Condensation energy in Eliashberg theory – from weak to strong coupling

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We consider two issues related to the condensation energy in superconductors described by the Eliashberg theory for various forms of the pairing interaction, associated either with phonon or electronic mechanisms of superconductivity. First, we derive a leading correction to the BCS formula for the condensation energy to first order in the coupling $\lambda$. Second, we show that at a given $\lambda$, the value of the condensation energy strongly depends on the functional form of the effective pairing interaction $\Gamma(\omega)$.

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A non-monotonic doping dependence of superconductivity in high $T_c$ cuprates revived the interest to the issue of the condensation energy in strongly coupled superconductors. The condensation energy $E_c$ is the energy gain in a superconducting state compared to a normal state at the same $T$. In a BCS superconductor, $E_c$ smoothly increases below $T_c$ and at $T = 0$ reaches $E^{\text{BCS}}_c = -V N_0 \Delta^2/2$, where $V$ is the volume, $\Delta$ is the superconducting gap and $N_0$ is the fermionic density of states. The decrease in the total energy upon pairing results from a fine competition between an increased kinetic energy and a decreased potential energy, both of which are much larger than $E_c$. Within BCS theory, the condensation energy is related to the jump of the specific heat at $T_c$ as $C_s - C_n \approx 6.08 E_c/T_c$.

The BCS formula for the condensation energy is valid at weak coupling. Experimental discoveries of strong fermionic self-energy in the normal state of the cuprates stimulated the studies of the condensation energy away from the BCS limit. In earlier papers Haslinger and one of us analyzed the condensation energy vs coupling for spin-mediated $d$–wave superconductivity. It was found numerically that the condensation energy rapidly deviates from the BCS form as coupling increases, then saturates and then even decreases at strong coupling, due to feedback on the bosonic spectrum from the pairing. The crossover from weak to moderate coupling, however, has not been analyzed in detail in Ref. [8].

In the present paper, we consider condensation energy in superconductors described by the Eliashberg theory, for various forms of the pairing interaction $\Gamma(\omega) \propto (\omega_D^2 + \omega^2)^{-\gamma/2}$ ($0 < \gamma < 2$), associated either with phonon or electronic mechanisms of superconductivity (we discuss the examples below). We address two issues that were not discussed in Ref. [8]. First, we analyze, both analytically and numerically, the leading correction to the BCS form of the condensation energy at weak coupling. We show that the relative correction scales as a dimensional coupling $\lambda$ and does not depend on the functional form of the pairing interaction (i.e., on $\gamma$). Second, we compare the condensation energy for fixed $\lambda$, as a function of $\gamma$. In the limit of $\lambda \to \infty$, $E_c$ is the largest at $\gamma = 2$, and for this $\gamma$ it actually diverges as $\log \lambda$.

However, we found that this behavior only holds for extremely large $\lambda \sim 10^2 - 10^3$. At moderate $\lambda$, we found numerically an opposite trend: a strong increase of $E_c$ with decreasing $\gamma$. We understood this behavior analytically as originating already within the BCS theory and coming from the strong $\gamma$ dependence of the prefactor of the superconducting gap.

We consider a model in which low-energy fermions are interacting by exchanging either phonons or collective spin or charge fluctuations. This exchange gives rise to an attraction in one of pairing channels, such that at $T = 0$, the system is in the superconducting state. At weak coupling, both phonon-mediated and collective mode-mediated pairings can be treated within BCS theory. At moderate and strong coupling, we assume that the Eliashberg theory is valid, i.e., that the self-energy is large, but it predominantly depends on frequency, and vertex corrections can be still neglected. Eliashberg theory can be straightforwardly justified for phonon superconductors due to the smallness of the sound velocity compared to the Fermi velocity. For electronic mechanism of pairing, it is justified on different reasons, but still, at low energies bosonic excitations turn out to be slow modes compared to electrons, i.e., the effective bosonic velocity is smaller than $v_F$. We discuss the justification of the Eliashberg theory for electronic pairing mechanism in some detail at the end of the paper, after we discuss the results.

The smallness of (real of effective) bosonic velocity compared to $v_F$ implies that in the pairing problem, the momentum integration is factorized: the one over momenta transverse to the Fermi surface involves only fermions, while the one along the Fermi surface involves the bosonic propagator $\chi(q||, \omega)$. As a consequence, the theory operates with the effective “local” pairing interaction $\Gamma_\omega \propto \int dq|| \chi(q||, \omega)$. This interaction quite generally can be cast in the form

$$\Gamma_\omega = (1 + \omega^2/\omega_D^2)^{-\gamma/2}. \quad (1)$$

where $\omega_D$ is characteristic frequency. The case $\gamma = 2$ corresponds to phonon-mediated superconductivity, where $\omega_D$ is a Debye frequency. Other values of $\gamma$ correspond to electronic pairing. For instance, $\gamma = 1/3$ corresponds
to the pairing mediated by 2D ferromagnetic Ising spin fluctuations or long-wavelength charge fluctuations \[12\]. In both cases, \(\chi(q, \omega) \propto (\xi^{-2} + q^2 + |\omega|/q)\). Integrating over \(q\), one immediately finds \(\Gamma_x \to \text{const}\) at \(x \to 0\) and \(\Gamma_x \propto (x/\xi^{-3})^{-1/3}\) at large \(x\), in agreement with \[12\] for \(\gamma = 1/3\). The behavior at intermediate \(x\) is more complex than in \[11\] but this does not affect the physics. Similarly, \(\gamma = 1/2\) corresponds to the pairing mediated by 2D overdamped spin or charge fluctuations peaked at a finite momentum \[13\] \[14\], while \(\gamma = 1\) corresponds to the pairing mediated by propagating spin or charge density waves. The case \(\gamma \to 0\) describes all 3D pairings mediated by either charge or spin fluctuations \[17\].

The variables of the Eliashberg theory are the pairing gap \(\Delta(\omega)\) and the quasiparticle renormalization factor \(Z(\omega)\). They are related to the fermionic self-energy \(\Sigma(k, \omega)\) and the pairing vertex \(\Phi(k, \omega)\) by \(\omega + \Sigma(\omega) = \omega Z(\omega)\), \(\Delta(\omega) = \Phi(\omega)/Z(\omega)\). The equation for \(\Delta\) is decoupled from that for \(Z\) regardless of the form of \(\Sigma\) and is obtained by straightforward extension of that for phonons \[11\].

\[
\Delta_{\omega_m'} = \pi T \lambda \sum_{m=\infty}^{\infty} \frac{\Delta_{\omega_m} - \Delta_{\omega_m'} \omega_m' \omega_m}{\sqrt{\omega_m^2 + \Delta_{\omega_m}^2}} \Gamma_{\omega_m'} \omega_m (2)
\]

If we approximate \(\Delta_{\omega}\) in the first term by a constant, this term yields a BCS condensation energy which at \(T = 0\) is \(E_{c,\text{BCS}} = -N_0 \Delta^2/2\). The combination of the second and the third terms in \[14\], and the frequency dependence of \(\Delta_{\omega}\), account for the corrections to the BCS formula. We analyzed both corrections and found that at small \(\lambda\), the leading correction comes from the combination of second and third terms. At \(T = 0\), the sum of these two terms reduces to

\[
\delta E_c = -\frac{N_0 \lambda}{4} \int_0^\infty d\omega d\omega' \left( \frac{(\sqrt{1 + D_{\omega'}^2} - \sqrt{1 + D_{\omega}^2})^2}{\sqrt{1 + D_{\omega'}^2} \sqrt{1 + D_{\omega}^2}} \right) \left( \frac{1}{(1 + ((\omega - \omega')/\omega_D)^2)^{1/2}} - \frac{1}{(1 + ((\omega + \omega')/\omega_D)^2)^{1/2}} \right)
\]

Simple considerations show that the dominant contribution to the double integral comes from the range when either \(\omega \sim \omega_D\), and \(\omega' \sim \Delta\), or vice versa. Since at weak coupling, \(\Delta \ll \omega_D\), one can expand in the smaller frequency in the last term in \[15\]. One then obtains from

The dimensionless \(\lambda\) is defined as \(\lambda = (\bar{g}/\omega_D)^\gamma\) where \(\bar{g}\) is the effective fermion-boson interaction. This definition implies that at \(\omega_D \to 0\), the gap equation becomes independent of \(\omega_D\) as it should be as \(\omega_D \to 0\) just implies that a pairing boson becomes gapless, i.e., the pairing occurs near a quantum critical point (QCP). As in previous studies \[10\], we fix \(\bar{g}\) to set the overall energy scale, and compute \(E_c\) as a function of \(\lambda\). The choice to measure \(E_c\) in units of \(\bar{g}\) is justified on the grounds that near QCP, \(\bar{g}\) does not critically depend on the distance to criticality.

Once \(\Delta_{\omega_m'}\) is found by solving \[2\], \(Z_{\omega_m}\) is immediately obtained from

\[
Z_{\omega_m} = 1 + \pi T \lambda \sum_{m=\infty}^{\infty} \frac{1}{\omega_m^2 + \Delta_{\omega_m}^2} \frac{\omega_m}{\omega_m'} \Gamma_{\omega_m'} - \omega_m (3)
\]

The expression for the condensation energy in the Eliashberg theory for phonons \(\gamma = 2\) has been obtained by Wada and Bardeen and Stephen \[10\]. The extension to arbitrary \(\gamma\) is straightforward \[11\]. In terms of \(D_m = \frac{\Delta_{\omega_m}}{\omega_m'}\) and \(\Gamma_{\omega_m}\) the condensation energy reads

\[
\delta E_c = -\frac{N_0 \lambda}{4} \int_0^\infty \frac{d\omega d\omega'}{(\sqrt{1 + D_{\omega'}^2} - 1)^2} \sum_{m=\infty}^{\infty} \frac{1}{\sqrt{1 + D_{\omega'}^2} \sqrt{1 + D_{\omega}^2}} \left( \frac{1}{(1 + ((\omega - \omega')/\omega_D)^2)^{1/2}} - \frac{1}{(1 + ((\omega + \omega')/\omega_D)^2)^{1/2}} \right) \]

\[
\int_0^\infty \frac{d\omega' d\omega}{\sqrt{1 + D_{\omega'}^2}} \frac{(\sqrt{1 + D_{\omega'}^2} - 1)^2}{\sqrt{1 + D_{\omega}^2}} \]
The last integral is the same one that yields a BCS condensation energy. Evaluating the first integral, we obtain

\[ \delta E_c = \lambda E_{c,BCS} \]  

such that

\[ E_c = -N_0 \frac{\Delta^2}{2} (1 + \lambda) \]  

(7)

Note that the relative correction to the BCS result depends only on \( \lambda \), but not on \( \gamma \).

Eq. (8) for \( E_c \) can be formally obtained if one assumes that the quasiparticle renormalization factor \( Z(\omega) \) can be approximated by a constant, and this constant does not change between the superconducting and the normal state, where \( Z = 1 + \lambda \) [10]. For a constant \( Z \), the full Green’s function differs from the BCS result only by the renormalization \( \epsilon_k \rightarrow \epsilon_k^* = \epsilon_k/Z \). Since the condensation energy is the integral over \( \epsilon_k \) of the product of the Green’s function and the self-energy, the effect of \( Z \) can be absorbed into \( d\epsilon_k = Z \, d\epsilon_k^* \). Obviously then \( E_c = E_{c,BCS} (1 + \lambda) \) as in Eq. (8) [10]. It is not a priori clear, however, whether the change in \( Z \) between the normal and the superconducting state can be neglected, as, by rough estimates, the contribution to \( E_c \) from \( Z_{sc} - Z_n \) is of the same order as in [7]. We checked this explicitly for \( \gamma = 2 \) using the Bardeen-Stephen formula for \( E_c \) and found that the correction to \( E_c \) due to \( Z_{sc} - Z_n \) is small, because of an extra frequency integration involved, and scales as \( \lambda E_{c,BCS} \, (\Delta/\lambda \omega_D)^2 \ll \lambda E_{c,BCS} \). Our explicit calculation of \( \delta E_c \) above shows that this smallness survives for all \( \gamma \).

To test this result, we computed \( E_c \) numerically for a range of small to intermediate \( \lambda \).

The equation for \( \Delta_{\omega_m} \) was solved using an iterative computational method. Two representative sets of results for

\[ \Delta_{\omega_m}, Z_{\omega_m}, \Sigma_{\omega_m}, \Phi_{\omega_m} \] for \( \lambda = 0.3 \) and \( \gamma = 2 \) and \( \gamma = 1 \) are shown in Fig. 1. The condensation energy vs \( \lambda \) is plotted in Fig. 2. At the lowest \( \lambda < 0.5 \), we indeed reproduced the BCS result \( E_{c,BCS} = -N_0 \frac{\Delta^2}{2} \). We see, however, that at intermediate \( \lambda \leq 1 \), the condensation energy deviates from the BCS formula, but closely follows Eq. (8). At even larger \( \lambda \), \( E_c \) deviates even from the modified BCS expression.

We next discuss the behavior of the condensation energy at large \( \lambda \). Here the dependence on \( \gamma \) becomes crucial. First, we found from numerical computation that for \( \gamma = 2 \), the condensation energy never saturates and keeps slowly increasing with \( \lambda \) (see Fig. 3 and Fig. 4). This can be easily understood analytically: using \( \omega_D = \tilde{g}/\sqrt{\lambda} \) and substituting \( \lambda \Gamma_{\omega_m} = \tilde{g}/(\omega_m^2 + \lambda^{-1} \tilde{g}^2) \) into Eq. (8), one obtains that the second term in (9) diverges as \( \log \lambda \) [11]. A more careful examination shows [11] that this divergence actually comes from the divergence of the free energy of the normal state [17]

\[ F_n = N_0 \pi^2 T^2 \tilde{g}^2 \sum_{m,m'} \left( \frac{1 - \text{sgn}(\omega_m) \text{sgn}(\omega_{m'})}{(\omega_m - \omega_{m'})^2 + \lambda^{-1} \tilde{g}^2} \right) \]  

(9)

At \( T = 0 \) and \( \lambda \to \infty \) (i.e., \( \omega_D \to 0 \), the 2D integral in (9) diverges as \( \log \lambda \).

At the same time, in the superconducting state, the
As the frequency integral in $F_{\text{sc}}$ now converges. Carrying out the integration, we obtain an effective BCS formula

$$D = \frac{1}{\chi} \int_0^\infty dx \frac{1}{x(x^2+1)^\frac{3}{2}}$$

where $D_0 = D_0/\omega_D$. At $\gamma \to 0$ (i.e., when the pairing interaction tends to a constant), the integral diverges at the upper limit. This divergence is artificial as in reality the integration must not go beyond $x_{\text{max}} \sim E_F/\omega_D$. We, however, will focus on finite $\gamma$, when the integral converges. Carrying out the integration, we obtain an effective BCS formula

$$\Delta \sim \omega_D e^{-\frac{1}{\chi}} \exp \left[ \frac{\Psi(1) - \Psi(\frac{1}{2})}{2} \right]$$

where $\Psi(x)$ is the digamma function. The first term in the r.h.s. of Eq. (12) is the conventional weak-coupling result for a phonon superconductor. The dependence on $\gamma$ emerges through the second factor. We found that the dependence on $\gamma$ is actually quite strong already at intermediate $\gamma$. We plot our numerical $\Delta(\gamma)$ obtained for $\lambda = 0.5$ against Eq. (12) in Fig. 6. We see that the agreement between numerical and analytic $\Delta^2$ is quite good. As, to a very good accuracy, the condensation energy for $\lambda = 0.5$ scales as $E_c \propto D_0^2$, the good agreement in Fig. 6 implies that the origin of a very strong variation of $E_c$ with $\gamma$ is indeed a strong $\gamma$-dependence of the magnitude of $\Delta$.

Finally, we discuss the validity of the Eliashberg theory. For phonon superconductors, Eliashberg theory is based on the smallness of the ratio of the electron mass and the ionic mass, or, alternatively, with the smallness of the sound velocity $v_s$ compared to the Fermi velocity $v_F$. The theory is valid as long as $\lambda v_s/v_F < 1$, where $\lambda$ is the dimensionless coupling constant. On the scale of this parameter, one can neglect vertex corrections which
analyze both weak coupling $\lambda$ dimensionless $\lambda_0$ for phonons) becomes relevant, and for $\gamma$ Landau damping mechanism (which was unimportant to this regime, Eliashberg theory is valid. Note, however, that unlike the case of electron-phonon interaction, Eliashberg theory for electron-electron interaction is only applicable at $\lambda \geq 1$.

There are two other complications for collective mode-mediated pairing. First, the interaction is generally momentum-dependent, and the pairing is not of $s$-type. This does not invalidate Eliashberg theory as vertex corrections still remain small, and the momentum integration in the gap equation is still factorized. As a result, $\Delta_{\omega} \approx \Delta_k \Delta_{\omega}$, and the momentum dependence of the gap only affects the functional form of $\Gamma_\omega$, but does not change the structure of the equation for $\Delta_{\omega}$. Second complication is that the propagator of a collective mode by itself changes once the system enters a superconducting state. This, roughly, implies that $\gamma$ changes with $T/T_c$. In the analysis above we focused on $T = 0$, assuming that all feedback effects are already incorporated into $\Gamma_\omega$.

To conclude, in this paper we computed the condensation energy $E_c$ for Eliashberg superconductors for a wide range of coupling strengths and for several different physically motivated forms of the pairing interaction (parameterized by $\gamma$), representing both phonon ($\gamma = 2$) and electronic collective mode mediated superconductivity ($0 < \gamma < 2$). We found analytically and confirmed numerically that for weak coupling, $E_c = E_{c,BCS}(1 + \lambda)$, where $E_{c,BCS} = -N_0\Delta^2/2$ is BCS result. This result holds for all $\gamma$. We also found that in the opposite limit of very large $\lambda$, $E_c$ diverges as $\log \lambda$ if the pairing is mediated by phonons, but remains finite for electronic mechanisms of pairing and decreases with decreasing $\gamma$. However, for moderate $\lambda \geq 1$, we found an opposite trend – the condensation energy at a given $\lambda$ strongly increases with decreasing $\gamma$. We argued that this behavior holds in the regime where $E_c \propto \Delta^2$, and is a consequence of the strong $\gamma$ dependence of the pairing gap $\Delta$. We computed $E_c(\gamma)$ analytically and numerically and obtained a very good agreement between the two results.

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[17] Eqs. (9) and (10) require clarifications. Both normal and superconducting Free energies obtained from Luttinger-Ward functional contain an extra term $F_{ex} = -N_0 \left[ 2\pi T \sum_m |\omega_m| + \lambda \pi^2 T^2 \bar{\gamma}^2 \sum_{m,m'} \Gamma_{\omega_m-\omega_m'} \right]$. The first term in this extra piece does not depend on $\lambda$ and formally diverges at any $\lambda$ and any $T$, the second diverges as power of $\lambda$ at $\lambda \to \infty$ due to self-action piece with $m = m'$. This $F_{ex}$ is, however, irrelevant from physics perspective as the first term is independent on the interaction, while the second term is just the frequency integral of the interaction potential, and it does not distinguish between superconducting and normal states. We therefore can safely subtract $F_{ex}$ from the Free energy. This leads to Eqs. (9) and (10).
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