A look at the crossover region between BCS superconductivity and Bose Einstein Condensation

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Pair fluctuation theory has been used to study the crossover from the weak coupling BCS theory to the strong coupling Bose Einstein Condensation. The effect of fluctuations has been studied over the whole crossover regime. It has been shown that the pair fluctuations are enhanced considerably in both two and three dimensions and hence mean field theory is inadequate to study the physical properties in this regime. A self consistent scheme for calculating the pair susceptibility is given.

The study of crossover from BCS to Bose Einstein Condensation has been a subject of intense study in recent times. The motivation for this study has been from the point of view of trying to model High $T_c$ superconductors. These materials share many properties with BCS superconductors, however, the coherence length $\xi$ in these materials is unusually small. The short coherence length feature is also apparent in the phenomenon of Bose Einstein Condensation (BEC) where the coherence length $\xi$ is expected to be of the order of an atomic spacing. Moreover, in the BEC process the temperature at which pairing occurs is different from the pair condensation temperature. The phenomenon of BEC was was known as Schafroth condensation in the pre BCS days of superconductivity. Recently this has lead to a formulation of theories based on occurence of pseudo gaps in the normal state of these materials. The crossover from BCS to BEC has been studied as a case of weak to strong attractive coupling theory in details during recent years within the mean field theory or RPA. These results agree with the expected behavior at the two extreme limits (i.e. the weak coupling BCS limit and the strong coupling BEC limit) and predict a smooth crossover from one limit to the other. However, the intermediate regime, to which the High $T_c$ superconductors are believed to belong within this theory, has not been well understood. The theory is based on the existence of two parameters which can be varied - the electronic density $n$ and the coupling strength $g$. Coupled self consistent equations for these two parameters leads to the calculation of $T_c$, the transition temperature and the chemical potential $\mu$. For a constant density, if the coupling strength is varied, there is smooth crossover from the weak coupling BCS superconductivity to the strong coupling Bose Einstein condensation. In principle, however, both the parameters can be varied. If this is done such that $T_c$ remains constant and $\mu$ is varied there is a crossover with respect to $\mu$, where for large positive $\mu$ ($\mu \sim \epsilon_F$, the Fermi temperature) the results for the BCS superconductors are recovered and for large negative $\mu$ the BEC results are recovered. Thus, the intermediate regime can be interpreted in this regime as the region close to $\mu = 0$. In what follows, we shall take this point of view in order to study the crossover.

In this work, we wish to study the crossover regime from the point of view of pair fluctuations. The main aim of this work is to ask the question - how important are fluctuation contributions to this phenomenon of crossover, especially in the region close to the crossover ? As has already been mentioned before, most of the studies in this subject have taken recourse to mean field theory. If fluctuation contributions do become important, then, mean field theory is bound to breakdown. We therefore set up an equation for the pair susceptibility within the mean fluctuation field approximation (MFFA) where the effect of fluctuations are included in a self consistent manner. This self consistent equation is then solved to obtain the inverse pair susceptibility over the whole regime of crossover from the BCS limit (where $\mu \gg T$) to the BEC limit (where $-\mu \gg T$).

The starting point for the calculation is the BCS Hamiltonian in the momentum space with an s-wave attractive potential which is given by,

$$H - \mu N = \sum_{p,\sigma} \epsilon_p C_{p,\sigma}^\dagger C_{p,\sigma} - \frac{1}{2} g \sum_{p, p', q, \sigma} C_{p+q,\sigma}^\dagger C_{-p, -\sigma}^\dagger C_{p', -\sigma} C_{p'+q, \sigma},$$

(1)

where $\epsilon_p = p^2/2m$ is the free electron kinetic energy, and $g$ is the interaction strength. The mean field results for this Hamiltonian are well known for both the BCS limit and the BEC limit.

The functional integration technique is a convenient method for treating the fluctuation problem microscopically. For the case of superconductors the technique was developed by Langer, Rice and others. We follow the procedure adopted by Rice in what follows. Using the functional integral technique the partition function can be expressed as,

$$Z/Z_0 = \int \prod \frac{Dx_{q,m}}{\pi} \exp \{ -\beta F[x_{q,m}] \}$$

(2)
where \( Z_0 \) is the partition function of non-interacting system and \( x_{q,m} \) is the (bosonic) auxiliary field with momentum \( q \) and frequency \( \omega_m \). The pairing correlation is the only one which has been considered here. A diagrammatic expansion of \( F[x_{q,m}] \) in powers of \( x_{q,m} \) is possible and leads to the Ginzburg Landau functional. The corresponding expression for the free energy functional is given by,

\[
F^{(1)}[x_{q,m}] = \frac{1}{\beta} \sum_{q,m} (1 + gK^{(1)}_q)x^*_{q,m}x_{q,m} + \frac{1}{\beta} g^2 \sum_{q,m} K^{(2)}_{q_1,q_2,q_3}x^*_{q_1}x_{q_2}x_{q_3}x_{q_1+q_2-q_3}.
\]

These terms are shown in Fig. (1).

\[\text{FIG. 1. Lowest order diagrams for Free Energy}\]

The Eq. 3 represents the free energy of interacting electrons near a superconductive instability in terms of interacting pair fluctuation field. The first term is the “free” or the RPA term (Fig. 1a), while the second term represents the interaction between pair fields (Fig. 1b). Parameters of this model, e.g. transition temperature, collective mode dispersion, fluctuation spectrum, fluctuation coupling vertices are determined by properties of the underlying fermion system. Expanding \( K^{(1)} \) and \( K^{(2)} \) in powers of \( q \) and \( \omega_m \) and retaining the lowest powers we get,

\[
\beta F[x_{q,m}] = [a + cq^2 - i\omega_m] |x_{q,m}|^2 + b |x_{q,m}|^4.
\]

The coefficients \( a, b, c \) and \( d \) are given by,

\[
a = \frac{1}{g} - \frac{1}{\beta} \sum_{p,\nu_l} \frac{1}{((\epsilon_p - \mu)^2 + \nu_l^2)}
\]

\[
b = \frac{1}{2\beta} \sum_{p,\sigma,l} \frac{1}{((\epsilon_p - \mu - i\nu_l)^2 - \nu_l^2)^2}
\]

\[
c = \frac{2m}{\beta} \sum_{p,\nu_l} \frac{1}{((\epsilon_p - \mu)^2 + \nu_l^2)^2} \left[(\epsilon_p - \mu) - \eta \epsilon_p \left((\epsilon_p - \mu)^2 + \nu_l^2\right)\right]
\]

\[
d = \frac{1}{\beta} \sum_{p,\nu_l} \frac{(\epsilon_p - \mu)}{((\epsilon_p - \mu)^2 + \nu_l^2)^2},
\]

where \( \nu_l = (2l + 1)\pi/\beta \). The value of \( \eta \) comes out to be 2 in 2D and 4/3 in 3D. At \( T = T_c \), \( a = 0 \), which leads to the Thouless criterion, \( 1 + gK^{(1)}_0 = 0 \),

\[
\frac{1}{g} = \frac{1}{\beta_c} \sum_{p,\nu_l} \frac{1}{((\epsilon_p - \mu_c)^2 + \nu_l^2)} = \frac{1}{2} \int_0^\infty d\epsilon \rho(\epsilon) \frac{\tanh[\beta_c(\epsilon - \mu_c)/2]}{(\epsilon - \mu_c)}
\]

The integral on the right hand side is UV divergent. In the conventional weak coupling theory this is taken care of by putting an upper cutoff at the Debye energy. However, since we are interested in the crossover from weak to strong coupling behavior this restriction on the energy integration has to be removed. The singular behavior is taken care of by replacing the bare \( g \) by the low energy limit of the two body \( T \) matrix,

\[
\frac{1}{g} = -\frac{1}{t} + \sum_{2k} \frac{1}{2\epsilon_k},
\]
where $1/t$ turns out to be $m/4\pi a_s$ for $d = 3$ and $(m/4\pi)\ln(E_b/2)$ for $d = 2$. Here $a_s$ is the s-wave scattering length and $E_b = 1/ma_s^2$.

The number density of electrons $n$ and the coupling strength $g$ determine the transition temperature and also specify whether one is in Bose or the BCS regime of pairing. These are related to the transition temperature $T_c$ and the chemical potential $\mu$ through Eqs. (3) and the equation for the number density, viz.

$$n = \sum_k (1 - \tanh \frac{\beta(k - \mu)}{2}),$$

which are to be solved self consistently. One can consider ($n$ and $g$) or ($T_c$ and $\mu$) combination as the parameters in the problem. We find convenient to consider the latter pair, particularly when dealing with the crossover region. The region around $\mu \sim 0$ marks the crossover. We write $a$ etc. in terms of $T_c$ and $\mu_c$, i.e.,

$$a = \frac{1}{2} \left( \int_0^\infty d\rho(\epsilon) \frac{\tanh[\beta(\epsilon - \mu_c)/2]}{(\epsilon - \mu_c)} - \int_0^\infty d\rho(\epsilon) \frac{\tanh[\beta(\epsilon - \mu)/2]}{(\epsilon - \mu)} \right).$$

The expressions for $b, c$ and $d$ are nonsingular at $T_c$.

The pair susceptibility can be calculated in this scheme as,

$$\chi(q, \omega_m) = \langle |x_{q,m}|^2 \rangle = \int dx_{q,m} dx_{q,m}^* |x_{q,m}|^2 \exp -\beta F[x_{q,m}] / \int dx_{q,m} dx_{q,m}^* \exp -\beta F[x_{q,m}]. \quad (10)$$

We now write down a self consistent equation for the inverse of pair susceptibility within the mean fluctuation field approximation. This amounts to writing the quartic term, in the expansion of the free energy functional in terms of the pair field, as a quadratic form (i.e. $|x_{q,m}|^4 = \langle x_{q,m}^2 \rangle$) and taking average over the effective Gaussian distribution. The technique is well known [17]; we, however, follow the earlier work on spin fluctuations [14]. The pair susceptibility is given by,

$$\chi(q, \omega_m) = \frac{1}{\alpha(T, \mu) + cg^2 + id\omega_m}, \quad (11)$$

where,

$$\alpha(T, \mu) = a + b \sum_{q', \omega_{m'}} \chi(q', \omega_{m'}). \quad (12)$$

FIG. 2. Mean fluctuation field diagram

To calculate the susceptibility one needs values of Ginzburg-Landau coefficients, $a$, $b$, $c$ and $d$. On performing the summation over the Matsubara frequencies, one gets in 3 dimensions,

$$b = \frac{1}{8} \int_0^\infty d\epsilon \rho_{3D}(\epsilon) \Phi(\epsilon), \quad c = \frac{1}{12} \int_0^\infty d\epsilon \rho_{3D}(\epsilon) \epsilon \Phi(\epsilon), \quad \text{and} \quad d = \frac{1}{8} \int_0^\infty d\epsilon \rho_{3D}(\epsilon)(\epsilon - \mu) \Phi(\epsilon). \quad (13)$$

Here, $\rho_{3D}(\epsilon) = (2m)^{3/2}\sqrt{\tau}/4\pi^2$ is the density of states in 3 dimensions and

$$\Phi(\epsilon) = \{2 \tanh[\beta(\epsilon - \mu)/2] - \beta(\epsilon - \mu)\sech^2([\beta(\epsilon - \mu)/2]/(\epsilon - \mu)^3. \quad (14)$$

It is not possible to evaluate the energy integral analytically throughout the parameter space. Only in the extreme limits the results are available. In the BCS limit $\beta\mu \gg 1$, $a = \ln(\pi\epsilon^2/[8e\gamma\beta\mu]) - \ln(\pi\epsilon^2/[8e\gamma\beta\mu_c])\rho_{3D}(\mu_c), \quad (15)$
\[ b = \frac{7(\zeta(3)/8\pi^2)}{\rho_{BD}(\mu)} c = \frac{7(\zeta(3)/12\pi^2)}{\rho_{BD}(\mu)} \beta^2, \quad d = \ln(8\gamma\beta\mu/\pi) \rho_{BD}(\mu)/4\mu. \]

In the Bose Einstein regime \((-\beta\mu \gg 1)\) the corresponding value are, \[ a = (\pi/2)\rho_{BD}(\mu) - \rho_{BD}(\mu_c), \quad b = \rho_{BD}(\mu)(\pi/32 | \mu |^2), \]
\[ c = \rho_{BD}(\mu)(\pi/16 | \mu |), \quad d = \rho_{BD}(\mu)(\pi/8 | \mu |). \]

Similarly, in two dimensions, the summation over the Matsubara frequencies gives,
\[ b = \frac{1}{4} \int_0^\infty d\epsilon \rho_{2D}(\epsilon) \Phi(\epsilon), \quad c = \frac{1}{4} \left( \frac{7(\zeta(3)/2\pi^2)}{\rho_{2D}(\epsilon)} \beta^2 \mu(\mu) + | \mu | \int_{|\mu|} d\xi \rho_{2D}(\epsilon) \frac{\text{tanh}(\beta\xi/2)}{\xi^3} \right), \quad d = \frac{\rho_{2D}(\epsilon) \text{tanh}(\beta\mu/2)}{4\mu}, \]

(15)

where \( \rho_{2D}(\epsilon) = m/2\pi \). Again, in the BCS limit, \[ a = \rho_{2D} \ln(\beta_\mu/\beta\mu), \quad b = \frac{7(\zeta(3)/8\pi^2)}{\rho_{2D}} \beta^2, \quad c = \frac{7(\zeta(3)/8\pi^2)}{\rho_{2D}} \beta^2, \]
\[ d = \rho_{2D}/4\mu; \text{ and in the Bose Einstein limit}, \quad a = (1/2) \rho_{2D} \ln(\mu_c), \quad b = \rho_{2D}/8 | \mu | \text{ and } d = \rho_{2D}/4 | \mu |. \]

Since the values for the GL coefficients are expressible analytically only in the two limiting cases we use the full expression for these coefficients to calculate the susceptibility and take recourse to the numerical evaluation of the integrals.

Before proceeding further we want to make some remarks regarding these coefficients. In the BCS limit the temperature dependence of \( c \) (which is related to \( \xi^2 \)) and the coefficient of the fourth order term are similar. (In fact \( b \) and \( c \) are related in both the limits). The reason for this can be traced to the diagrammatic representation of these terms. The quadratic term has two internal fermion lines and to get the coefficient \( c \) we differentiate \( K^{(1)} \) twice with respect to momentum. This makes it equivalent to four fermion lines which is similar to four fermion lines in the fourth order term, particularly when vanishing momentum limit is taken. Moreover, \( b \) and \( c \) are singular as \( T \approx T_c \to 0 \).

This may have interesting consequences when one considers the possibility of quantum phase transition in this limit. The second remark is regarding the BE limit. In this limit the coefficients, in both two and three dimensions, are independent of temperature. The GL expansion look similar to one for system near an antiferromagnetic instability [23]. Thus in this limit, one can expect that in the limit of \( T_c \to 0 \) (in case it is possible) a non-Fermi liquid like behavior in some transport and thermodynamic properties may be seen and the temperature dependence of these quantities will be similar to that in antiferromagnets.

To calculate the pair susceptibility the equation for \( \alpha(T,\mu) \) must be solved self-consistently. For this we first note that,
\[ \frac{1}{\beta} \sum_{q,m} \chi(q,\omega_m) = \frac{d}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\omega}{(\alpha(T) + eq^2)^2 + d^2 \omega^2} \frac{1}{(e^{\beta\omega} - 1)} \]
\[ = \frac{1}{\pi} \ln[y - (2y)^{-1} - \psi(y)], \]

where \( \psi(y) \) is the digamma function and \( y \) is given by, \( \alpha + eq^2)/2\pi dT \). A good interpolation for \( \ln[y - (2y)^{-1} - \psi(y)] \) which is valid for large as well as small \( y \) is \( 1/(2y + 12y^2) \). Thus, the self-consistent equation for \( \alpha(T,\mu) \) can be written as,
\[ \alpha(T,\mu) = a + \frac{b}{\pi} \int_0^{q_c} dq \frac{q^{D-1}}{2y + 12y^2} \]

\[ (17) \]

where \( D \) denotes the dimension of the system. Our interest is in how \( \alpha(T,\mu) \) which has been obtained within the fluctuation theory compares with the mean field value \( a \). We calculate \( \alpha(T,\mu) \) as a function of \( \mu \) at temperatures just above \( T_c \).

The results of self consistent calculation of Eq. (17) with the numerical evaluation of the coefficients \( b \), \( c \) and \( d \) in three and two dimensions is plotted along with the corresponding mean field value \( a \) in Fig. (3). The parameters are taken as \( \beta_c = 100 \) and \( \beta = 90 \). The behavior of the curves is not very different in two and three dimensions qualitatively. In the calculation of the coefficient \( a \), we have assumed that \( \mu \) at temperature just above \( T_c \) is the same as its value at \( T_c \), i.e. \( \mu_c \). This is reasonable for temperatures close to \( T_c \). This is why in the extreme negative \( \mu \) regime (the BEC regime) \( a \) is identically equal to zero since in this regime \( a \) is independent of temperature. From the figure two things stand out very clearly - the first is that in the extreme limits (both the BCS and the BEC), the effect of fluctuations is negligible. Secondly, as one moves away from the two extreme limits by reducing \( | \mu | \), the effect of fluctuations increases leading to a dominant contribution to the pair susceptibility as \( \mu \to 0 \). In the the BEC regime as one moves towards the crossover regime the value of \( a \) also increases but the fluctuation contribution is much larger. It is also apparent that, the fluctuation contribution in two dimensions is an order of magnitude higher than in three dimensions for the same set of parameters. The curves are shown for relatively small transition
temperature. Preliminary results indicate that as the parameter $\beta_c$ is reduced from the value $\beta_c = 100$ towards $\beta_c = 20$ corresponding to an increase in the transition temperature, the crossover region as well as the fluctuation contribution both increase.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{Inverse susceptibility within the mean fluctuation field approximation ($\alpha(T,\mu)$) and within the mean field approximation ($\alpha'(T,\mu)$) plotted as a function of $\mu$ in three dimensions (a) and in two dimensions (b). Note that the scale for the plot in two dimensions (b) is one order of magnitude larger than that in three dimensions (a).}
\end{figure}

In conclusion, we have studied the crossover from BCS to BEC from the point of view of pair fluctuations. We find that the effects of fluctuations are large in the crossover regime, where $\mu$ is close to zero. This shows that a mean field calculation will be inadequate in this regime. The enhanced fluctuation effects show that the behavior of physical properties can be qualitatively different in this regime. If a parallel is drawn with the results of Spin Fluctuation theory, then it can be predicted that the physical properties of the system may show a non-Fermi liquid behavior if parameters are such that one is close to $T_c$, with $T_c \to 0$. The non-Fermi liquid behavior of some high $T_c$ materials can be modeled in this scheme. Our discussion has been confined to isotropic two- or three-dimensional systems, while the anisotropy seems to play an important role in the High $T_c$ materials. This is especially true for the layered High $T_c$ compounds. However, in the layered materials, the coherence length along the $a-b$ plane is also of the order of that expected for the bulk material. Hence, the normal state properties of the $a-b$ plane, which are different from the properties along the $c$ axis, should in fact follow our two dimensional result. The other important point is that the form of the pairing potential which we have chosen here is s-wave. It is now quite well agreed upon that the pairing potential in most of the High $T_c$ materials, especially the layered materials, is d-wave. In our opinion the enhancement of fluctuations will occur in this case also along with the reflection of the inherent anisotropy brought in by the d-wave nature of the pair wave function. Work in this direction is in progress.

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