Phonon-Induced Renormalization and Interaction: An Improvement on Frohlich Transformation

H. Zheng
Department of Applied Physics, Shanghai Jiao Tong University, Shanghai, P. R. China

Abstract
Starting from the Flohlich electron-phonon model, which has a history of 50 years, a new unitary transformation is proposed to implement the perturbation treatment. Our main results are: (1) The phonon-induced interaction shows a crossover from the BCS-like potential when the phonon frequency $\omega_p$ is much smaller than the Fermi energy $E_F$ to that of the small polarons when $\omega_p/E_F \geq 1$. (2) The jump of momentum distribution of electron number $n_k$ at the Fermi surface goes to zero when the dimensionless coupling constant $\lambda$ increases to the critical value $\lambda_c \geq 1$, which means a possible broken down of the Fermi-liquid description.

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It is a well-known fact that within the Migdal-Eliashberg (ME) description\cite{1, 2, 3, 4} of electrons and phonons coupled by the linear electron-phonon interaction there is no instability (where the Fermi-liquid description may break down) at any value of the dimensionless coupling constant $\lambda$. People tried to study the polaronic collapse of the electron band starting from the Lang-Firsov (LF) transformation\cite{5} followed by the small polaron approximation\cite{6, 7}. Note that the LF transformation together with the small polaron approximation cannot lead to those results which can be obtained via the ME approach. For example, Bardeen, Cooper, and Schrieffer\cite{8} (BCS) proposed a square-well potential for electrons in momentum space, that is, only those electrons within a layer of width $\omega_p$ (the characteristic phonon frequency) near the Fermi surface can attract with each other. This potential is localized in momentum space, so it is extended in real space and leads to large coherence length of Cooper pairs. But the LF transformation results in an attractive potential for all electrons in Fermi sea\cite{5, 7}, which is a localized potential in real space. As far as we know, there is no theories which can describe successfully the crossover between the two pictures. In this letter we propose a new approach which can (1) describe the crossover and (2) lead to a possible broken down of the Fermi-liquid description.

The Frohlich Hamiltonian of electron-phonon coupling system is\cite{9}

$$H = \sum_{k,\sigma} (\epsilon_k - \mu_0) d_{k,\sigma}^\dagger d_{k,\sigma} + \sum_q \omega_q b_q^\dagger b_q + \frac{1}{\sqrt{N}} \sum_q \sum_{k,\sigma} g_q d_{k+q,\sigma}^\dagger d_{k,\sigma} (b_{-q}^\dagger + b_q).$$

(1)

$N$ is the number of sites, $\epsilon_k$ is the bare band function, $b_q$ and $d_{k,\sigma}$ are usual notations for phonon or electron operators, respectively. $\mu_0$ is the chemical potential, $\omega_q$ the phonon frequency and $g_q$ the electron-phonon coupling. We set $\hbar = 1$ and $k_B = 1$.

Frohlich used a unitary transformation to treat $H$: $H' = \exp(S) H \exp(-S)$. The transformation can proceed order by order,

$$H' = H_0 + H_1 + [S, H_0] + [S, H_1] + \frac{1}{2} [S, [S, H_0]] + O(g_q^3),$$

where $H = H_0 + H_1$ and $H_0$ contains the first two terms and $H_1$ the last one. Frohlich let $H_1 + [S, H_0] = 0$ to get the generator $S$. The transformation leads to a phonon-induced...
interaction with the potential
\[ V_F(k + q, k) = \frac{g_q^2 \omega_q}{|\epsilon_{k+q} - \epsilon_k|^2 - \omega_q^2}, \] (2)
which can be attractive or repulsive with a singularity at the energy shell: \(|\epsilon_{k+q} - \epsilon_k| = \omega_q\). Frohlich noted that, although the transformation can eliminate the first order terms completely, because of the singularity one has to set a constraint \(|\epsilon_{k+q} - \epsilon_k| - \omega_q > \epsilon\) (\(\epsilon > 0\) is a constant) in the transformation. Because of the constraint the elimination of the first-order terms is not complete.

The BCS theory simplifies the Frohlich potential as
\[ V_{BCS}(k + q, k) = \begin{cases} -\frac{g_q^2}{\omega_p}, & \text{for } |\epsilon_{k+q} - \epsilon_k| < \omega_p, \\ 0, & \text{otherwise}. \end{cases} \] (3)

We propose to improve the Frohlich transformation by a new generator
\[ S = \frac{1}{\sqrt{N}} \sum_q \sum_{k,\sigma} g_q d^\dagger_{k+q,\sigma} d_{k,\sigma} (b^\dagger_{-q} - b_q) \delta(k + q, k), \] (4)
where \(\delta(k + q, k)\) is a function of the energies of incoming and outgoing electrons in the electron-phonon scattering process,
\[ \delta(k + q, k) = \delta(\epsilon_{k+q}, \epsilon_k; \omega_q) = \left(1 + \frac{|\epsilon_{k+q} - \epsilon_k|}{\omega_q}\right)^{-1}. \] (5)
The reason of choosing this generator will become clear later. After transformation the first order terms in \(H'\) are
\[ H_{11} = H_1 + [S, H_0] = \frac{1}{\sqrt{N}} \sum_q \sum_{k,\sigma} g_q \frac{d^\dagger_{k+q,\sigma} d_{k,\sigma}}{\omega_q + |\epsilon_{k-q} - \epsilon_k|} \left(b^\dagger_{-q} - b_q\right) \delta(k + q, k), \]
\[ \times \left\{ |\epsilon_{k-q} - \epsilon_k| - (\epsilon_{k-q} - \epsilon_k) b^\dagger_{-q} + |\epsilon_{k-q} - \epsilon_k| + (\epsilon_{k-q} - \epsilon_k) b_q \right\}. \] (6)
The second order terms in \(H'\) are:
\[ H_{12} = [S, H_1] + \frac{1}{2} [S, [S, H_0]] \]
\[ = \frac{1}{2N} \sum_{k,q} \sum_{\sigma} g_q^2 \left(b^\dagger_{-q} b_{-q} + b_q b^\dagger_{q}\right) \frac{|\epsilon_k - \epsilon_{k+q}|}{\omega_q} \left(d^\dagger_{k+q,\sigma} d_{k+q,\sigma} - d^\dagger_{k,\sigma} d_{k,\sigma}\right) \]
\[ - \frac{1}{N} \sum_{k,k',q,\sigma,\sigma'} g_q^2 \delta(k + q, k') \left[2 - \delta(k' - q, k')\right] d^\dagger_{k+q,\sigma} d_{k,\sigma} d^\dagger_{k'-q,\sigma'} d_{k',\sigma'}. \] (7)
where the non-diagonal phonon terms are neglected. $H_{I2}$ contains a phonon-induced interaction with potential

$$V(k + q, k) = -\frac{g_q^2}{\omega_q}\delta(k + q, k)[2 - \delta(k, k + q)].$$

Fig. 1 shows $V(k', k)$ as functions of $\epsilon_{k'} - \epsilon_k$ for different ratios $\omega_p/E_F$ where $E_F$ is the Fermi energy. For comparison we also show $V_{BCS}(k', k)$, which is a narrow square-well in the middle, and the potential for small polarons which can be obtained via the LF transformation: $V_{LF} = -g^2/\omega_p$ for all electrons.

The purpose of our transformation is to find a better way to divide the Hamiltonian into the unperturbed part and the perturbation. After transformation $H' = H'_0 + H_{I1} + H_{I2}' + O(g_q^3)$. The unperturbed part is

$$H'_0 = \sum_q \omega_q b_q^\dagger b_q + \sum_{k, \sigma} (E_k - \mu_0) d_{k, \sigma}^\dagger d_{k, \sigma} - \sum_{k, \sigma} \Delta(k) \left( d_{k, \uparrow}^\dagger d_{-k, \downarrow} + d_{-k, \downarrow} d_{k, \uparrow} \right),$$

$$E_k = \epsilon_k + \frac{1}{N} \sum_q \frac{g_q^2}{\omega_q} \coth\left(\frac{\omega_q}{2T}\right) \frac{\epsilon_{k+q} - \epsilon_k}{\omega_q} \delta^2(k + q, k)$$

$$- \frac{1}{N} \sum_q \frac{g_q^2}{\omega_q} \delta(k + q, k)[2 - \delta(k + q, k)] \frac{E_{k+q} - \mu_0}{\xi_{k+q}} \tanh\left(\frac{\xi_{k+q}}{2T}\right),$$

$$\Delta(k) = \frac{1}{N} \sum_q \frac{g_q^2}{\omega_q} \delta(k + q, k)[2 - \delta(k + q, k)] \frac{\Delta(k + q)}{\xi_{k+q}} \tanh\left(\frac{\xi_{k+q}}{2T}\right),$$

$$\xi_k = \sqrt{(E_k - \mu_0)^2 + \Delta^2(k)},$$

which can be solved exactly. The perturbation is $H_{I1} + H_{I2}'$ where $H_{I2}' = H_{I2} - (H'_0 - H_0)$. $E_k$ and $\Delta(k)$ have been determined by the condition that the lowest order contribution of $H_{I2}'$ to the self-energy is zero.

A renormalized chemical potential $\mu$ and a band renormalization factor $\rho(\epsilon_k)$ can be introduced, $E_k - \mu_0 = \rho(\epsilon_k)(\epsilon_k - \mu)$. The equation to determine $\mu$ is

$$1 - n = \frac{1}{N} \sum_k \frac{\rho(\epsilon_k)(\epsilon_k - \mu)}{\xi_k} \tanh\left(\frac{\xi_k}{2T}\right),$$

where $n$ is the electron number density. The equation to determine $\rho(\epsilon_k)$ will be given later.
The Green’s function of $H'_0$ is

$$G_0(k, \omega) = (\omega + E_k - \mu_0)/(\omega^2 - \xi^2(k)), \quad F_0^\dagger(k, \omega) = -\Delta(k)/(\omega^2 - \xi^2(k)).$$

The contribution of $H_{I1}$ to the self-energy (to the second order of $g_q$) is
taken

$$\Sigma(k, \omega) = -\frac{1}{N} \sum_q g_q^2 \left\{ \frac{\beta}{i\omega_n - \omega_q} \sum_n G_0(k - q, \omega - i\omega_n) \right\},
$$

\[ W(k, \omega) = 0. \tag{14} \]

The abnormal self-energy $W(k, \omega) = 0$ because it contains a factor $|\epsilon_{k-q} - \epsilon_k|^2 - (\epsilon_{k-q} - \epsilon_k)^2$ in the $q$-summation. Generally, the normal self-energy $\Sigma(k, \omega) \neq 0$. But for the normal state ($\Delta(k) = 0$) and when $T = 0$, we have

$$\Sigma_n(\epsilon_k = \mu, \omega) = 0, \tag{15}$$

that is, the normal self-energy is zero at the Fermi surface. As the spectrum of elementary excitations in the normal state is $\omega = \rho(\epsilon_{k-q})(\epsilon_{k-q} - \mu) + \Sigma_n(k, \omega)$, the mass renormalization at Fermi surface is

$$\frac{m}{m^*} = \left[ \rho(\epsilon_k) + \frac{\partial}{\partial \epsilon_k} \Sigma_n(k, \omega) \right] \left[ 1 - \frac{\partial}{\partial \omega} \Sigma_n(k, \omega) \right]_{\epsilon_k = \mu} = \rho(\epsilon_k = \mu). \tag{16}$$

Eqs.(14), (15), and (16) are main reasons for the choice of the functional form of $\delta(k + q, k)$ in (5). Now one can see clearly the purpose of our unitary transformation: The transformed $H'$ is divided into the unperturbed part $H'_0$, which contains the main physics of the problem, and the perturbation $H_{I1} + H'_{I2}$, which is small as shown by Eqs.(14), (15), and (16).

Gap equation (11) can be rewritten as an integral equation by introducing the Eliashberg function $\alpha^2 F[3, 4]$

$$\Delta(\epsilon) = \int_{-\infty}^{+\infty} d\epsilon' \int d\Omega \frac{N(\epsilon')}{N(\mu)} \alpha^2 F(\Omega) \frac{\Omega}{(\Omega + |\epsilon|)^2} \frac{\Delta(\epsilon')}{\xi(\epsilon')} \tanh \frac{\xi(\epsilon')}{2T}. \tag{17}$$
\(N(\epsilon)\) is the density of states (DOS). The integration over \(\epsilon'\) is from the bottom \((-D)\) of the band to the top \((D)\). The equation for \(\rho(\epsilon_k)\) can be rewritten in the same way,

\[
\rho(\epsilon) = 1 + \int_{-D}^{D} d\epsilon' \int_{0}^{\infty} d\Omega \frac{N(\epsilon')}{N(\mu)} \alpha^2 F(\Omega) \coth\left(\frac{\Omega}{2T}\right) \times \left\{ \frac{\epsilon' - \epsilon}{(\Omega + |\epsilon' - \epsilon|)^2} - \frac{\epsilon' - \mu}{(\Omega + |\epsilon' - \mu|)^2} \right\} / (\epsilon_k - \mu) - \int_{-D}^{D} d\epsilon' \int_{0}^{\infty} d\Omega \frac{N(\epsilon')}{N(\mu)} \alpha^2 F(\Omega) \left\{ \frac{\Omega + 2|\epsilon' - \epsilon|}{(\Omega + |\epsilon' - \epsilon|)^2} - \frac{\Omega + 2|\epsilon' - \mu|}{(\Omega + |\epsilon' - \mu|)^2} \right\} \frac{\rho(\epsilon')(\epsilon' - \mu)}{(\epsilon - \mu)\xi(\epsilon')} \tanh\left(\frac{\xi(\epsilon')}{2T}\right)
\]

(18)

These two equations are very similar to the Eliashberg equations[2, 3, 4].

For calculating the physical quantities we must calculate the thermodynamical potential and the average of electron or phonon operators. The thermodynamical potential is

\[
\Omega = -\frac{1}{\beta} \ln \text{Tr exp}[\beta H] = -\frac{1}{\beta} \ln \text{Tr exp}[\beta H'] \approx -\frac{1}{\beta} \ln \text{Tr exp}[\beta H_0].
\]

(19)

The last "\(\approx\)" is because of Eqs.(14) and (15), that is, to the order \(O(g_q^2)\) the contribution of \(H_{I1} + H_{I2}'\) is very small in the lowest temperature region. Hence, for the normal state

\[
\Omega \approx -\frac{2}{\beta N} \sum_k \ln \{1 + \exp[-\beta \rho(\epsilon_k)(\epsilon_k - \mu)]\} + \text{phonon part}.
\]

(20)

The heat capacity can be calculated as \(C = -T \partial^2 \Omega / \partial T^2 = C_0 / \rho(\epsilon_k = \mu)\), where \(C_0\) is the heat capacity for free electrons and

\[
\rho(\epsilon_k = \mu) = 1 - \lambda + \lambda \frac{\omega_p(\omega_p + D)}{(\omega_p + D)^2 - \mu^2}.
\]

(21)

In calculating we assume a constant DOS and \(\lambda = 2 \int d\Omega \alpha^2 F(\Omega) / \Omega\). The enhancement factor at \(\omega_p/D \rightarrow 0\) is \(1/(1 - \lambda)\) which should be compared with the same factor in ME theory \(1 + \lambda^{[4]}\).

We have to take into account the effect of the unitary transformation when calculating the thermodynamical average of electron or phonon operators. The Green's
function for the original Hamiltonian $H$
\[
\tilde{G}(k, \tau) = -\text{Tr} \left\{ T_\tau \exp[-\beta(H - \Omega)]d_{k,\sigma}(\tau)d_{k,\sigma}^\dagger \right\} \\
= -\text{Tr} \left\{ T_\tau \exp[-\beta(H' - \Omega)]d_{k,\sigma}'(\tau)d_{k,\sigma}'^\dagger \right\},
\]
(22)
where $T_\tau$ means $\tau$ ordering\(\textsuperscript{[11]}\). The transformation of a single fermion operator can proceed as
\[
d_{k,\sigma}' = e^S d_{k,\sigma} e^{-S} = d_{k,\sigma} + [S, d_{k,\sigma}] + \frac{1}{2}[[S, [S, d_{k,\sigma}]] + O(g^3).\]

Fig. 2 shows $n_k$ as functions of $\epsilon_k$ around the Fermi surface. For smaller coupling (dashed line) or the larger frequency (dash-dotted line), there is a finite jump of $n_k$ at Fermi surface. But for smaller frequency (solid line) and $\lambda \sim 1$, the Fermi surface is smeared by the electron-phonon coupling. The jump of $n_k$ at Fermi surface $\epsilon_k = \mu$ is $\rho(\epsilon_k = \mu$) (Eq.(25)) and it predicts an instability of the Fermi liquid state at
\[
\lambda_c = \left( 1 - \frac{\omega_p(\omega_p + D)}{(\omega_p + D)^2 - \mu^2} \right)^{-1}.
\]
(23)
$\lambda_c \to 1$ when $\omega_p \to 0$. For comparison, ME theory predicts a jump $1/(1 + \lambda$ and there is no instability.
At the end, as the transformation is truncated after the second order of $g_q$, we justify the cutoff by showing the small expansion parameter. Roughly speaking, in three-dimension it is $\lambda \omega_p/E_F$ when $\omega_p/E_F < 1$ but $\lambda E_F/\omega_p$ when $\omega_p/E_F > 1$. Note that they are the same as that of ME theory or LF transformation.
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Figure Captions

Fig.1  The phonon-induced interaction.

Fig.2  The phonon-induced renormalization of the momentum distribution $n_k$ on and near the Fermi surface.
$$\omega_p / E_F = 0.01$$

$$\omega_p / E_F = 0.1$$

$$\omega_p / E_F = 1$$
\[ \eta_k = \frac{\varepsilon_k - \mu}{D} \]