Role of the superconducting gap opening on vertex corrections

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The nonadiabatic effects due to the breakdown of Migdal’s theorem in high-$T_c$ superconductors are strongly affected by the opening of the superconducting gap. Here we report how the momentum-frequency dependence of vertex corrections is modified by the gap. A general effect is that the positive region of the vertex corrections is increased leading to an enhancement of their relevance. This has a number of physical consequences that we discuss in details in relation to specific experiments.

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I. INTRODUCTION

A common peculiar characteristic of many unconventional high-$T_c$ superconductors (cuprates, $A_3C_{60}$ compounds,...) is the narrowness of the electronic bands crossing the Fermi level, leading to Fermi energies $\epsilon_F$ of the same order of magnitude of the phonon energies $\omega_{ph}$ ($\omega_{ph}/\epsilon_F \approx 0.2 - 0.3$). In such a situation, the adiabatic assumption ($\omega_{ph}/\epsilon_F \ll 1$) on which Migdal’s theorem rests cannot be used anymore to justify the omission of vertex corrections in a diagrammatic theory. Motivated by this observation, a renewed interest has recently arose about the possible effects due to inclusion of the vertex corrections in the electron-phonon (or any kind of bosonic mediator) interaction. This task is even more relevant for the purely electronic interaction models (Hubbard, of $t-J$), where no justification exists at all to neglect such corrections.

In this perspective, in previous papers, we have performed an intensive study of the vertex corrections in the normal state, and, afterwards, we have generalized the conventional Migdal-Eliashberg theory in order to include the first nonadiabatic corrections due to the breakdown of Migdal’s theorem. We have investigated the effect of the Migdal corrections on different quantities related to both the superconducting and the normal state properties, as for instance the superconducting critical temperature, or the isotope effect on the effective electron mass. It was shown that an important feature of these corrections is the non trivial structure in momenta and frequencies space, so that the actual relevance of their inclusion can, or cannot, affect in a significant way the properties of the system depending on the effective parameters of the systems. In particular, the critical temperature $T_c$ is found to be sensitive to the momentum transfer of the electron-phonon interaction, and it would be interesting to evaluate the effect of the vertex corrections to the gap-$T_c$ ratio. Moreover, a negative isotope effect is predicted on the effective electron mass $m^*$ in the normal state. This is in quite good agreement with recent experiments that show a large isotope effect on $m^*$. However, this result is based on measurements performed in the superconducting state, where a nonadiabatic generalization of Migdal-Eliashberg theory to include vertex corrections is still missing, and no prediction on the effect of vertex corrections can be yet done.

As a first step to overcome this lack, we are going to analyze in some detail, in the present paper, the vertex function and its momentum-frequency dependence in the superconducting state. Our conclusions show that, as soon as a superconducting gap is opened, the momentum and frequency structure of the vertex corrections is drastically changed, driving the system towards an effective strengthening of the electron-phonon coupling.

The paper is organized as follows: in the next section we introduce the vertex function in the normal state while in Sec. we study the modifications induced by the opening of a superconducting gap. Section is devoted to a general discussion on the possible implications on physical quantities.

II. THE VERTEX FUNCTION IN THE NORMAL STATE

The lowest order correction due to the breakdown of Migdal’s theorem in the normal state is diagrammatically depicted in Fig. 1, which defines the vertex function $\Gamma(q, \omega_n; k, \omega_m)$:

$$\Gamma(q, \omega_n; k, \omega_m) = \sum_p \frac{2|g(k-p)|^2}{\omega(k-p)} T \sum_{l} \frac{\omega(k-p)^2}{(\omega_m - \omega_l)^2 + \omega(k-p)^2} \frac{1}{i\omega_l - \epsilon(p)} \frac{1}{i\omega_l + i\omega_n - \epsilon(p+q)}.$$ (1)
Here, $\epsilon(p)$ and $\omega(k - p)$ are electronic and phononic dispersions and $g(k - p)$ is the matrix element of the electron-phonon interaction, $T$ is the temperature and $\omega_n$, $\omega_m$, and $\omega_l$ are Matsubara frequencies.

As it was discussed in Ref. 3, the qualitative behavior of the momentum-frequency structure of $\Gamma(q, \omega_n; k, \omega_m)$, is well caught by two characteristic limits, the static and the dynamical one, $\Gamma_s$ and $\Gamma_d$, defined as follows: $\Gamma_s = \Gamma(q \to 0, \omega_n = 0; k, \omega_m)$, $\Gamma_d = \Gamma(q = 0, \omega_n \to 0; k, \omega_m)$. In fact, it can be show that the difference between these two limits is in general finite and it is given by the following expression:

$$\Gamma_d - \Gamma_s = \sum_p \frac{2|g(k - p)|^2 \partial f[\epsilon(p)]}{\omega(k - p)} \frac{\omega(k - p)^2}{\epsilon(p) + \omega(k - p) - i\omega_m}.$$  \hspace{1cm} (2)

An analytic calculation of the vertex function $\Gamma$, valid for small $q$, was also derived by considering an Holstein model, with Einstein phonon dispersion $\omega(q) = \omega_0$, a constant electron-phonon bare vertex $g(q) = g$, and a flat electron density of states for a band of width $E$. Within this model, at zero temperature and for a negligible external frequency $\omega_m$, Equation (2) simplifies to:

$$\Gamma_d - \Gamma_s = \lambda,$$ \hspace{1cm} (3)

where $\lambda = 2g^2N(0)/\omega_0$ is the electron-phonon coupling constant and $N(0)$ is the electronic density of states at the Fermi level. The two limits read

$$\Gamma_d = \lambda/(1 + 2\omega_0 / E),$$

$$\Gamma_s = -\lambda/(1 + E/2\omega_0),$$ \hspace{1cm} (4)

where $2\omega_0 / E$ represents, in this model, the adiabatic parameter of Migdal’s theorem.

The sign of the vertex function is plotted in Fig. 2 as function of the exchanged momentum $q$ and frequency $\omega_n$. The non-analyticity of the vertex at $(q = 0, \omega_n = 0)$ is here clear, where the negative static limit is recovered on the vertical axis, and the positive dynamical limit on the horizontal one. This complex structure in momentum and frequency has important consequences on the role of the vertex corrections for different quantities. For instance, the renormalized electron mass $m^*$, and so its isotope effect, is mainly related to the static limit only, while for the superconducting critical temperature the full $(q, \omega_n)$ dependence of the vertex function is relevant.

This difference can be reflected in a stronger dependence of $T_c$, and its isotope effect, on the microscopical parameters than the isotope effect on $m^*$, as it is experimentally seen.

However, we would like to stress that the above predictions are derived in the normal state. How are these results affected by the onset of the superconductivity? Despite the difficulty to build a generalization of Migdal-Eliashberg theory including the nonadiabatic corrections to the Migdal’s theorem in the superconducting state, some preliminary answers at this question can be obtained by analyzing the modifications on the vertex function induced by the superconducting order parameter.

### III. The Vertex Function in the Superconducting State

The existence of a long-range superconducting order parameter modifies the vertex correction in two ways (Fig. 3). On one hand, the single particle propagators involved in the diagram (Fig. 3a) are affected by the opening of the superconducting gap. On the other hand, a new diagram appears, involving two anomalous Green’s functions (Fig. 3b). We label them $\Gamma^{on}$ and $\Gamma^{off}$, respectively, reminding that they are related to on-diagonal and off-diagonal propagators. In order to preserve the analogy with the previous calculations at $T > T_c$ (Fig. 1), $\Gamma^{on}$ and $\Gamma^{off}$ are obtained by using Green’s functions renormalized only by anomalous self-energies, and the normal state renormalization is not taken in account. Within this approximation, the normal and anomalous propagators are given by:

$$G(k, i\omega_n) = \frac{-i\omega_n + \epsilon(k)}{\omega_n^2 + E(k)^2},$$ \hspace{1cm} (5)

$$F(k, i\omega_n) = \frac{\Delta}{\omega_n^2 + E(k)^2},$$ \hspace{1cm} (6)

where $E(k) = \sqrt{\epsilon(k)^2 + \Delta^2}$ is the BCS superconducting excitation spectrum and $\Delta$ is the order parameter. In this paper we consider only isotropic $s$-wave symmetry, however most of the results will be valid also for anisotropic $s$-wave and $d$-wave type of symmetries. By using the propagators defined above, the extension of Eq. (1) in the superconducting state reads:

$$\Gamma(q, \omega_n; k, \omega_m) = \Gamma^{on}(q, \omega_n; k, \omega_m) + \Gamma^{off}(q, \omega_n; k, \omega_m) =$$

$$= \sum_p \frac{2|g(k - p)|^2}{\omega(k - p)} \int \left[ \frac{\omega(k - p)^2}{\omega_m - \omega_l + \omega(l + \omega_m)^2 + E(p + q)^2} \frac{i\omega_l + \epsilon(p)}{\omega_l^2} + \frac{i\omega_l + \epsilon(p)}{\omega_l^2} + \frac{\Delta}{\omega_l^2 + E(p + q)^2} \right].$$ \hspace{1cm} (7)
The first important difference of the above expression with respect to the vertex function in the normal state, Eq. (1), is already evident by looking at the difference between the dynamical and static limits:

\[ \Gamma_d - \Gamma_s = \sum_{\mathbf{p}} \frac{2g(\mathbf{k} - \mathbf{p})^2}{\omega(\mathbf{k} - \mathbf{p})} \frac{\partial f[E(\mathbf{p})]}{\partial E(\mathbf{p})} \frac{\omega(\mathbf{k} - \mathbf{p})^2 [E(\mathbf{p})^2 - \omega(\mathbf{k} - \mathbf{p})^2 - \omega_m^2 + 2i\omega_n \epsilon(\mathbf{p})]}{[\omega(\mathbf{k} - \mathbf{p})^2 + \omega_m^2 - E(\mathbf{p})^2]^2 + [2\omega_n E(\mathbf{p})]^2}. \]  

(8)

In fact, contrary to Eq. (1), the right hand side of Eq. (8) vanishes when \( T \to 0 \) because of the gap opening in the quasiparticle spectrum. One can realize such a result by noticing that for \( T \ll \Delta \) the integral over the Brillouin zone has roughly the weight factor

\[ \frac{\partial f[E(\mathbf{p})]}{\partial E(\mathbf{p})} \sim - \frac{\exp(-\Delta/T)}{T}, \]  

(9)

which goes to zero for \( T \to 0 \). The vanishing of \( \Gamma_d - \Gamma_s \) at zero temperature is an intrinsic feature related to the opening of a gap in the excitation spectrum. It is easy to verify that such a result holds true also for a \( d \)-wave symmetry of the order parameter. Therefore the equality \( \Gamma_d = \Gamma_s \) at zero temperature characterizes the deep modification of the vertex correction due to the onset of superconducting long-range order.

In order to compare in more details the effect of the superconducting gap opening on the vertex function we consider the same model discussed in Ref. [4], that we remind here briefly: the phonon dispersion is taken as a Einstein one \( \omega_0(\mathbf{q}) = \omega_0 \), the electron-phonon matrix element constant \( g(\mathbf{q}) = g \), the electronic density of states flat:

\[ \Gamma(Q, \omega_n) = \frac{\lambda}{E \Omega} T \sum_{\mathbf{p}} \left[ \frac{\omega_0^2}{\omega_1^2 + \omega_0^2} \right] \int_{-E/2}^{E/2} d\epsilon \int_{-E_{\Omega}}^{E_{\Omega}} \frac{\epsilon(\epsilon + y) - \omega(\omega_n + \omega)}{[\omega_1^2 + \epsilon^2 + \Delta^2] [\omega_1^2 + \epsilon^2 + \Delta^2]} \frac{d\omega}{\omega_1^2 + \epsilon^2 + \Delta^2}, \]  

(10)

where, as before, \( \lambda = 2g^2N(0)/\omega_0 \). The sum over \( \omega_1 \) can be performed exactly by using the Poisson’s formula at \( T = 0 : T \sum_{\mathbf{p}} \to \int_{-\infty}^{\infty} d\omega/2\pi \). In this way, the static and dynamical limits can be analytically obtained. The derivation is quite cumbersome, but straightforward, and does not present particular difficulties. Namely, we obtain

\[ \Gamma_s = \frac{\lambda}{E \Omega} \int_{-E/2}^{E/2} \frac{\omega_0 d\epsilon}{2(\omega_0 + \sqrt{\epsilon^2 + \Delta^2})^2} = \lambda \left[ \frac{\delta^2}{4[1 - \delta^2]^{3/2}} \ln \left| \frac{\sqrt{1 + \delta^2 m^2} - \sqrt{1 - \delta^2} m^2 - \delta^2 m^2}{\sqrt{1 + \delta^2 m^2} + \sqrt{1 - \delta^2} m^2 - \delta^2 m^2} \right| \frac{m \sqrt{1 - \delta^2} + 1}{m \sqrt{1 - \delta^2} - 1} + \frac{m - \sqrt{1 + \delta^2 m^2}}{1 - \delta^2} \right], \]  

(11)

where, for the sake of shortness, we have set \( m = 2\omega_n/E \) and \( \delta = \Delta/\omega_0 \). Comparing Eq. (1) with Eq. (4) we can see that the onset of the long-range superconducting order parameter leads to a drastic change of the structure of the vertex function. In particular, while the dynamical limit is affected in a smooth way by a finite \( \Delta \), the value of the static limit immediately jumps to the positive value \( \Gamma_s = \Gamma_d \) as soon as the gap is open. This result is not surprising, since similar modifications of the analytical properties of different susceptibilities (and the electron-phonon vertex can be described as a particular susceptibility) were already recovered.

The global change of \( \Gamma(Q, \omega_n) \) due to the opening of
the superconducting gap is also evident in Fig. 4, where we plot the sign of the vertex function in the $Q - \omega_n$ space, as calculated directly by Eq. (11), without any small $Q$ assumption. With respect to the normal state, marked by the dashed line in Fig. 4, the change of sign in the superconducting state is shifted towards larger values of $Q$, leading to an enlargement of the region of positivity of the vertex function. Moreover, the non-analyticity of the vertex function in the normal state at the point $(q = 0, \omega_n = 0)$ is completely removed. For zero exchanged frequencies $\omega_n = 0$, the vertex changes sign at a finite value $Q_\Delta$ of the exchanged momentum, roughly given by $Q_\Delta \sim \Delta/\omega_0$. This feature can be attributed to the presence of a characteristic length which we identify with the superconducting coherence length $\xi_0$. The interplay of the vertex function and the coherence length will be discussed from the physical point of view in Sec. IV.

In addition to the increase of the region where $\Gamma(Q, \omega_n) > 0$, the opening of the superconducting gap leads also to an amplification of the global magnitude of the vertex. This behavior is clearly shown in Fig. 5, where we plot the average of the vertex function over the Brillouin zone and over the relevant exchanged frequencies:

$$\langle \Gamma \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\omega_0}{\omega^2 + \omega_0^2} \int_0^1 2Q \Gamma(Q, \omega) dQ. \quad (12)$$

When $\Delta = 0$ the positive and negative contributions of the vertex function nearly cancel each other giving a negligible total effect also for intermediate values of $\omega_0/E_F$. The case $\Delta \neq 0$ gives instead an imbalance in favour of the positive contribution resulting into an enhancement of $\langle \Gamma \rangle > 0$. This result is a consequence of both the enlargement of the positive sign region and at the same time an increase (suppression) of the magnitude of the positive (negative) values of $\Gamma(Q, \omega_n)$. Despite of the deep modifications induced by the opening of gap, the vertex function still fulfills the adiabatic limit of Migdal’s theorem $\lim_{\omega_n/E_F \to 0} (\langle \Gamma \rangle) = 0$.

The importance of small momentum transfer selection for the global sign of the vertex function in the normal state has already been outlined in Refs. 4, 5. There, an upper cut-off $Q_c$ was introduced in order to select values of the momentum transfer $Q < Q_c$. In this way the average procedure of Eq. (11) was modified to restrict the integration over $Q$ according to the constraint $Q < Q_c$. The so defined constrained average turns out to be very sensitive to $Q_c$, since it modifies the balance of the positive and negative regions of $\Gamma(Q, \omega_n)$. In particular, small values of $Q_c$ lead to an effective enhancement of $\langle \Gamma \rangle$. This situation is quite altered by the opening of a finite gap. In fact, from Fig. 4 it can be realized that an upper cut-off $Q_c$ has less important effects on the global magnitude when $\Delta \neq 0$. Therefore, in the superconducting state, the $Q_c$ dependence of $\langle \Gamma \rangle$ is more and more weakened by increasing the value of $\Delta$. This feature is described in Fig. 6 where we compare $\langle \Gamma \rangle$ for $\Delta = 0$ and $\Delta = 0.5\omega_0$ as a function of $Q_c$. However, more than the magnitude of $\langle \Gamma \rangle$, the most significant quantity to look at is the sensitivity of the average vertex, that can be expressed as the derivative $\partial(<\Gamma>/\partial Q_c)$, (insert of Fig. 6). For small $Q_c$’s, that in our perspective is the relevant region for the high-$T_c$ materials, the sensitivity of the averaged vertex function $\langle \Gamma \rangle$ is much less pronounced for $\Delta \neq 0$, implying that microscopical variations of $Q_c$ lead to smaller modifications of $\langle \Gamma \rangle$ in the superconducting state than in the normal one.

As we are going to discuss below, all these modifications on the vertex structure induced by the gap opening can have important implications on physical quantities of the superconducting state.

IV. DISCUSSION

As we have seen in the above calculations, the onset of a long-range superconducting order parameter changes substantially the momentum-frequency structure of the vertex function. In particular, the region of positivity is enlarged with respect the normal state, and its relevance for small adiabatic parameter is increased. The main modifications can be sketched by the static and dynamical limits. The dynamical limit $\Gamma_d$ is just slightly affected by the onset of superconductivity, and it remains always positive, whereas the static limit $\Gamma_s$ is drastically changed switching from a negative to a positive value. In particular, at zero temperature these two limits are strictly equal for $\Delta \neq 0$. This behavior can be understood by considering that the dynamical limit, which is essentially independent of the many-particle properties, is related to the static lattice distortions, and as matter of fact it defines the attractive electron-phonon coupling. On the other hand, the static limit depends on many-body effects due to the Pauli exclusion principle, so that it is strongly determined by the fermionic picture of the single-particle properties of the electrons. Such a picture is completely destroyed in the superconducting state where all the Fermi electrons are condensed in Cooper pairs, and Pauli principle is ineffective. As a result, no more difference between dynamical and static limits is found. Moreover, the presence of a finite value $Q_\Delta$ of the momentum transfer $Q$ for which at zero exchanged frequency the vertex changes sign is a consequence of the presence of the superconducting coherence length $\xi_0$.

Therefore, based on this result, which kind of physical predictions can be done?

First of all, it is straightforward to expect that the vertex corrections beyond Migdal’s theorem become more and more important in the superconducting state with the magnitude of the gap, and, since the positive part of the vertex function is increased, this leads to a strengthening of the electron-phonon coupling. We remind that the magnitude of the superconducting gap $\Delta(0)$ is of the same order of the phonon frequencies in the high-$T_c$ materials, so that such a situation gives a huge increase of the positive part of the vertex function. As a first consequence, the zero temperature quantities, as for instance $\Delta(0)$, will feel a much stronger effect of vertex corrections with respect $T_c$, and the ratio $2\Delta/T_c$ is expected to increase the BCS value 3.53. The modifications induced
by the superconducting gap on the vertex corrections are essentially ruled by ratio $\Delta(0)/\omega_0$, so that materials with high phonon energies, as the $C_{60}$ compounds, should show a lighter enhancement of $2\Delta/T_c$ with respect the cuprates, where the phonon energies involved are smaller. This is actually recovered by experimental measurements.

In addition we can argue that the superconducting properties are much more robust inside the superconducting phase than the properties related to the onset of superconducting instabilities. In fact, as the positive and negative parts of the vertex function are almost equivalent in the normal state, the critical temperature is strongly affected by the implicit possible predominance of forward small $q$ scattering, that will select the positive part. Such a situation is naturally given by taking into account the strong electronic correlation due to the on-site Coulomb interaction that is considered to be a crucial ingredient of the high-\(T_c\) superconductors. The relevance of the forward scattering is strongly affected by microscopic parameters, like the adiabatic ratio and the doping. As a consequence, the critical temperature itself is expected to be strongly related to these parameters. On the other hand, due to the opening of the superconducting gap, the vertex corrections involved in the zero temperature gap $\Delta(0)$ are essentially positive, and the small $q$ selection given by the strong correlation is less relevant. This could explain the different behavior of $\Delta(0)$ and $T_c$ as function of the doping $\delta$.

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**Figures:**

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FIG. 1. The lowest order vertex correction diagram. Solid lines are electronic propagators, dashed lines are phonon propagators.

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FIG. 2. Positive and negative regions of the vertex function in the normal state (Ref. 4). It was derived by a small $Q$ expansion. The adiabatic parameter is $2\omega_0/E = 0.5$. 
\[ \Gamma = \begin{array}{c}
\text{(a)} \\
\text{(b)}
\end{array} \]

FIG. 3. First order vertex diagram in the superconducting state.

FIG. 4. Comparison between positive and negative regions of the vertex function in the normal state ($\Delta = 0$) and in the superconducting state ($\Delta = 0.1\omega_0$) for $2\omega_0/E = 0.5$.

FIG. 5. Momentum-frequency average of the vertex function $\langle \Gamma(Q, \omega) \rangle$ as function of the adiabatic parameter $2\omega_0/E$ for different gap magnitudes. $\lambda$ is set equal 1.

FIG. 6. Plot of $\langle \Gamma \rangle$ as function of the momentum cut-off $Q_c$, for $2\omega_0/E = 0.3$ and $\lambda = 1$. Insert: the corresponding derivative: $\partial \langle \Gamma \rangle / \partial Q_c$. 

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