The Ward identity and nonadiabatic corrections to the quasiparticle self-energy

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Abstract

In some newly discovered materials the ratio of phonon to electron energies is no longer small. We have investigated the basement of the recently proposed gauge-invariant self-consistent method and found conditions of its applicability.

When describing electron-phonon interaction in usual metals, so-called adiabatic approximation is used. It assumes that due to electroneutrality fast electrons must follow "slow" ions. Narrow bandwidths and strong electron-phonon interaction make the orders of these velocities comparable. A question appears: Does this result in a breakdown of adiabaticity and increase of interelectron interaction (and in the result $T_c$)?

Traditionally such corrections were considered to be small as the Migdal parameter $\Omega_{ph}/W$ was small \cite{1, 2, 3, 4}. But recently there were discovered materials (for example, fullerenes and high $T_c$ superconductors) where $\Omega_{ph} \sim W$. So Migdal’s theorem about smallness of adiabatic corrections \cite{1, 4} is violated. This gives the grounds for not just discussing these corrections, but even for considering an antiadiabatic limit $\Omega_{ph} \gg W$. For example, it is stated that this results in increase of interelectron interaction and can increase $T_c$ for superconductors \cite{5}. But even with small $\Omega_{ph}/W$ there are contradictory conclusions about importance of such corrections (the author of Ref. \cite{1} considers them to be negligible, in contradiction to the authors of Refs. \cite{3, 4}).

There are two methods to take nonadiabatic corrections into account. One of them, which can be called Migdal’s one, is based on the solution to the Bethe-Salpeter equation for the vertex function \cite{1, 2, 3, 7}. In the lowest approximation, the first correction to the unit vertex is determined by the diagram in Fig. 1 (a). Then with the found vertex function the self-energy $\Sigma$ is calculated (see Fig. 1 (b)).
This traditional method does not allow to take into account higher order diagrams analytically because of complexity of integration over momenta.

Recently Y. Takada offered another method [6] which he called the gauge-invariant self-consistent (GISC). In this method, based on the Ward identity [2], the vertex function is chosen as a functional of the self-energy which is supposed to be independent from momentum. So, when comparing this method with Migdal’s one, we discuss validity of such approach. The parameter \( \Omega_{ph}/W \) is considered to be small.

For simplicity in the Letter we consider the model of the Fermi liquid with the usual Fröhlich Hamiltonian [4] and the Einstein phonon spectrum. This corresponds to

\[
a^2 F_E(\Omega) = \frac{1}{2} \lambda \Omega_{ph} \delta(\Omega - \Omega_{ph}) \tag{1}
\]

where \( \Omega_{ph} \) is the phonon frequency independent from momentum, and \( \lambda \) is the mass-enhancement parameter. It is assumed that the density of states is the constant \( N(0) \) for \(-W < \varepsilon < W\) where \( 2W = 2p_Fv_F \) is the bandwidth. The chemical potential equals zero which corresponds to a half-filled band.

We are interested in the quasiparticle self-energy \( \Sigma \) on the imaginary axis which is determined by the diagram in Fig. 1 (b). The phonon Green’s function \( D_0(i\omega_\nu) = -\Omega_{ph}^2(\omega_\nu^2 + \Omega_{ph}^2)^{-1}, \omega_\nu = 2\nu\pi T \), and the electron Green’s function \( G(i\omega_n, \vec{p}) = (i\omega_n - \varepsilon_{\vec{p}} - \Sigma(i\omega_n, \vec{p}))^{-1}, \omega_n = (2n + 1)\pi T, \varepsilon_{\vec{p}} \) is the electron spectrum.

Assuming that \( \Sigma(i\omega_n, \vec{k}) \) weakly depends on \( \vec{k} \), we take \( |\vec{k}| = p_F = \text{const} \), and so \( \Sigma = \Sigma(i\omega_n) \). Then the diagram in Fig. 1 (b) corresponds to

\[
\Sigma(i\omega_n) = \int_0^\infty d\Omega a^2 F_E(\Omega)T \sum_{\omega_\nu} \frac{2\Omega}{\omega_\nu^2 + \Omega^2} \frac{1}{N(0)} \times \sum_{\vec{q}} G(i\omega_n - i\omega_\nu, \vec{k} - \vec{q}) \Gamma(i\omega_n, i\omega_n - i\omega_\nu, \vec{q}) \tag{1}
\]

Takada’s and Migdal’s methods differ by a choice of the vertex function, and this is discussed below. We will obtain the results for \( T = 0 \) and the variables will change as follows: \( \omega_n \longrightarrow \omega, \omega_\nu \longrightarrow \omega' \) remaining on the imaginary axis.

According to Takada’s GISC method, the vertex function can be chosen as a functional of the self-energy \( \Gamma_T = \Gamma_T[\Sigma_T] \). This choice is based on the Ward identity [2]

\[
i\omega_\nu \Gamma(i\omega_n, i\omega_n - i\omega_\nu, \vec{k} - \vec{q}) - \vec{q} \Gamma(i\omega_n, i\omega_n - i\omega_\nu, \vec{k} - \vec{q})
= G^{-1}(i\omega_n, \vec{k}) - G^{-1}(i\omega_n - i\omega_\nu, \vec{k} - \vec{q}), \tag{2}
\]

valid for all \( \omega_\nu \) and \( \vec{q} \). It is essential that the phonon Green’s function does not depend on momentum. Only in this case one may use the Ward identity for finite momentum \( \vec{q} \) [2]. In Ref. [5] Takada proposes to use this identity for \( v_F|\vec{q}| \ll |\omega_\nu| \)
and choose \( \Sigma \)

\[
\Gamma_T[\Sigma] = \Gamma_T(i\omega_n, i\omega_n - i\omega_p) = 1 + \left( -\frac{\Sigma_T(i\omega_n)}{2i\omega_n} - \frac{\Sigma_T(i\omega_n - i\omega_p)}{2(i\omega_n - i\omega_p)} \right),
\]

which corresponds to the estimates of Refs. [2, 3] in this limit.

The set of equations (1), (3) is proposed to be solved by iterations. At the first step \( G = G^{(0)}, \Gamma = \Gamma^{(1)} \) give \( \Sigma_T = \Sigma_T^{(1)} \) (Fig. 2 (a)). For \( T = 0 \)

\[
\Sigma_T^{(1)}(i\omega) = -i\lambda \Omega_{ph} \arctan \frac{\omega}{\Omega_{ph}} + i\lambda \Omega_{ph} \arctan \frac{\omega}{W + \Omega_{ph}},
\]

which corresponds to the results of Refs. [2, 5]. At the second step \( G = G[\Sigma_T^{(1)}], \) and the correction \( \Gamma_T^{(2)} \) for \( \Omega_{ph}/W \ll 1 \) gives:

\[
\Sigma_T^{(2)}(i\omega) = i\lambda^2 \Omega_{ph} b(m), \text{ where } m = \omega/\Omega_{ph}, b(m) = b_1(m) + b_2(m).
\]

\[
b_1(m) = -\frac{1}{2m} \arctan^2 m,
\]

\[
b_2(m) = \frac{1}{4} \int_{-\infty}^{+\infty} dy \frac{1}{y^2 + 1} \frac{\arctan(m - y)}{m - y} \text{sign}(y - m), \quad y = \omega'/\Omega_{ph}.
\]

So

\[
b(m) = -\begin{cases} 
\left( \frac{1}{4} + \frac{\pi^2}{16} \right)m, & |m| \ll 1, \\
\frac{\pi^2}{4} \frac{1}{m}, & |m| \gg 1.
\end{cases}
\]

Here \( \Sigma_T^{(2)} \) is obtained by using (4) with infinite limits of integration over \( d\varepsilon. \)

During this calculation the vertex \( \Gamma_T^{(2)} \) is of the order of \( \lambda \) for any \( q \) which is incorrect. So in Takada’s method the leading term of the corrections does not have the small parameter \( \Omega_{ph}/W, \) that is in this approach Migdal’s theorem does not hold for the self-energy. This can be explained by the fact that the region \( v_F|\vec{q}| \ll |\omega'| \) where \( \Gamma \sim \lambda \) gives in reality a small contribution to \( \Sigma. \) If, on the contrary, \( v_F|\vec{q}| \gg |\omega'|, \) the vertex \( \Gamma \sim \lambda \Omega_{ph}/W \) which gives \( \Sigma^{(2)} \sim \lambda \Omega_{ph}^2/W. \) At the same time, the sign of the vertex correction to the self-energy in GISC method is opposite to that in Migdal’s one (see below).

In the method which can be called Migdal’s one, there is considered the first correction to the unit vertex function \( \Gamma^{(1)}. \) It is shown on Fig. 1 (a). It has been
estimated in many papers [1, 3], but now it is becoming especially significant [5] as it has appeared that the parameter $\lambda \Omega_{ph}/W$ can be not very small.

The diagram in Fig. 1 (a) corresponds to the expression

$$
\Gamma^{(2)}(i\omega_n, i\omega_n - i\omega_V, q) = T \sum_{\omega_{n'}} \sum_{\vec{q}'} \int_0^\infty d\Omega \frac{\alpha^2 F_E(\Omega) 2\Omega}{N(0)(\omega_{n'}^2 + \Omega^2)} 
\times G^{(0)}(i\omega_n - i\omega_{n'}, \vec{p} - \vec{q}'')G^{(0)}(i\omega_n - i\omega_V - i\omega_{n'} - \vec{q}') \times \frac{\lambda \Omega_{ph}^2}{qv_F} \arctan \left( \frac{qv_F}{\omega'} \right)
- \arctan \left( \frac{W + \Omega_{ph}}{W + \Omega_{ph}} \right) + \arctan \left( \frac{\omega - \omega'}{W + \Omega_{ph}} \right) \right).
$$

(9)

Assuming that $|\vec{p} - \vec{q}'| \sim p_F$ and expanding $\varepsilon(\vec{p} - \vec{q}' - \vec{q}) \approx \varepsilon(\vec{p} - \vec{q}') - qv_F \cos \theta$, we get for $T = 0$:

$$
\Gamma^{(2)}(i\omega, i\omega - i\omega', \vec{q}) = \lambda \frac{\Omega_{ph}^2}{qv_F} \arctan \left( \frac{qv_F}{\omega'} \right) \left( \arctan \left( \frac{\omega}{\Omega_{ph}} \right) - \arctan \left( \frac{\omega - \omega'}{\Omega_{ph}} \right) \right).
$$

(10)

At $v_F|\vec{q}| \ll |\omega'|$ this expression corresponds to the Ward identity (2) and to the choice of a functional (3). For $v_F|\vec{q}| \gg |\omega'|$ the correction $\Gamma^{(2)}(i\omega, i\omega - i\omega', \vec{q}) \sim \lambda \Omega_{ph}/qv_F \sim \lambda \Omega_{ph}/W$, that is Migdal’s theorem for the vertex function does hold in this method.

The corresponding self-energy then equals (see Fig. 2)

$$
\Sigma = \Sigma^{(1)} + \Sigma^{(2)}.
$$

$\Sigma^{(1)}$ is equal to $\Sigma_T^{(1)}$ as it also corresponds to $\Gamma^{(1)} = 1$. For the correction due to $\Gamma^{(2)}$, $\Sigma_v^{(2)}$, one can get at $\Omega_{ph}/W \ll 1$:

$$
\Sigma^{(2)}_v(i\omega) = i\lambda^2 \frac{\Omega_{ph}^2}{W} d_v(m) \text{ where } m = \frac{\omega}{\Omega_{ph}},
$$

$$
d_v(m) = \frac{\pi}{4} \int_{-\infty}^{\infty} dy \frac{1}{y^2 + 1} \text{sign}(y) \text{sign}(y - m) (\arctan m - \arctan(m - y)).
$$

(11)

In the limiting cases

$$
d_v(m) = \begin{cases} 
\frac{\pi^2 m}{8}, & |m| \ll 1, \\
\frac{\pi^2}{4} \frac{1}{m}, & |m| \gg 1.
\end{cases}
$$

(12)

The sign of the correction $\Sigma_v^{(2)}$ is opposite to that of $\Sigma^{(1)}$ which favour tendency towards instability [4, 3].
In this approximation one can find the vector vertex function $\vec{\Gamma}$ and show that it really cannot be neglected. Using electron-hole symmetry, in our model, $\vec{\Gamma}(i\omega, i\omega - i\omega', \vec{k}, \vec{k} - \vec{q}) = \vec{\Gamma}^{(1)} + \vec{\Gamma}^{(2)}$ where $\vec{\Gamma}^{(1)} \approx \frac{\vec{k}}{m}$.

$$q\vec{\Gamma}^{(2)} = -i\lambda\Omega_{ph}(1 - \frac{\omega'}{qv_F}\arctan\frac{qv_F}{\omega})(\arctan\frac{\omega}{\Omega_{ph}} - \arctan\frac{\omega - \omega'}{\Omega_{ph}}).$$

The diagram in Fig. 1 (a) corresponds to $\vec{\Gamma}^{(2)}$ if one substitutes $\Gamma^{(1)}$ by $\vec{\Gamma}^{(1)}$ and $\Gamma^{(2)}(i\omega_n, i\omega_n - i\omega_n, -\vec{q})$ - by $\vec{\Gamma}^{(2)}(i\omega, i\omega - i\omega', -\vec{q})$.

If one designates $x = \omega'/qv_F$, then using at $\Omega_{ph}/W \ll 1$ the expression (11) for $\Gamma^{(2)}$, we can find that the terms $\omega'\Gamma^{(2)}$ and $q\vec{\Gamma}^{(2)}$ from (2) become of the same magnitude if $x_0\arctan(1/x_0) = 1 - x_0\arctan(1/x_0)$, from which $x_0 = 0.43$. If, however, $\omega'/qv_F < x_0$, the vector term dominates and it may not be neglected.

So in the Letter there is consistently considered contribution of nonadiabatic effects to the electron self-energy in first orders in $\lambda$. The two methods of taking into account the nonadiabatic corrections were compared: 1) Migdal’s and 2) the GISC proposed by Takada.

It is shown that the latter gives for the self-energy physically incorrect result. This is connected with the fact that the leading contribution to $\Sigma$ is made by the region $qv_F \gg \omega'$ where $\Gamma \sim \lambda\Omega_{ph}/W$. This means that in the Ward identity one may not neglect the vector term as proposed by Takada. In the frame of the standard (Migdal’s) approach, in the lowest order, there is evaluated the parameter $x = \omega'/qv_F$ at which contributions of the vector and scalar terms become the same (see Fig. 3). They are equal at $x_0 = 0.43$. As it was shown above, the region of large $q$’s indeed gives the main contribution to the self-energy. That is why the GISC method, which works only for small $q$’s, may not be applied.

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**Figure Captures**

Fig. 1. (a) The equation for the vertex function $\Gamma^{(2)}$ in Migdal’s method. The outgoing lines are shown for clearness and are not included in the definition of $\Gamma$. (b) The equation for the self-energy $\Sigma$. The wavy line is a bare phonon Green’s function $D_0$, the double solid line is an electron Green’s function $G$, and the hatched triangle is a vertex function $\Gamma$.

Fig. 2 (a), (b). Diagrams which are included when calculating the self-energy $\Sigma$. The solid straight line is a bare electron Green’s function $G^{(0)}$.

Fig. 3. The ratio of the vector to the scalar terms in the Ward identity. The GISC method may only be used for large $x$’s (small $q$’s).
(a) \[ \Gamma^{(2)}(i\omega_n, i\omega_n - i\omega_\nu, q) = \Gamma^{(1)} \]

(b) \[ \Sigma(i\omega_n) = \Gamma(i\omega_n, i\omega_n - i\omega_\nu, q) \]
\( \Sigma^{(1)}(i\omega_n) = \)

\( i\omega_n, q \)

\( i\omega_n - i\omega_q, k = q \)

\( \Sigma^{(2)}(i\omega_n) = \)

\( i\omega_n, q \)

\( i\omega_n - i\omega_q - i\omega_{\nu'}, k - q' \)

\( i\omega_n - i\omega_{\nu'}, k - q' \)

\( i\omega_{\nu'}, q' \)

\( i\omega_n - i\omega_{\nu}, k - q \)
