Nonadiabatic Superconductivity: Electron-Phonon Interaction Beyond Migdal's Theorem

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We generalize Eliashberg's equations to include nonadiabatic effects like vertex corrections, cross phonon scattering, and others arising from the breakdown of Migdal's theorem. This generalization is imposed by the fact that all high T_c superconductors (oxides, fullerene compounds, etc.) have a very small Fermi energy (E_F). Nonadiabatic effects show a complex structure as a function of the exchanged frequency and momenta. In particular, a predominance of small momentum scattering leads to positive contributions with respect to T_c. This situation is actually realized in a correlated Fermi liquid with small E_F that naturally leads to an enhancement of T_c and to various other consequences for the phenomenology of both the superconductive and normal phases.

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The observation of high-temperature superconductivity in the layered cuprates and in the C_{60} compounds has led to a fascinating theoretical challenge that is still quite open and controversial. The magnetic properties of the oxides have stimulated a large effort toward exotic superconductivity mechanisms that would not involve phonons. For the C_{60} compounds instead, the presence of a large isotopic effect and other standard properties seemed to point toward a normal superconductivity mechanism in which the only problem is the calculation of the parameters. Recently both situations have evolved in a somewhat converging trend. The oxides appear more normal in many ways and especially in their superconductivity phenomenology [1]. For the C_{60} compounds instead, the band filling as a function of doping turned out to be anomalous because, among the compounds A_xC_{60} ($A = K, Cs, \ldots$), only the case $x = 3$ is metallic and superconductor [2]. In addition, the comparison between K_3C_{60} and the graphite intercalation compound KC_8, which has a very small $T_c \simeq 0.2$ K, clarifies that also the fullerene compounds are genuine high T_c superconductors that cannot be understood within the standard theory [3].

One possibility is therefore that two new superconductivity theories are needed. The alternative is instead to conceive that the essential mechanism will be only one, the same for both classes of compounds. In this case one should focus on the few common elements of the two classes. This is the point of view we will adopt in this Letter by considering that an important common element of the two classes is that the Fermi energy (E_F) is very small, of the order of the Debye frequency (ω_D) [4]. This implies the breakdown of Migdal's theorem [5] which is at the basis of the many-body electron phonon theory [6] and of the Eliashberg theory of superconductivity [7,8]. For the C_{60} compounds one can estimate [3] $\omega_D \simeq 0.2$ eV and $E_F \simeq 0.2$–0.4 eV, so that $\omega_D/E_F \simeq 0.5$–1. A somewhat lower value can be estimated for the oxides [4] for which, however, the identification of the effective Fermi energy is more problematic.

In this Letter we describe the generalization of Eliashberg equations to include the first nonadiabatic effects. These are the vertex corrections, the cross phonon scattering, and some technical modifications to the self-energy and the gap equation that are necessary if Migdal's theorem does not hold. This generalization brings us in a more general framework in which the limitations of the usual theory do not hold anymore and various new effects are possible. The value of the critical temperature T_c can be enhanced or reduced by the nonadiabatic effects, depending on the properties of the systems. In particular, we show that a strong enhancement of T_c can be obtained if the electron phonon scattering is dominated by small momentum transfer. This situation may be realized in a strongly correlated Fermi liquid or in the vicinity of a strong peak in the density of states.

The generalization of the gap equation to include the first nonadiabatic effects is shown in Fig. 1. The double electronic lines are supposed to include all the self-energy effects. To lowest order these effects are of the order of λ, the usual dimensionless electron-phonon (el-ph)

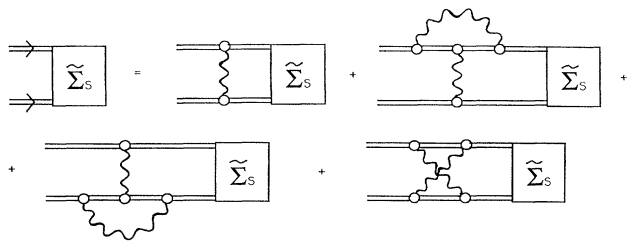

FIG. 1. Self-consistent equation for the scattering amplitude $\tilde{\Sigma}_s$ (related to the gap equation), including the first corrections beyond Migdal's theorem. These are the two vertex corrections and the cross phonon scattering. The generalization of Eliashberg equations for $\omega_0/E_F \neq 0$ implies also some technical differences for the standard self-energy and other effects.

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coupling. In the Eliashberg equations [7], which would correspond to our first term in Fig. 1, these effects are resummed to all orders. The nonadiabatic effects induced by the breakdown of Migdal's theorem can be included perturbatively in terms of the parameter $\lambda(\omega_D/E_F)$, where ω_D is the Debye frequency and E_F the Fermi energy. To first order in this parameter, we have two vertex correction diagrams and the cross phonon scattering process as shown in Fig. 1. Therefore, our scheme is limited to small values of λ if $\omega_D/E_F \approx 1$, but for $\omega_D/E_F \leq 1$ it extends also to relatively large values of λ.

It is interesting to consider in some detail the vertex correction function [9]. The correction that multiplies the bare vertex (g) to include the first contribution beyond Migdal is (Fig. 2)

$$\Lambda(\omega_n, \omega_m, q; \omega_0, E) = 1 + \lambda P_V(\omega_n, \omega_m, q; \omega_0, E), \tag{1}$$

$$P_v(\omega_n, \omega_m, q; \omega_0, E) = -\frac{T}{N_0}\sum_{\omega_s}\sum_{k_s}\left[\frac{1}{i\omega_s - \varepsilon(\mathbf{k}_s)}\right] \times \left[\frac{-\omega_0^2}{(\omega_n - \omega_s)^2 - \omega_0^2}\right] \times \left[\frac{1}{i(\omega_s - \omega_m) - \varepsilon(\mathbf{k}_s - \mathbf{q})}\right]. \tag{2}$$

In Eqs. (1) and (2) we use the usual Matsubara notations [6], and the ω_0^2 in the numerator corresponds to the fact that we consider the coupling g as already renormalized and N_0 is the density of states. The vertex function P_V depends on the variables q and ω_m of the exchanged phonon and on the parameters ω_0, the frequency of an Einstein phonon and $E = 2E_F$. The dependence on E on the right-hand side of the equation will arise from the dispersion and the limits of integration. Usually we will neglect the dependence on ω_n by considering only the case $\omega_n = 0$ (in the $T \to 0$ limit). In fact, the dependence on the value of the incoming frequency is weak because the process depends essentially on the exchanged frequency [10,11].

The first estimate of the vertex function is of course due to Migdal [5] who showed that P_V is of the order of ω_0/E_F. The original Migdal estimate, however, did not provide a specific result for the vertex function nor could one estimate its sign. A more detailed calculation was performed by Grabowsky and Sham [12] in the context of plasmon mediated superconductivity. They computed P_V in a particular limit and showed that $\lim_{q\to 0}\lim_{\omega_m\to 0} P_V < 0$. This result appeared reasonable because it allowed one to reduce to more realistic values the too high values of T_c that one obtains for the plasmon interaction. This paper generated the opinion that vertex corrections should, in general, be negative. Recently this problem has received further attention, but mainly in situations in which it is not possible to discuss its momentum dependence [13,14] or by considering particular averages over frequency and momentum [15].

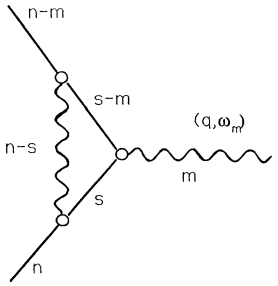

FIG. 2. First-order vertex correction diagram. The resulting vertex function can be positive or negative depending on the values of the momentum (q) and frequency (ω_m) of the emitted phonon.

A detailed calculation of Eq. (2) keeping the full dependence of ω_m and q shows in fact a rich and complex behavior [9,11]. In Fig. 3 we report the sign of the vertex function P_V as a function of $Q = q/E$ and $\omega = \omega_m$ with $\omega_n = 0$. Our calculation requires drastic simplifications for the band structure and for the density of states of the system. However, given the various averages that are contained in Eq. (2), we do not expect these effects to be crucial in general. From Fig. 3 we can see that in the limit $\omega \to 0$ followed by $Q \to 0$ we indeed obtain a negative value in agreement with Ref. [10]. This, however, is not representative because there is also a large positive area. In Fig. 4 we report the value of $P_V(\omega)$ for different values of Q. It is important to note that for small values of Q the positive part of P_V becomes predominant. This situation is in evidence of the importance of an eventual Q dependence of the el-ph scattering $g(Q)$.

A similar study can be performed for the cross-scattering term that also shows a complex behavior as function of Q and ω, somewhat similar to the one we have discussed for P_V. At this point it is possible to generalize the Eliashberg equations to include these effects. In the critical region the generalized equations can be written as [10,11]

$$\Delta(i\omega_n)Z(i\omega_n) = \pi T_c\sum_m \frac{\lambda_\Delta(\omega_n, \omega_m, Q_c; \omega_0, E)\omega_0^2}{(\omega_n - \omega_m)^2 + \omega_0^2} \times \frac{\Delta(i\omega_m)}{|\omega_m|}\frac{2}{\pi}\arctan\left[\frac{E}{2Z(i\omega_m)|\omega_m|}\right], \tag{3}$$

$$Z(i\omega_n) = 1 + \frac{\pi T_c}{\omega_n}\sum_m \frac{\lambda_z(\omega_n, \omega_m, Q_c; \omega_0, E)\omega_0^2}{(\omega_n - \omega_m)^2 + \omega_0^2}\frac{\omega_m}{|\omega_m|} \times \frac{2}{\pi}\arctan\left[\frac{E}{2Z(i\omega_m)|\omega_m|}\right], \tag{4}$$

in which we have introduced the effective couplings λ_Δ and λ_z defined as follows:

$$\lambda_\Delta(\omega_n, \omega_m, Q_c; \omega_0 E) = \lambda[1 + 2\lambda P_V(\omega_n, \omega_m, Q_c; \omega_0 E) + \lambda P_c(\omega_n, \omega_m, Q_c; \omega_0 E)], \tag{5}$$

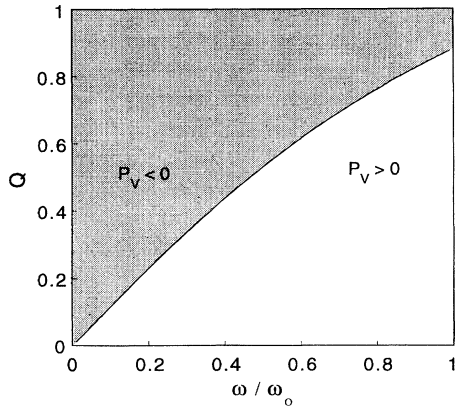

FIG. 3. Sign of the vertex correction function $P_V(Q,\omega)$ for the case $\omega_0/E_F = 1$. The white areas correspond to $P_V > 0$ and the dark areas to $P_V < 0$. The general structure of $P_V(Q,\omega)$ is therefore rather complex, and its role in the gap equation depends in detail on the scattering properties of the system.

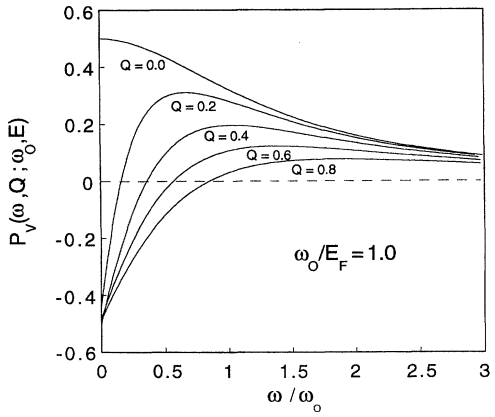

FIG. 4. Behavior of $P_V(\omega)$ for different values of Q. For small Q values the positive part of the vertex function becomes predominant. This figure refers to the case $\omega_n = 0$ and $\omega_m = \omega$.

$$\lambda_\Delta(\omega_n,\omega_m,Q_c;\omega_0,E) = \lambda[1+\lambda P_V(\omega_n,\omega_m,Q_c;\omega_0,E)]. \tag{6}$$

As mentioned, we consider the case $\omega_n = 0$ in P_V and P_c. The ω_m dependence will find a natural cutoff in ω_0 when these functions are used in the gap equation. The situation is more delicate for the Q dependence for which different physical mechanisms for the scattering can lead to quite different nonadiabatic effects. For this reason we introduce an upper cutoff Q_c for the el-ph scattering and discuss our results as a function of Q_c. Namely, the Q dependence of the function P_V and P_c is averaged between 0 and Q_c. Given our scheme of calculation, an average over the whole Brillouin zone corresponds roughly to setting $Q_c = 1$. The use of different values ($Q_c < 1$) is meant to reproduce the effect of an upper cutoff in $g(Q)$. In order to compare the results for different values of Q_c as corresponding to same values of λ, we normalize $g(Q)$ in such a way that the average $\langle g\rangle$ over the Brillouin zone is the same for different values of Q_c.

In order to obtain analytical expressions, a good approximation, which we have tested numerically, is to neglect the frequency dependence in P_V and P_c by taking their values at $\omega_m = \omega_0$. This leads to [10,11]

$$P_V(m,Q_c) = -A(m) + \left[\frac{\pi}{4} - \arctan\left(\frac{m}{1+m}\right) + A(m)\right]\frac{m^2}{4Q_c^4} \times \left\{\sqrt{1+\left(\frac{4Q_c^2}{m}\right)^2} - 1 - \ln\left[\left[1+\sqrt{1+\left(\frac{4Q_c^2}{m}\right)^2}\right]\Big/ 2\right]\right\}, \tag{7}$$

where $m = \omega_0/E_F$ is the Migdal parameter and

$$A(m) = \frac{m(1+m)[(1+m)^2+2m^2]}{[(1+m)^2+2m^2]^2}. \tag{8}$$

For the cross function the average over Q cannot be performed analytically and we approximate it just by considering its value $Q \simeq Q_c/2$. This leads to [12]

$$P_c(m,Q_c) = -A(m) + \left[\frac{\pi}{4} - \arctan\left(\frac{m}{1+m}\right) + A(m)\right] \times \frac{m}{4Q_c^2[1-(Q_c/2)^2]} \times \arctan\{(4/m)[1-(Q_c/2)^2 Q_c^2]\}. \tag{9}$$

The generalized Eliashberg's Eqs. (3) and (4) can be solved numerically to determine T_c, and we will discuss this point in detail elsewhere [10,11]. It is useful, however, to derive an approximate analytical expression for T_c following the scheme of McMillan [16] or the more accurate one of Combescot [17]. We obtain [12]

$$T_c = \left[\frac{1.13\omega_0}{\sqrt{e}(1+m)}\exp\left[\frac{1}{2}\frac{m}{1+m}\right]\right] \times \exp\left[\frac{-\{1+\lambda_z[1/(1+m)]\}}{\lambda_\Delta}\right] \tag{10}$$

that agrees well with our numerical solutions over a broad range of parameters. In Fig. 5 we show the value of T_c as a function of the Migdal parameter $m = \omega_0/E_F$ for $\lambda = 0.5$ and for different values of the momentum cutoff Q_c. The case $m = 0$ corresponds to Migdal's limit. One can see that for relatively small values of Q_c a substantial enhancement with respect to the standard theory ($m = 0$) can be obtained.

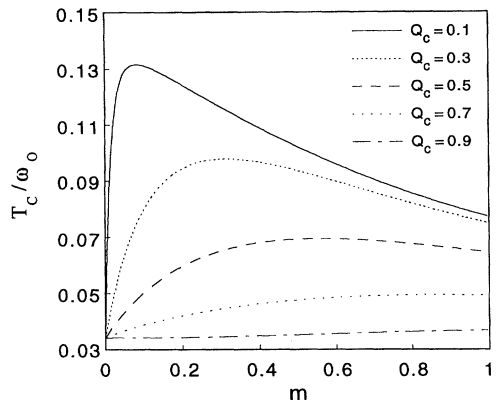

FIG. 5. Critical temperature T_c as a function of the Migdal parameter $m = \omega_0/E_F$ for $\lambda = 0.5$ and different values of the upper cutoff for the exchanged momentum Q_c. The limit $m \to 0$ corresponds to the Migdal-Eliashberg limit. Small values of Q_c (mainly forward scattering) lead to a large enhancement of T_c.

An important element to consider at this point is the relation of our highly simplified calculation to the complexity of real materials. For example, we have neglected the Coulomb repulsion term μ^* [16] not because we believe it to be negligible, but rather because in the high T_c materials the study of μ^* cannot be limited to a single narrow band, but other bands or states have to be involved [18]. The limitation of the phonon scattering to a single narrow band is justified by the fact that the Debye frequency is lower than the gaps between different bands. In any case our results show that, in the regime of positive nonadiabatic effects, the effective el-ph coupling for the Cooper channel can be strongly enhanced so to overcome also relatively large values of μ^*.

We have seen that an essential point of our results is the Q dependence of the nonadiabatic effects. In particular a predominance of small Q scattering leads to appreciable enhancements of T_c. This situation can be realized if there are peaks in the density of states near the Fermi surface but also, more generally, if one includes in the problem the effects of electronic correlations due to Coulomb interactions. Various authors [19–21] have recently considered this problem with different approaches. In all cases the effect of electronic correlations is to enhance small Q scattering with respect to large Q scattering.

In addition to the enhancement of T_c nonadiabatic effects are expected to have many other implications on both the superconducting and normal properties. For example, the isotope effect can become negligibly small if $\omega_0 \geq E_F$, but also anomalously large ($\alpha > 1/2$) in an intermediate region [10,11]. The introduction of μ^* in the theory is expected to reduce the value of α. Various anomalous properties of the high T_c superconductors like the absence of the Hebel-Slichter peak, the ratio $2\Delta_0/T_c$, and the second peak in $\Delta(\omega)$ can be reproduced in appreciable detail using the standard Eliashberg equations with an unrealistically large value of the coupling $\lambda \geq 3$ [22]. It is possible to show that the use of our generalized theory [Eqs. (3)–(5)], even though only to first order in the nonadiabatic effects, would allow the same phenomenology to be reproduced with a more realistic value $\lambda \leq 1$ [23]. This shows the important result that nonadiabatic effects in a regime of medium-weak coupling can give rise to a phenomenology that, from the usual point of view, would appear as corresponding to very strong coupling. Vertex corrections should also play an important role on various other properties of the normal state like transport, photoemission lines, lifetime effects, etc.

In summary, we have presented a new perspective for the phenomenon of high T_c superconductivity. The crucial point is the breakdown of Migdal's theorem that requires the inclusion of nonadiabatic effects and the generalization of Eliashberg equations. Electronic correlations are also important because they bring the system into a favorable regime that leads to an enhancement of T_c and to various other effects. In our opinion, the conceptual strength of the present approach is that the small value of E_F is a well-established experimental fact common to all high T_c superconductors [24].

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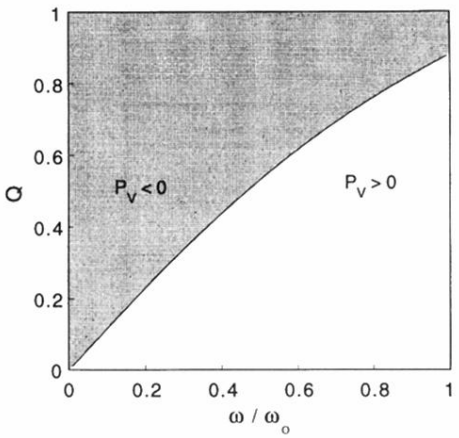

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