the experimental values are about 48% and 39%, respectively, giving a renormalized gap of 12 meV and a renormalized critical temperature of 56 K. As a consequence of the larger renormalization of $\Delta$ in comparison with $T_c$, the ratio $2\Delta_\lambda/k_BT_{c\lambda}$ reduces to 4.98, a value very close to the ratio of Bi (see Table 3). We remark that some conventional low-$T_c$ very strong-coupling superconductors, like Pb$_{0.5}$Bi$_{0.5}$, have $\lambda$ and $2\Delta/k_BT_c$ values as large as 3 and 5.12, respectively [16].

Finally, in Figure 3, we show the dependence of the critical temperature of BSCCO on $q_c$ and $m$ as determined from Eqs. 3 to 5. The light gray circle on the contour map approximately shows the region of the parameters corresponding to the solution of the system presented in Table 3. There are two interesting observations: (i) it is clear from Fig. 3 and it was already stressed in the original papers [11] that, at the increase of the breakdown of Migdal’s theorem ($m \to 0.5$), $T_c$ increases only if $q_c$ is small. For $q_c$ of the order of 0.8-1, the increase of $m$ produces a reduction of $T_c$; (ii) the action of removing the effects due to the deviations from the standard Migdal-Eliashberg theory, that we have tentatively done in the last part of the present paper, does not mean to perform the limits $m \to 0$ and $q_c \to 1$ but $m \to 0$ while $q_c$ remains constant (in this case $q_c = 0.15$). As a matter of fact, $T_{c\lambda} \simeq 56$ K determined by the direct solution of the Eliashberg equations is consistent with $m \simeq 10^{-3}$ and $q_c \simeq 0.15$ as shown by the hollow circle in Fig.3. This guarantees a self-consistency to our approach, since it has been calculated that $\lambda \simeq 2$ is compatible with a ratio $T_c/\omega_0 \simeq 0.2$ [16] which is the value we obtain by using $T_{c\lambda}$ for the critical temperature.

In conclusion, the results of this paper show that the breakdown of Migdal’s theorem, certainly present at various degrees in high-$T_c$ superconductors, yields to a relevant increase of the experimental e-p coupling constant $\lambda^{ex}$ in comparison with the bare one. This increase appears roughly proportional to the degree of violation of Migdal’s theorem expressed by $m \cdot \lambda$. By solving in direct way the standard Eliashberg equations, we have shown that, in
first approximation, $T_c$ and $\Delta$ are also increased by the effects of the approximate first-order vertex corrections described in Refs. 2-6. The amount of such an increase is greater for $\Delta$ than for $T_c$ thus leading to an amplified value of the experimental ratio $2\Delta/k_BT_c$. In BSCCO, the renormalized values $\lambda = 1.85$ and $2\Delta_\lambda/k_BT_{c\lambda} = 4.98$ are quite compatible with a conventional strong-coupling electron-phonon origin of superconductivity.

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### TABLES

**Table 1:**

|        | $\lambda^{ex}$ | $\mu^{ex}$ | $\Delta^{ex}(meV)$ | $T^{ex}_c(K)$ | $2\Delta/k_BT_c$ |
|--------|----------------|------------|---------------------|---------------|-----------------|
| La     | 0.98           | 0.039      | 0.89                | 5.04          | 4.10            |
| Bi     | 2.46           | 0.091      | 1.30                | 6.11          | 4.90            |
| BKBO   | 1.23           | 0.04       | 4.5                 | 24.5          | 4.64            |
| BSCCO  | 3.34           | 0.0093     | 23                  | 93            | 5.74            |

**Table 2:**

|        | $\omega_0(meV)$ | $\omega_{max}(meV)$ | $E_F(meV)$ | $m$   |
|--------|-----------------|----------------------|------------|-------|
| La     | 4.49            | 15                   | 3300       | 0.0014|
| Bi     | 2.87            | 14                   | 9900       | 0.0003|
| BKBO   | 14.57           | 62                   | 103        | 0.1415|
| BSCCO  | 21.91           | 90                   | 84         | 0.2608|

**Table 3:**

|        | $\lambda$ | $\lambda_\Delta$ | $q_c$ | $m \cdot \lambda$ | $\rho$ | $\Delta_{\lambda}(meV)$ | $T_{c\lambda}(K)$ | $2\Delta_{\lambda}/k_BT_{c\lambda}$ |
|--------|-----------|------------------|-------|---------------------|-------|--------------------------|-------------------|-------------------------------------|
| La     | 0.98      | 0.98             | 0.3-1 | 0.0013              | 1.00  | 0.89                     | 5.04              | 4.10                                |
| Bi     | 2.46      | 2.46             | 0.2-1 | 0.0007              | 1.00  | 1.30                     | 6.11              | 4.90                                |
| BKBO   | 1.01      | 1.4              | 0.6   | 0.1429              | 1.22  | 3.05                     | 17.71             | 4.00                                |
| BSCCO  | 1.85      | 7.65             | 0.15  | 0.4825              | 1.81  | 12.10                    | 56.34             | 4.98                                |
FIGURE CAPTIONS

Fig. 1 Experimental electron-phonon spectral functions $\alpha^2 F(\omega)$ of La (upper graph) and Bi (lower graph) taken from Ref. 11. The vertical lines indicate the energy positions $\omega_0$ of the Dirac’s functions that play the role of the spectral functions in the approximate vertex-corrected Migdal-Eliashberg theory.

Fig. 2 Experimental electron-phonon spectral functions $\alpha^2 F(\omega)$ of BKBO (upper graph, from Ref. 12) and BSCCO (lower graph, from Ref. 14). Details are as in Fig.1.

Fig. 3 Contour map of the calculated critical temperature of BSCCO as a function of $q_c$ and $m$. For details see the text.
La \( \omega_0 = 4.49 \text{ meV} \)
\( \lambda = 0.98 \quad \mu^* = 0.039 \)

Bi \( \omega_0 = 2.87 \text{ meV} \)
\( \lambda = 2.46 \quad \mu^* = 0.091 \)

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Fig. 1
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Fig. 2
Fig. 3