

Nonadiabatic superconductivity and vertex corrections in uncorrelated systems

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We investigate the issue of the nonadiabatic superconductivity in uncorrelated systems. A local approximation is employed coherently with the weak dependence on the involved momenta. Our results show that nonadiabatic vertex corrections are never negligible, but lead to a strong suppression of T_c with respect to the conventional theory. This feature is understood in terms of the momentum-frequency dependence of the vertex function. In contrast to strongly correlated systems, where the small \mathbf{q} selection probes the positive part of vertex function, vertex corrections in uncorrelated systems are essentially negative resulting in an effective reduction of the superconducting pairing. Our analysis shows that vertex corrections in nonadiabatic regime can never be disregarded independently of the degree of electronic correlation in the system.

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One of the characteristics of the high transition temperature superconductors (HTSC) is the small density of charge carriers.¹ As a consequence, the scale of the electronic dynamics, the Fermi energy E_F , is comparable with the typical phonon frequencies ω_{ph} and the adiabatic parameter ω_{ph}/E_F becomes significant. This situation opens the way to a scenario in which nonadiabatic effects are relevant. From a diagrammatic point of view, nonadiabatic effects can be taken into account by the inclusion of vertex corrections arising from the breakdown of Migdal's theorem.² However, in general, this amounts to consider an infinite set of nonadiabatic diagrams whose resummation is a formidable task. Nevertheless, it is possible to formulate a perturbative theory by assuming that the order of magnitude of the first vertex corrections $\lambda \omega_{\text{ph}}/E_F$,² is small enough to be treated as an expansion parameter.^{3,4} In principle, this assumption is fulfilled by nonadiabatic weak coupling systems ($\lambda < 1$ and $\omega_{\text{ph}}/E_F \sim 1$) or moderately nonadiabatic strong coupling materials ($\lambda \sim 1$ and $\omega_{\text{ph}}/E_F < 1$).

In previous studies we have shown how such a perturbative approach accounts for some of the anomalous properties of the HTSC materials. In particular, large values of T_c , compared with the ones predicted by the Migdal-Eliashberg (ME) theory, are related in a natural way to the opening of nonadiabatic channels in the Cooper pairing with no need of assuming large values of λ .^{5,6} To understand from a microscopical point of view in which way the nonadiabatic channels affect the superconducting properties, and in particular the critical temperature T_c , a detailed study of the momentum-frequency structure of the vertex function is needed. In fact, vertex function presents a complex behavior with respect to the momentum \mathbf{q} and the frequencies ω of the exchanged phonon.^{3,4} In particular the vertex function has been shown to be positive for small values of \mathbf{q} and negative for large values of \mathbf{q} compared to ω , leading respectively to an enhancement and to a decrease of the superconducting pairing. The evaluation *a priori* of the nonadiabatic effects on T_c is thus not at all easy, since it will depend on the total

balance of negative and positive parts of the vertex function. In this perspective, specific properties of real materials become very important, since they can modify the balance favouring or disfavouring positive or negative parts and determining an enhancement or a suppression of the critical temperature.

In particular, in strongly correlated systems the electron correlation due to onsite Coulomb repulsion has shown to be actually responsible for a predominance of small- \mathbf{q} scattering yielding an effective modulation of the electron-phonon coupling.^{7,8} In this situation the positive part of the nonadiabatic vertex corrections is mainly probed, leading to a net increase of the coupling in Cooper channel and to a corresponding enhancement of the critical temperature T_c .⁴⁻⁶ On the other hand in uncorrelated systems the \mathbf{q} dependence is weak and the negative part of the vertex corrections at large momenta is expected to lead to a resulting decrease of the Cooper pairing and of T_c .

The aim of this short communication is twofold. First, we show that nonadiabatic effects cannot be neglected also in uncorrelated materials (structureless electron-phonon interaction) and vertex corrections play a primary role in suppressing the superconducting pairing as long as ω_{ph}/E_F is not negligible. Second, we argue that the nonadiabatic superconductivity developed by us for the small \mathbf{q} scattering regime is also a rather good approximation of the uncorrelated case, providing therefore a unified and reasonable description of both the correlated and uncorrelated cases.

In conventional metals, according to Migdal's theorem,² the smallness of the adiabatic parameter ω_{ph}/E_F permits us to describe successfully the electron-phonon coupled system by neglecting the vertex corrections in the electron-phonon interaction. The application of Migdal's theorem to the superconducting state has led to the ME equations of superconductivity,⁹ which accurately describe the properties of conventional superconductors.¹⁰ A different situation is encountered in nonadiabatic materials, as we have briefly discussed above, where the breakdown of Migdal's theorem

is expected. The relevance of the nonadiabatic corrections can be established by evaluating the vertex function schematized as

$$P(\omega_n, \omega_m; \mathbf{q}) = g^2 \sum_{p, \omega_l} D(\omega_n - \omega_l) G(\mathbf{p}, \omega_l) \times G(\mathbf{p} + \mathbf{q}, \omega_l + \omega_m), \quad (1)$$

where D and G represent respectively the phonon and the electron propagators, g is the electron-phonon matrix element, and ω_n , ω_m , and ω_l are fermionic Matsubara frequencies. We adopt a simple Einstein spectrum with frequency ω_0 for the phonon propagator $D(\omega_n - \omega_l) = -\omega_0^2 / [\omega_0^2 + (\omega_n - \omega_l)^2]$.

As shown by Migdal in his pioneering work,² the vertex function, given in Eq. (1), scales as $\lambda \omega_{\text{ph}} / E_F$, where $\lambda = 2N_0 g^2 / \omega_0$ is the dimensionless electron-phonon coupling and N_0 is the electronic density of states (DOS) at the Fermi level. To obtain this result typical phonon momenta are assumed to be of the order of the Debye momentum $q_D \sim k_F$. However, as briefly above discussed, this assumption breaks down in strongly correlated systems where the predominance of small- \mathbf{q} scattering is important to establish the enhancement of the critical temperature.

The small- \mathbf{q} selection due to strong Coulomb repulsion in strongly correlated systems can be simulated by a cutoff q_c in the exchanged momentum space so that $\sum_{\mathbf{q}} \rightarrow \sum_{\mathbf{q}} \theta(q_c - |\mathbf{q}|)$ which restricts the momentum integrations. In this situation we replace the vertex function $P(\omega_n, \omega_m; \mathbf{q})$ by its average over momenta $P(\omega_n, \omega_m; q_c)$ that depends only on the frequencies and on the cutoff q_c :

$$P(\omega_n, \omega_m; q_c) = \frac{\sum_{\mathbf{q}} \theta(q_c - |\mathbf{q}|) P(\omega_n, \omega_m; \mathbf{q})}{\sum_{\mathbf{q}} \theta(q_c - |\mathbf{q}|)}. \quad (2)$$

We can generalize the ME equations to include the momentum average of the first order vertex corrections due to the breakdown of Migdal's theorem. The generalized ME equations in the nonadiabatic regime for the self-energy renormalization function Z and for the superconducting gap Δ are the following:⁴

$$Z(\omega_n) = 1 + \frac{T_c}{\omega_n \omega_m} \sum_{\omega_m} \Gamma_Z(\omega_n, \omega_m, Q_c) \eta_m, \quad (3)$$

$$Z(\omega_n) \Delta(\omega_n) = T_c \sum_{\omega_m} \Gamma_{\Delta}(\omega_n, \omega_m, Q_c) \frac{\Delta(\omega_m)}{\omega_m} \eta_m, \quad (4)$$

where $\eta_m = 2 \arctan\{E_F / [Z(\omega_m) \omega_m]\}$ and $Q_c = q_c / 2k_F$ is the dimensionless cutoff. The kernels of Eqs. (3) and (4) are, respectively, given by

$$\Gamma_Z(\omega_n, \omega_m, Q_c) = \lambda D(\omega_n - \omega_m) [1 + \lambda P(\omega_n, \omega_m, Q_c)],$$

$$\Gamma_{\Delta}(\omega_n, \omega_m, Q_c) = \lambda D(\omega_n - \omega_m) [1 + 2\lambda P(\omega_n, \omega_m, Q_c)] + \lambda^2 C(\omega_n, \omega_m, Q_c).$$

Explicit expressions of the vertex P and cross C functions have been obtained analytically for small values of Q_c in

Refs. 3 and 11. Higher order nonadiabatic corrections in Γ_Z and Γ_{Δ} , here not taken into account, should be explicitly included in the extreme nonadiabatic regime where $\lambda P \sim 1$ ($\lambda C \sim 1$).¹² This intriguing issue is, however, beyond the purpose of our paper, and all the following results apply only when $\lambda \omega_{\text{ph}} / E_F$ is small enough to permit truncation of higher order vertex corrections.

The nonadiabatic equations of superconductivity Eqs. (3) and (4) have been numerically solved and the resulting T_c has found to be strongly enhanced with respect to the adiabatic case due to the inclusion of vertex corrections and to the presence of electronic correlation that favors small- \mathbf{q} scattering.^{5,6} A different situation is encountered when we look at uncorrelated systems where the \mathbf{q} dependence of the relevant physical quantities is weak. In this case no restriction in the momenta integration is expected and the momentum average of the vertex function becomes an almost exact approximation. As easily seen from Eq. (2) this corresponds to a local theory in which the vertex function becomes

$$P_{\text{loc}}(\omega_n, \omega_m) = \sum_{\mathbf{q}} P(\omega_n, \omega_m; \mathbf{q}) = g^2 \sum_{\omega_l} D(\omega_n - \omega_l) G_{\text{loc}}(\omega_l) G_{\text{loc}}(\omega_l + \omega_m), \quad (5)$$

where G_{loc} is the local electron propagator

$$G_{\text{loc}}(\omega_n) = \int d\epsilon \frac{N(\epsilon)}{i\omega_n Z(\omega_n) - \epsilon}.$$

For a direct comparison we adopt the same simplifications of Refs. 3 and 4, namely, we considered a half-filled constant DOS band with $N(\epsilon) = N_0$, $-E_F \leq \epsilon \leq E_F$. E_F represents then the Fermi energy.

The nonadiabatic equations of superconductivity for uncorrelated systems are thus formally obtained by substituting the local vertex function given by the Eq. (5) in the kernels Γ_Z and Γ_{Δ} of Eqs. (3) and (4). The numerical solution of such equations in local regime follows the usual scheme. Therefore, without entering in details, we are going to discuss the results.

In Fig. 1(a) we show the superconducting transition temperature T_c of uncorrelated nonadiabatic systems as function of dimensionless electron-phonon coupling λ for three different adiabatic parameters. To evidence the effects of the vertex corrections, the results of the nonadiabatic local theory are compared with those obtained by the conventional one for values of λ up to the unphysically large $\lambda = 3$, where of course the perturbative approach breaks down ($\lambda \omega_0 / E_F \sim 1$). Solid lines represent the ME solutions where nonadiabatic effects are just included by considering finite energy bandwidth. This is thus equivalent to a noncrossing approximation (NCA). Dashed lines are the numerical results of Eqs. (3) and (4), where the vertex function is given in the local theory by Eq. (5). From top to the bottom, different lines correspond to adiabatic parameters $\omega_0 / E_F = 0.1, 0.4, 0.7$.

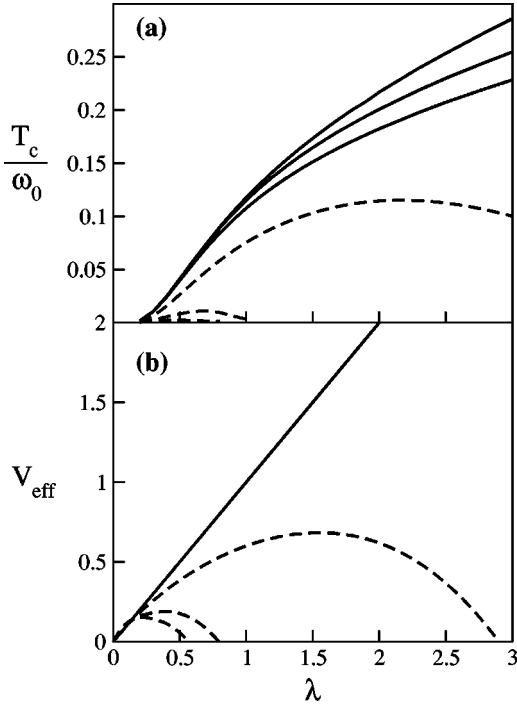


FIG. 1. (a) T_c as function of λ in uncorrelated nonadiabatic systems. Solid lines correspond to the noncrossing approximation; dashed lines correspond to the nonadiabatic local theory. Both the cases are shown (from top to bottom) for $\omega_0/E_F = 0.1, 0.4, 0.7$. (b) Behavior of effective pairing interaction V_{eff} as function of λ in noncrossing approximation (solid line) and in the nonadiabatic local theory (dashed lines).

As shown in Fig. 1(a) nonadiabatic effects in uncorrelated systems lead to a drastic reduction of the critical temperature T_c with respect to the conventional theory. This result confirms the above qualitative discussion suggesting that in uncorrelated systems the negative part of the vertex function is more relevant yielding therefore an effective reduction of the pairing. The increase of this effect by increasing both the electron-phonon coupling λ and the adiabatic parameter ω_0/E_F seems also to point towards a similar conclusion, since the vertex corrections scale as $\lambda \omega_0/E_F$.

In order to quantify this concept we parametrize the magnitude of the “effective” superconducting pairing V_{eff} with the static limit of the superconductive kernel $V_{\text{eff}} = \Gamma_{\Delta}(\omega_n = 0, \omega_m = 0)$. In conventional ME theory V_{eff} reduces to the simply bare electron-phonon coupling constant $V_{\text{eff}} = \lambda$, while the opening of nonadiabatic channels strongly affects V_{eff} through the vertex function calculated in the local theory. The dependence of the effective interaction V_{eff} on the bare electron-phonon coupling λ in both the cases is plotted in Fig. 1(b). The similarity between the behaviors of T_c and V_{eff} is striking pointing out that this particular limit of the superconductive kernel and of the vertex function is directly reflected on the critical temperature T_c : the static negative limit³ of the vertex function reduces V_{eff} and induces a strong suppression of T_c . The nonmonotonic behavior of T_c in uncorrelated nonadiabatic systems is thus simply related to the non monotonic underlying behavior of V_{eff} : the maximum is determined roughly by the value of λ which gives $dV_{\text{eff}}/d\lambda$

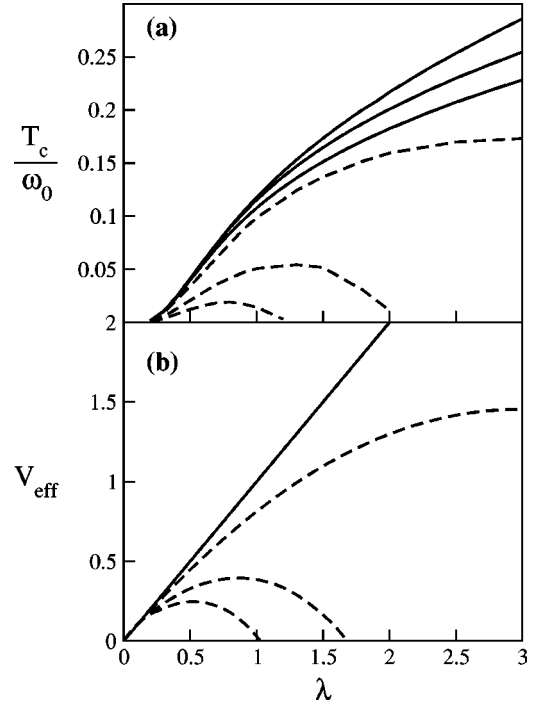


FIG. 2. T_c (a) and V_{eff} (b) calculated by the small- \mathbf{q} expansion of the vertex corrections for $Q_c = 1$. Solid and dashed lines as defined in the previous caption.

$= 0$ corresponding to $4\lambda P_{\text{loc}}(\omega_n = 0, \omega_m = 0) = -1$ (cross function is negligible and can be omitted for the discussion). We conclude that nonadiabatic effects are dominant also in uncorrelated systems where they lead to a strong reduction of T_c .

Let us address now whether the nonadiabatic theory developed in Refs. 4 and 5 for small momentum transfers (small Q_c) are capable of reproducing the results of the local theory ($Q_c = 1$). In fact, it would be interesting to define a common approach which would permit to span from uncorrelated to correlated cases. From this point of view, the small- Q_c expansion of the vertex function used in Refs. 3 and 4 appears a promising tool to extrapolate to intermediate Q_c 's. In particular, as we can see from Eq. (2), the uncorrelated case corresponds in this framework to a $Q_c = 1$. We stress that the equivalence between this procedure and the local theory is only formal since using $Q_c = 1$ in a small- Q_c expansion is obviously an approximation.

In Fig. 2 the critical temperature T_c and the “effective” superconducting pairing V_{eff} calculated within the small- \mathbf{q} approach with $Q_c = 1$ are shown. The overall features of both T_c and V_{eff} are quite the same as in the local theory with a slight overestimation of T_c and V_{eff} . This is not unexpected since the small- \mathbf{q} expansion emphasizes the positive region of the vertex function and as a consequence underestimates the net negative magnitude of it. However, the qualitative agreement between Figs. 1 and 2 is quite good suggesting that the nonadiabatic evaluation of the vertex function based on the small- \mathbf{q} expansion can actually interpolate from weak to large correlation.

This is confirmed in Fig. 3 where we plot the evolution of

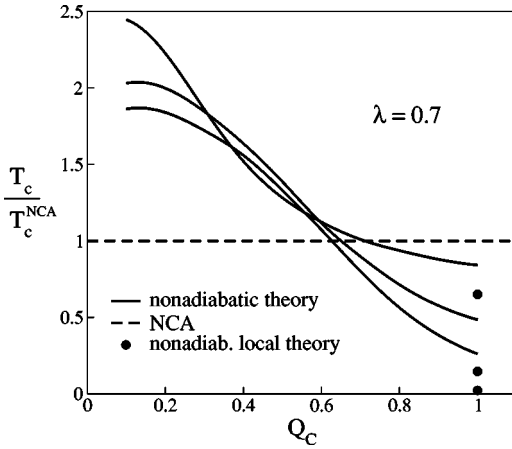


FIG. 3. T_c as function of Q_c as evaluated by the small- \mathbf{q} expansion (solid lines). Dashed lines represents T_c in non crossing approximation and filled circles the nonadiabatic local theory for uncorrelated systems. From top to bottom: $\omega_0/E_F=0.1, 0.4, 0.7$

the critical temperature T_c in nonadiabatic regime calculated within the small- \mathbf{q} approach (solid lines) as function of Q_c . In an exact theory the solid lines would end at $Q_c=1$ in the filled circles, representing the nonadiabatic local theory. The discrepancy is shown to be quite small and almost independent of the nonadiabatic parameter. In general, we can identify two different regimes: the first one, for small Q_c 's, is relevant for strong correlated systems where the critical temperature is effectively enhanced with respect the conventional theory by nonadiabatic effects; the second one which represent weakly correlated compounds where nonadiabatic vertex corrections produces a significant reduction of T_c . While the first regime is expected to be well described by the small- \mathbf{q} approach, Fig. 3 shows that it works qualitatively

well also in uncorrelated systems providing therefore a unique tool to evaluate the nonadiabatic effects on the critical temperature. This appears even more important since the analytical study of the vertex function in small- \mathbf{q} expansion allows to understand from a microscopic point of view the way through the which the nonadiabatic vertex function enhances or reduces T_c , respectively, in correlated and uncorrelated systems.

In conclusion, we have investigated the nonadiabatic effects in uncorrelated systems. We have shown that the breakdown of Migdal's theorem and the consequent inclusion of vertex diagrams lead to a strong suppression of the critical temperature T_c . Nonadiabatic effects cannot be neglected in uncorrelated materials as well as in correlated ones when the Fermi energy is comparable to the phonon frequencies. We show also that the nonadiabatic theory based on a small- \mathbf{q} expansion, early introduced in previous papers, works quite well even in uncorrelated systems where no predominance of forward scattering is present. Of course, as already stressed above, this conclusion holds true as long as higher order vertex corrections can be neglected ($\lambda\omega_{ph}/E_F$ sufficiently small).

As a final observation, we would like to remark that the present analysis has been restricted to the half-filling case. Away from half-filling, and in particular for Fermi levels very close to the bottom (top) of the band, the vertex function changes significantly its structure becoming roughly shapeless in momentum space and mainly positive.¹³ In such a situation nonadiabatic vertex corrections can give rise to an enhancement of T_c even for uncorrelated systems.¹⁴ This case can be for instance relevant for the recently discovered superconductivity at $T_c \approx 40$ K in MgB_2 ,¹⁵ where the chemical potential is very close to the top of the σ bands, with $E_F \approx 0.5$ eV, thus comparable to the phonon frequencies.

¹Y. J. Uemura *et al.*, Phys. Rev. Lett. **66**, 2665 (1991).

²A. B. Migdal, Zh. Eksp. Teor. Fiz. **34**, 1438 (1958) [Sov. Phys. JETP **7**, 996 (1958)].

³L. Pietronero, S. Strässler and C. Grimaldi, Phys. Rev. B **52**, 10 516 (1995).

⁴C. Grimaldi, L. Pietronero, and S. Strässler, Phys. Rev. B **52**, 10 530 (1995).

⁵C. Grimaldi, L. Pietronero, and S. Strässler, Phys. Rev. Lett. **75**, 1158 (1995).

⁶E. Cappelluti, C. Grimaldi, L. Pietronero, and S. Strässler, Phys. Rev. Lett. **85**, 4771 (2000).

⁷R. Zeyher and M. L. Kulić, Phys. Rev. B **53**, 2850 (1996).

⁸M. L. Kulić, Phys. Rep. **338**, 1 (2000).

⁹G. M. Eliashberg, Zh. Eksp. Teor. Fiz. **38**, 966 (1960) [Sov. Phys. JETP **11**, 696 (1960)].

¹⁰J. P. Carbotte, Rev. Mod. Phys. **62**, 1027 (1990).

¹¹M. Scattoni, C. Grimaldi, and L. Pietronero, Europhys. Lett. **47**, 588 (1999).

¹²O. V. Dolgov, D. A. Kirzhnits, and E. G. Maksimov, Rev. Mod. Phys. **53**, 81 (1981).

¹³A. Perali, C. Grimaldi, and L. Pietronero, Phys. Rev. B **58**, 5736 (1998).

¹⁴J. K. Freericks, Phys. Rev. B **50**, 403 (1994).

¹⁵J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, and J. Akimitsu, Nature (London) **410**, 63 (2001).