Anomalous impurity effects in nonadiabatic superconductors

M. Scattoni\(^1\), C. Grimaldi\(^12\)(\*), and L. Pietronero\(^12\)

\(^1\) Dipartimento di Fisica, Università di Roma I “La Sapienza”, Piazzale A. Moro, 2, 00185 Roma, Italy
\(^2\) Istituto Nazionale Fisica della Materia, Unità di Roma 1, Italy

(received ; accepted )

PACS. 71.38+i – Polarons and electron-phonon interactions.
PACS. 74.20Mn – Nonconventional mechanisms.
PACS. 74.62Dh – Effects of crystal defects, doping and substitution.

Abstract. – We show that, in contrast with the usual electron-phonon Migdal-Eliashberg theory, the critical temperature \(T_c\) of an isotropic s-wave nonadiabatic superconductor is strongly reduced by the presence of diluted non-magnetic impurities. Our results suggest that the recently observed \(T_c\)-suppression driven by disorder in \(K\_3C\_60\) (Phys. Rev. B 55, 3866 (1997)) and in \(Nd_{2-x}Ce_xCuO_4-\delta\) (Phys. Rev. B 58, 8800 (1998)) could be explained in terms of a nonadiabatic electron-phonon coupling. Moreover, we predict that the isotope effect on \(T_c\) has an impurity dependence qualitatively different from the one expected for anisotropic superconductors.
distinguish this regime from the ME and the polaronic ones we use the concept of nonadiabatic fermions, which we define as quasiparticles (weakly) interacting nonadiabatically with phonons. In practice, such a regime can be formulated perturbatively by treating $\lambda \omega / E_F$ as the small parameter of the theory. At the zeroth order, the theory coincides with the ME limit while for finite values of $\lambda \omega / E_F$ the nonadiabatic fermions display anomalous behaviors, at the same time being faraway from the crossover to polarons. This latter feature is ensured by considering values of $\lambda$ smaller than the critical coupling $\lambda_c$ (which is of order unity) of the crossover to the polaronic state. The reliability of such a perturbative approach is suggested by the comparison with exact results for the one electron system \cite{8} and quantum Monte Carlo calculations for the many electrons case \cite{9}.

The results obtained by previous studies of the nonadiabatic regime interest both the superconducting transition and the normal state properties. For example, the inclusion of the first vertex corrections beyond Migdal’s limit have led to the possible enhancement of $T_c$ with respect to the adiabatic ME case \cite{10}. Another interesting outcome is certainly the nonzero isotope effect of the effective mass of the nonadiabatic fermions \cite{11}. The latter result provides a possible interpretation of recent measurements on cuprates \cite{12}.

In this paper, we present results on the non-magnetic impurity effects on the critical temperature $T_c$ and its isotope coefficient $\alpha_{T_c}$ for an isotropic s-wave nonadiabatic superconductor. We show that disorder strongly affect the nonadiabatic corrections and change their analytic properties substantially. As a result, $T_c$ can be strongly lowered with respect to the pure case, in contrast therefore with the adiabatic ME theory which, according to Anderson’s theorem \cite{13}, predicts an insensitivity of $T_c$ with respect to the presence of weak disorder for an isotropic s-wave superconductor.

Our results can be of particular interest in light of the disorder dependence of $T_c$ recently observed in the fullerene compound $K_3C_60$ and in the electron doped cuprate $Nd_{2-x}Ce_xCuO_4 - \delta$ \cite{14, 15}. Both compounds have a well-established s-wave symmetry of the gap, hence the disorder induced suppression of $T_c$ cannot be explained in terms of d-wave pairing \cite{16}. It is however true that anisotropies could lead to qualitatively the same effect also if the gap is nodeless \cite{17}. Our results therefore provide an alternative interpretation based solely on the nonadiabatic regime of the el-ph interaction.

To have a first idea of how disorder affects the critical temperature of a nonadiabatic superconductor, let us consider the first vertex correction in the normal state depicted in fig.1. In the figure, the solid and the wiggled lines are electron and phonon propagators, $G$ and $D$, respectively, while the filled circles represent the $el-ph$ matrix element $g(q)$ for momentum transfer $q$. From the usual rules for diagrams, the resulting vertex function $P(k + q, k)$ is:

\[
P(k + q, k) = \sum_{k'} g^2(k - k') D(k - k') G(k' + q) G(k').
\] (1)

Here, $\sum_k$ and $k$ are short notations for $-T \sum_{m} \sum_k$ and $k$, $i\omega_m$, respectively.

In the presence of impurities, the electron propagators entering eq. (1) are given by $G^{-1}(k) = i\omega_m - \epsilon(k) + i\Gamma\omega_m / |\omega_m|$, where $\epsilon(k)$ is the electronic dispersion and $\Gamma = 1/\tau$ is the impurity scattering rate \cite{18}. We neglect for the moment the self-energy due to the $el-ph$ coupling, the effects of the finite bandwidth on the impurity contribution and the momentum dependence of $g(k - k')$. By employing some approximations which will be specified later, the vertex function (1) can be evaluated as a function of the dimensionless momentum transfer $Q = q / 2k_F$, where $k_F$ is the Fermi momentum, and the exchanged frequency $\omega$. In fig. 2 we show the sign of the vertex function in the $Q - \omega$ plane for the half-filling case and for $\omega_0 / E_F = 0.5$. The different lines denote the boundaries where the vertex changes sign. On
the right side of the lines the vertex is positive while on the left side is negative. The effect of impurities is twofold. First, the non-analyticity in \(\omega = 0, Q = 0\) found for the pure case \[16\] (solid line) is removed when \(\Gamma \neq 0\). Second, by increasing the value of \(\Gamma\) the boundary lines shift toward higher values of the exchanged frequency, reducing therefore the region where the vertex is positive. When we average the vertex over the exchanged momentum and frequency, we find that by increasing \(\Gamma\) the average becomes negative. Since the vertex correction \[4\] enters into the generalized Eliashberg equation for a nonadiabatic superconductor \[16\], we expect from the above result that \(T_c\) should be lowered with respect to the pure case.

In order to confirm this hypothesis, we solve the Eliashberg equations beyond Migdal’s limit by including the effect of disorder in the Born approximation. The relevant diagrams for both the normal, \(\Sigma_N\), and anomalous, \(\Sigma_S\), self-energies are depicted in fig.3. In terms of the renormalized frequency \(W_n = \omega_n Z_n\), where \(Z_n = 1 - \Sigma_N(i\omega_n)/i\omega_n\), and the renormalized s-wave gap function \(\phi_n = Z(i\omega_n)\Delta(i\omega_n)\), the generalized Eliashberg equations reduce to:

\[
\phi_n \xi_n = \pi T_c \sum_m \left\{ \lambda_n \left[ I + 2\lambda P(Qc; n, m, l) \right] D(\omega_n - \omega_m) + \lambda^2 C(Qc; n, m) \right\} \frac{\phi_m}{|W_m|} \eta_m, \tag{2}
\]

\[
W_n \xi_n = \omega_n + \pi T_c \sum_m \lambda_n \left[ I + 2\lambda P(Qc; n, m, l) \right] D(\omega_n - \omega_m) \frac{W_m}{|W_m|} \eta_m, \tag{3}
\]

where \(\eta_m = (2/\pi) \arctan(E_F/|W_m|)\) is the finite band-width factor and \(\xi_n = 1 - \eta_n \Gamma/|W_n|\) is the renormalization induced by the elastic impurities \[3\].

In writing the above equations, we have assumed a dispersionless phonon spectrum with frequency \(\omega_0\) so that the phonon propagator is given by: \(D(\omega_l) = \omega_0^2/[(i\omega_l)^2 - \omega_0^2]\). The terms \(P(Qc; n, m, l)\) and \(C(Qc; n, m, l)\) are the vertex and cross corrections, respectively \[1, 4\].

The parameter \(Q_c = q_c/2k_F\) is an upper-cutoff over the momentum transfer which follows from the model we use for the \(el\)-\(ph\) coupling function \(g^2(Q) = (g^2/Q^2) \theta(Q_c - Q)\) where \(\theta\) is the Heaviside step function \[4, 17\]. This model simulates the effect of the strong electron correlations which lead to mainly forward \(el\)-\(ph\) scattering processes \[17\]. In fact, in a strongly correlated system, a single charge carrier is surrounded by the corresponding correlation hole whose linear size \(\xi_c\) can extend over many lattice units \[18\]. The charge carrier can therefore respond only to charge modulations with wave vector \(q_c \lesssim 1/\xi_c\).

The solution of equations (2)-(3) without the vertex and cross corrections \(P(Qc; n, m, l)\) and \(C(Qc; n, m, l)\) has been already reported by Choi in ref. \[19\]. The main result was that, for finite values of \(E_F\), \(T_c\) can be slightly lowered by the presence of impurities. Here, we solve instead the completely self-consistent equations with the inclusion of both the vertex and cross corrections. In evaluating \(P(Qc; n, m, l)\) and \(C(Qc; n, m, l)\) we use a density of states \(N_F\) constant over the entire electron bandwidth \(2E_F\) and we employ a small momentum transfer approximation which is valid for small values of the dimensionless cutoff parameter \(Q_c\). From the above discussion, the small \(Q_c\) approximation should be suitable for strongly forward \(el\)-\(ph\) couplings resulting from the effect of strong electron correlation. After the integration over the energy and the s-wave average over the momentum transfer \(Q\) have been performed, the vertex and cross corrections reduce to the following form:

\[
P(Qc; n, m, l) = T_c \sum_l D(\omega_n - \omega_l) \left\{ B(n, m, l) + \frac{A(n, m, l) - B(n, m, l)(W_l - W_{l-n+m})^2}{(2E_FQ^2)^2} \right\} \times \left[ 1 + \left( \frac{4E_FQ^2}{W_l - W_{l-n+m}} \right)^2 \right]^{1/2} \ln \left( \frac{1}{2} + \left( \frac{4E_FQ^2}{W_l - W_{l-n+m}} \right)^2 \right), \tag{4}
\]
To obtain the critical temperature $T_c$, we solve numerically the self-consistent equations (3)-(7) for different values of the adiabatic parameter $\alpha$. Our self-consistent calculations confirm the results of ref.\[7, 16\], i.e. small values of $Q_c$ lead to an enhancement of $T_c$ with respect to the Migdal limit. Moreover, at $\omega_0/E_F = 0$, $T_c$ is independent of $\Gamma$ in agreement with Anderson’s theorem [10]. On the other hand, when $\omega_0/E_F > 0$ the impurities lower $T_c$ for all values of $Q_c$ and $\omega_0/E_F$. We interpret this behavior in terms of the enhanced negative contribution of the vertex and cross corrections induced by the presence of the impurities as depicted in fig.2. This negative contribution leads to a reduction of the effective nonadiabatic $el-ph$ pairing interaction resulting in the reduction of $T_c$.

In fig.5 we show $T_c$ as a function of $\Gamma$ for $\omega_0/E_F = 0.2$ (a) and $\omega_0/E_F = 0.4$ (b). The thin solid lines refer to the case without vertex and cross corrections and correspond to the approximation scheme used in ref.\[19\]. As seen also by the inserts of fig.5, when we include the vertex and cross corrections (thick lines), the reduction of $T_c$ with the increase of $\Gamma$ can be much stronger than the reduction given by only the finite bandwidth effects.

So far, we have investigated the effects of disorder on a nonadiabatic superconductor with an $s$-wave symmetry of the order parameter. However, anisotropies of the gap lead to an impurity dependence of $T_c$ which, to a first approximation, can be described by using the Abrikosov-Gorkov (AG) scaling law [20] modified in order to represent d-wave, anisotropic s-wave and other types of symmetries of the order parameter [13][14]:\[\ln(T_{c0}/T_c) = \chi[\Psi(1/2+\gamma) - \Psi(1/2)],\]\[\Psi\] is the digamma function and $\gamma = \Gamma/(2\pi T_c)$. The parameter $\chi$ is a measure of the anisotropy of the order parameter: $\chi = 1$ ($\chi = 0$) for a d-wave (s-wave) superconductor [14]. According to the AG law, for $\chi \neq 0$ the impurities induce a monotonous reduction of $T_c$ in a way qualitatively similar to the one observed for the nonadiabatic case.

Given the above situation it could therefore difficult to decide whether the $T_c$ suppression observed in K$_3$C$_{60}$ [11] and in Nd$_2-x$Ce$_x$CuO$_{4-\delta}$ [12] should be ascribed to anisotropies of the order parameter or instead to the nonadiabatic $el-ph$ interaction. Here, we propose that a more suitable quantity to look at could be the ion-mass dependence of the critical temperature. In fact, the isotope coefficient $\alpha_{T_c}$ resulting from the AG-type relation is:

$$\frac{\alpha_{T_c}}{\alpha_{T_{c0}}} = \left[1 + \frac{d\ln(T_c/T_{c0})}{d\ln\gamma}\right]^{-1},$$

\[\alpha_{T_{c0}}\] is the isotope coefficient for $T_{c0}$.
where $\alpha_{T_c}$ is the isotope coefficient for the pure system. Since $T_c/T_{c0}$ decreases by increasing $\gamma$, equation (8) predicts a monotonous impurity induced enhancement of $\alpha_{T_c}$ compared with the corresponding value in the pure limit. Such a behavior is qualitatively different from the one displayed by an isotropic s-wave nonadiabatic superconductor. In fact, as it is shown in Fig. 6, where we report numerical results for $\alpha_{T_c}$ for the same parameters as in Fig. 5(a), the decrease of $T_c/T_{c0}$ due to the impurities is accompanied by a non-monotonous dependence of $\alpha_{T_c}$ at least for small values of the momentum cut-off $Q_c$. Moreover, for larger values of $Q_c$, the isotope coefficient decreases with the impurity concentration showing therefore a behavior opposite to the one given by eq. (8). It would be therefore important to measure the isotope coefficient and its evolution with the amount of disorder in the two s-wave superconductors $K_3C_{60}$ and Nd$_{2-x}$Ce$_x$CuO$_{4-\delta}$. Such a measurement could in fact decide whether the observed $T_c$ suppression in these materials and Nd$_{2-x}$Ce$_x$CuO$_{4-\delta}$ is given by anisotropy or by the nonadiabatic regime of the $el-ph$ interaction. We note moreover that a measurement of $\alpha_{T_c}$ vs $T_c/T_{c0}$ could provide an experimental tool for an estimation of the typical momentum scattering $Q_c$ in addition to the one obtained by tunneling measurements.

In summary, we have shown that in the nonadiabatic regime the critical temperature is lowered by non-magnetic impurities which also lead to an unusual impurity dependence of the isotope coefficient. Our results together with recent measurements on $K_3C_{60}$ and Nd$_{2-x}$Ce$_x$CuO$_{4-\delta}$ suggest that the $el-ph$ interaction in these systems could be in the nonadiabatic regime. We propose also that in order to confirm or disregard this hypothesis, a suitable experiment could be the measurement of the isotope coefficient as a function of the amount of disorder. We conclude by noticing that, to our knowledge, there are no experimental results on the effect of disorder on the bismuth oxides. Since these materials are s-wave superconductors with estimated $\omega_0/E_F \simeq 0.14$, we predict that in these materials $T_c$ should be considerably lowered by non-magnetic impurities and eventually display an isotope effect with anomalies as described above.

C. G. acknowledges the support of a INFM PRA project (PRA-HTCS).

***

REFERENCES

1. Uemura Y. J., et al., Phys. Rev. Lett., 66 (1991) 2665.
2. Migdal A. B., Sov. Phys. JETP, 7 (1958) 996.
3. Schrieffer J. R., J. Low Temp. Phys., 99 (1995) 377.
4. Chakraverty B. K., Ranninger J., and Feinberg D., Phys. Rev. Lett., 81 (1998) 433.
5. Capone M., Ciuchi S., and Grimaldi C., Europhys. Lett., 42 (1998) 523.
6. Frericks J. K., Zlatić V., Chung W., and Jarrell M., Phys. Rev. B, 58 (1998) 11613.
7. Grimaldi C., Pietronero L., and Strässler S., Phys. Rev. Lett., 75 (1995) 1158.
8. Grimaldi C., Cappelluti E., and Pietronero L., Europhys. Lett., 42 (1998) 667.
9. Zhao G. M., Hunt M. B., Keller H. and Müller K. A., Nature, 385 (1997) 236.
10. Anderson P. W., J. Phys. Chem. Solid, 11 (1959) 26.
11. Watson S. K., et al., Phys. Rev. B, 55 (1997) 3866.
12. Woods S. I., et al., Phys. Rev. B, 58 (1998) 8800.
13. Radtke R. J., et al., Phys. Rev. B, 48 (1993) 653.
14. Openov L. A., JETP Lett., 66 (1997) 661.
15. Rickayzen G., Green’s Functions and Condensed Matter, (Academic, New York) 1980.
16. Pietronero L., Strässler S. and Grimaldi C., Phys. Rev. B, 52 (1995) 1995; Grimaldi C., Pietronero L. and Strässler S., Phys. Rev. B, 52 (1995) 10530.
[17] Zeyher R. and Kulić M., Phys. Rev. B, 54 (1996) 8985; Grilli M. and Castellani C., Phys. Rev. B, 50 (1994) 16880; Keller J., Leal C. E., and Forsthofer F., Physica C, 206-207 (1995) 739.

[18] Danylenko O. V. et al.: cond-mat/9710234, Preprint 1997.

[19] Choi H. Y., Phys. Rev. B, 53 (1996) 8591.

[20] Abrikosov A. A. and L. P. Gor’kov L. P., Sov. Phys. JETP, 12 (1961) 1243.

[21] Bill A., Kresin V. Z., and Wolf S. A., Z. Phys. B, 104 (1997) 759.

[22] Ummarino G. A. and Gonnelli R. S., Phys. Rev. B, 56 (1997) R14 279.

[23] Brawner D. A., Mamsen C., and Ott H. R., Phys. Rev. B, 55 (1997) 2788.
Fig. 1. – The electron-phonon scattering process. The filled circles represent $g(q)$. The last diagram is the first vertex correction $g(q)P(k + q, k)$ which in the adiabatic limit gives a negligible contribution according to Migdal’s theorem.

Fig. 2. – Sign of the vertex function for different values of the impurity scattering rate $\Gamma$ at $\omega_0/E_F = 0.5$. Solid line: $\Gamma = 0$; dashed line: $\Gamma = 0.1\omega_0$; dot-dashed line: $\Gamma = 0.5\omega_0$. 
Fig. 3. – (a): electronic self-energy including the first vertex correction beyond Migdal’s limit and the impurity contribution. (b): Self-consistent equation for the anomalous self-energy generalized to include the first nonadiabatic diagrams (vertex and cross) and the impurity contribution.

Fig. 4. – Critical temperature as a function of the adiabatic parameter $\omega_0/E_F$ for $\lambda = 0.7$. The solid lines refer to the pure case ($\Gamma = 0$) while the dashed lines are the results for $\Gamma = 0.5\omega_0$. Note that at $\omega_0/E_F = 0$ the critical temperature is independent of $\Gamma$. 
Fig. 5. – Critical temperature as a function of the impurity scattering rate $\Gamma$ for $\lambda = 0.7$, $\omega/E_F = 0.2$ (a) and $\omega_0/E_F = 0.4$ (b). The thick (thin) lines refer to the case with (without) the nonadiabatic corrections (4) and (5). Thick solid: $Q_c = 0.1$, thick dashed: $Q_c = 0.3$, thick dot-dashed: $Q_c = 0.5$. Inserts: same calculations rescaled with respect to the critical temperature $T_{c0}$ of pure systems.
Fig. 6. – Isotope coefficient $\alpha_{T_c}$ as a function of $T_c$ in the presence of non-magnetic impurities. Both quantities are normalized to their corresponding values $\alpha_{T_c0}$ and $T_{c0}$ for the pure limit. The curves refer to the case of fig. 5(a).