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 \( q \)-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 be never 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. As a consequence, the scale of the electronic dynamics, the Fermi energy \( E_F \), is comparable with the typical phonon frequencies \( \omega_{\text{ph}} \) and the adiabatic parameter \( \omega_{\text{ph}}/E_F \) 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. 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, \( \lambda \omega_{\text{ph}}/E_F \), is small enough to be treated as an expansion parameter. In principle, this assumption is fulfilled by nonadiabatic weak coupling systems \( (\lambda < 1 \text{ and } \omega_{\text{ph}}/E_F \sim 1) \) or moderately nonadiabatic strong coupling materials \( (\lambda \sim 1 \text{ and } \omega_{\text{ph}}/E_F < 1) \).

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 \( \lambda \). 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 behaviour with respect to the momentum \( q \) and the frequencies \( \omega \) of the exchanged phonon. In particular the vertex function has been shown to be positive for small values of \( q \) and negative for large values of \( q \) compared to \( \omega \), leading respectively to an enhancement and to a decrease of the superconducting pairing. The evaluation \( \text{a priori} \) 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-\( q \) scattering yielding an effective modulation of the electron-phonon coupling. In this situation the positive part of the nonadiabatic vertex corrections is mainly probed, leading to an net increase of the coupling in Cooper channel and to a corresponding enhancement of the critical temperature \( T_c \). On the other hand in uncorrelated systems the \( q \)-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 \( \omega_{\text{ph}}/E_F \) is not negligible. Second, we argue that the nonadiabatic superconductivity developed by us for the small \( q \) 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,3 the smallness of the adiabatic parameter \( \omega_{ph}/E_F \) permits 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,3 which accurately describe the properties of conventional superconductors. 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

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

where \( D \) and \( G \) represent respectively the phonon and the electron propagators, \( g \) is the electron-phonon matrix element, and \( \omega_n, \omega_m \) and \( \omega_l \) are fermionic Matsubara frequencies. We adopt a simple Einstein spectrum with frequency \( \omega_0 \) 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 work3 the vertex function, given in the Eq. (1), scales as \( \lambda \omega_{ph}/E_F \) where \( \lambda = 2N_0g^2/\omega_0 \) 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-\( q \) scattering is important to establish the enhancement of the critical temperature.

The small-\( q \) selection due to strong Coulomb repulsion in strongly correlated systems can be simulated by a cut-off \( q_c \) in the exchanged momentum space so that

\[
\sum_{\mathbf{q}} \to \sum_{\mathbf{q}} \theta(q_c - |\mathbf{q}|)
\]

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 cut-off \( q_c \):

\[
P(\omega_n, \omega_m; q_c) = \sum_{\mathbf{q}} \theta(q_c - |\mathbf{q}|)P(\omega_n, \omega_m; \mathbf{q}) \sum_{\mathbf{q}} \theta(q_c - |\mathbf{q}|).
\]

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 \( \Delta \) are the following:

\[
Z(\omega_n) = 1 + \frac{T_c}{\omega_n} \sum_{\omega_m} \Gamma_Z(\omega_n, \omega_m, Q_c) \eta_m,
\]

\[
Z(\omega_n)\Delta(\omega_n) = T_c \sum_{\omega_m} \Gamma_\Delta(\omega_n, \omega_m, Q_c) \frac{\Delta(\omega_m)}{\omega_m} \eta_m.
\]

where \( \eta_m = 2 \arctan( E_F/|Z(\omega_m)\omega_m|) \) and \( Q_c = q_c/2k_F \) is the dimensionless cut-off. The kernels of the equations (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 and cross C functions have been obtained analytically for small values of \( Q_c \) in Refs.3,6 Higher order nonadiabatic corrections in \( \Gamma_Z \) and \( \Gamma_\Delta \) have not been taken into account, should be explicitly included in the extreme nonadiabatic regime where \( \lambda P \sim 1 \) (\( \lambda C \sim 1 \)). This intriguing issue is however beyond the purpose of our paper, and all the following results apply only when \( \lambda \omega_{ph}/E_F \) 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 favours small-\( q \) scattering.3

A different situation is encountered when we look at uncorrelated systems where the \( q \)-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. (3) this corresponds to a local theory in which the vertex function becomes

\[
P_{loc}(\omega_n, \omega_m) = \sum_{\mathbf{q}} P(\omega_n, \omega_m; \mathbf{q})
\]

\[
= g^2 \sum_{\omega_l} D(\omega_n - \omega_l)G_{loc}(\omega_l)G_{loc}(\omega_l + \omega_m),
\]

where \( G_{loc} \) is the local electron propagator:

\[
G_{loc}(\omega_n) = \int d\epsilon \frac{N(\epsilon)}{\omega_n Z(\omega_n) - \epsilon}.
\]

For a direct comparison we adopt the same simplification as in Refs.3,6 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. (3) in the kernels \( \Gamma_Z \) and \( \Gamma_\Delta \) of the equations (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. 1a we show the superconducting transition temperature \( T_c \) of uncorrelated nonadiabatic systems as function of dimensionless electron-phonon coupling \( \lambda \) for three different adiabatic parameters. To evidence the
coupling constant $V_{\text{eff}} = \lambda$, while the opening of nonadiabatic channels strongly affects $V_{\text{eff}}$ through the vertex function calculated in the local theory. The dependence of the effective interaction $V_{\text{eff}}$ on the bare electron-phonon coupling $\lambda$ in both the cases is plotted in Fig. 1b. The similarity between the behaviours of $T_c$ and of $V_{\text{eff}}$ 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 limit of the vertex function reduces $V_{\text{eff}}$ and induces a strong supression of $T_c$. The non monotonic behaviour of $T_c$ in uncorrelated nonadiabatic systems is thus simply related to the non monotonic underlying behaviour of $V_{\text{eff}}$: the maximum is determined roughly by the value of $\lambda$ which gives $dV_{\text{eff}}/d\lambda = 0$ 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 Ref. 4,5 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. 3,4 appears a promising tool to extrapolate to intermediate $Q_c$’s. In particular, as we can see from Eq. (3), 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. 1b the critical temperature $T_c$ and the “effective” superconducting pairing $V_{\text{eff}}$ calculated within the small-$q$ approach with $Q_c = 1$ are shown. The overall features of both $T_c$ and $V_{\text{eff}}$ are quite the same as in the local theory with a slight overestimation of $T_c$ and $V_{\text{eff}}$. This is not unexpected since the small-$q$ 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. 1b and 2 is quite good suggesting that the nonadiabatic evaluation of the vertex function based on the small-$q$ expansion can actually interpolate from weak to large correlation. This is confirmed in Fig. 2b where we plot the evolution of the critical temperature $T_c$ in nonadiabatic regime calculated within the small-$q$ 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 rep-

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

effects of the vertex corrections, the results of the nonadiabatic local theory are compared with those obtained by the conventional one for values of $\lambda$ 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 non crossing approximation (NCA). Dashed lines are the numerical results of Eqs. (1)-3, where the vertex function is given in the local theory by Eq. (3). From top to bottom, different lines correspond to adiabatic parameters: $\omega_0/E_F = 0.1, 0.4, 0.7$.

As shown in Fig. 1b 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 $\lambda$ and the adiabatic parameter $\omega_0/E_F$ 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, $V_{\text{eff}}$, with the static limit of the superconductive kernel: $V_{\text{eff}} = \Gamma_\Delta(\omega_n = 0, \omega_m = 0)$. In conventional ME theory $V_{\text{eff}}$ reduces to the simply bare electron-phonon
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-$q$ approach, Fig. 1 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-$q$ expansion allows to understand from a microscopic point of view the way through 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 can not 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-$q$ 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. In such a situation nonadiabatic vertex corrections can give rise to an enhancement of $T_c$ even for uncorrelated systems. This case can be for instance relevant for the recently discovered superconductivity at $T_c \approx 40$ K in MgB$_2$, where the chemical potential is very close to the top of the $\sigma$-bands, with $E_F \simeq 0.5$ eV, thus comparable to the phonon frequencies.

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

FIG. 3. $T_c$ as function of $Q_c$ as evaluated by the small-$q$ 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: $\omega_0/E_F = 0.1, 0.4, 0.7$. 

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