A study on the coexistence of BEC and BCS states
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Abstract

We pointed out in this work that in dealing with the BEC-BCS crossover problem, the dynamic effect of $<b(t)>$ is not negligible. Accordingly, an equation of motion approach was devised to calculate the Green’s functions. Based on our result, we concluded that instead of crossover, BCS states and Bose-Einstein condensation always coexist.
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The physics of BCS states in a dilute system was first studied by Eagles[1] who proposed the possibility of forming Cooper pairs before the onset of superconductivity. The BEC-BCS crossover problem was discussed by Leggett[2] in 1980. He pointed out that there is no distinct boundary between Cooper pairs and Bose-Einstein condensation. As elaborated later by Nozières and Schmitt-Rink[3], in the strong coupling or low density limit, fermions will combine to form bosonic molecules and condense at sufficiently low temperature. As the coupling is weakened or density increases, the molecular wave functions overlap. With sufficient overlapping, the molecular BEC will be transformed into BCS states. The authors [2,3] saw no phase transition. In their opinion, the amplitudes of the states of phase coherence (BEC and BCS) undergo smooth variation.

On the other hand, there has been marvellous experimental progress[4-8] recently. Fermionic atoms in a trap can form bosonic molecules via Feshbach resonance[9]. The coupling strength can be adjusted by changing the applied magnetic field. The energy gap was found on both sides of resonance and its spectrum is compatible with theoretical calculation[10]. Hence, the scenario envisaged by Leggett[2] and Nozières and Schmitt-Rink[3] seems to be realized, with one complication: the fermions and bosons have internal degrees of freedom. They are the spins of electrons and nuclei. The above mentioned Feshbach resonance is fulfilled with the aid of hyperfine interaction. As a result, the state of electron spins of the atoms in the open channel are different, in general, from those in the closed channel.

Much theoretical work has been devoted to this subject. Kokkelmans et al.[11] made a thorough analysis of Feshbach resonance of the cold atom system. Their deduction greatly simplified further computation. Ohashi and Griffin[12] adopted the orthodox Feynman diagram approach. Stajic et al.[13] applied the concept of pseudogap originated from high $T_C$ superconductivity to explain the experimental results. In this paper we would like to raise a neglected point which has profound effect on one’s understanding of the BEC-BCS system.

We started with the of fermion-boson Hamiltonian[14]:

$$H = \sum_{p,\sigma} \varepsilon_p c_{p,\sigma}^\dagger c_{p,\sigma} + \sum_q (\omega_q + \nu) b_q^\dagger b_q - U \sum_{k,p,q} c_{p+q,\uparrow}^\dagger c_{k-q,\downarrow}^\dagger c_{k,\downarrow} c_{p,\uparrow}^\dagger + g \sum_{p,q} b_q^\dagger c_{-p+q/2,\downarrow}^\dagger c_{p+q/2,\uparrow}^\dagger + H.c. \quad (1)$$

where $c_{p,\sigma}$ and $b_q$ are the fermion and boson operators, $\varepsilon_p$ and $\omega_q$ are their energies, $\nu$ is the detuned energy of bosons, and $\sigma$ is the spin index. The terms in the second line denote the combination of atoms and dissociation of molecules. They are necessary because, as we stated before, the states of spins had been changed. Cooper pairs have different spin states from those in BEC. So they should be treated as different species.

Now we calculate the Green’s functions $G_\sigma(\tau, \tau'; k) = -\langle \hat{T}_{c_{k,\sigma}}(\tau)c_{k,\sigma}^\dagger(\tau') \rangle$ and $F_{\alpha\beta}(\tau, \tau'; k) = \langle \hat{T}_{c_{k,\alpha}}(\tau)c_{k,\beta}^\dagger(\tau') \rangle$ where $\hat{T}$ is the time-order operator. The
approach of equations of motion was applied.

\[
\frac{d}{d\tau} G^\tau_\nu(\tau, \tau'; \mathbf{k}) = -\delta(\tau - \tau') - \varepsilon_\mathbf{p} G^\tau_\nu(\tau, \tau'; \mathbf{k}) - [U F^\tau_{\uparrow \downarrow}(\tau, \tau) - g \langle b_0 \rangle] F^\tau_{\uparrow \downarrow}(\tau, \tau'; \mathbf{k}) \\
+ g \sum_q \langle T [b_q(\tau) - \langle b_0 \rangle] c^\dagger_{-\mathbf{k} + \mathbf{q}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle
\]  

(2)

and

\[
\frac{d}{d\tau} F^\tau_{\uparrow \downarrow}(\tau, \tau'; \mathbf{k}) = \varepsilon_\mathbf{p} F^\tau_{\uparrow \downarrow}(\tau, \tau'; \mathbf{k}) + [U F^\tau_{\uparrow \downarrow}(\tau, \tau) - g \langle b_0 \rangle] G_{\downarrow}(\tau, \tau'; \mathbf{k}) \\
+ g \sum_q \langle T [b^\dagger_q(\tau) - \langle b_0 \rangle] c_{\mathbf{k} + \mathbf{q}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle
\]  

(3)

where \( F_{\alpha \beta}(\tau, \tau) = \sum_{\mathbf{p}} \langle c_{-\mathbf{p}, \alpha}(\tau)c_{\mathbf{p}, \beta}(\tau) \rangle \). Here we assumed the Hartree-Fock terms can be absorbed into the single-particle energy. A term \( \langle b_{\mathbf{q}=0} \rangle \) had been intentionally added to and substracted from the right hand side to facilitate later decoupling.

While developing superconductivity theory, \( F_{\alpha \beta}(\tau, \tau) \) is usually set to be a real constant independent of \( \tau \). The prescription is to subtract \( N\mu \) from \( H[15] \). Similarly, in calculation involving BEC, \( \langle b_0(\tau) \rangle \) is also treated as a constant. In the case when both \( F_{\alpha \beta}(\tau, \tau) \) and \( \langle b_0(\tau) \rangle \) are present, this method in general, can only make either one of them a constant but not both. This point was ignored by the preceding works on the BEC-BCS crossover problem. In this paper, we chose to let \( F_{\alpha \beta}(\tau, \tau) = F_{\alpha \beta} \) be a constant and \( \langle b_0(\tau) \rangle \) a function of \( \tau \). This is the gist of this work.

With \( H \) replaced by \( H - N\mu \), we have to substitute \( \xi_\mathbf{k} \equiv \varepsilon_\mathbf{k} - \mu \) for \( \varepsilon_\mathbf{k} \) and \( \nu' = \nu - 2\mu \) for \( \nu \) in eqs. (1-3). If \( \langle b_0(\tau) \rangle \) was treated dynamically, we arrived at the next set of equations of motion:

\[
\frac{d}{d\tau} \langle T [b_\mathbf{q}(\tau) - \langle b_0 \rangle] c^\dagger_{-\mathbf{k} + \mathbf{q}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle \\
= [-\omega_\mathbf{q} + \nu'] + \xi_{\mathbf{k} - \mathbf{q}} \langle T [b_\mathbf{q}(\tau) - \langle b_0 \rangle] c^\dagger_{-\mathbf{k} + \mathbf{q}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle - \langle \omega_\mathbf{q} + \nu' \rangle \langle b_0 \rangle \langle T c^\dagger_{-\mathbf{k} + \mathbf{q}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle \\
+ U \sum_{\mathbf{p}, \mathbf{q}} \langle T [b_\mathbf{q}(\tau) - \langle b_0 \rangle] c^\dagger_{\mathbf{p} + \mathbf{q}, \downarrow}(\tau)c^\dagger_{-\mathbf{k} + \mathbf{q} - \mathbf{p}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau) \rangle \\
- g \sum_{\mathbf{p}} \langle T [b_\mathbf{p}(\tau) - \langle b_0 \rangle] c_{\mathbf{k} - \mathbf{q} + \mathbf{p}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle \\
+ \langle T c_{\mathbf{q} - \mathbf{p}, \downarrow}(\tau)c^\dagger_{\mathbf{p}, \uparrow}(\tau)c^\dagger_{\mathbf{k} - \mathbf{q}, \downarrow}(\tau)c^\dagger_{\mathbf{k}, \uparrow}(\tau') \rangle
\]  

(4)
and

\[
\frac{d}{d\tau} \langle \hat{T} [b_{q}^\dagger (\tau) - (b_{q}^\dagger)] c_{k+q,\downarrow} c_{k,\downarrow}^\dagger (\tau') \rangle
= [(\omega_{q} + \nu') - \xi_{k+q}^\prime] \langle \hat{T} [b_{q}^\dagger (\tau) - (b_{q}^\dagger)] c_{k+q,\downarrow} c_{k,\downarrow}^\dagger (\tau') \rangle + (\omega_{q} + \nu') \langle b_{q}^\dagger (\tau') c_{k+q,\downarrow} c_{k,\downarrow}^\dagger (\tau') \rangle \\
+ U \sum_{p,q} \langle \hat{T} [b_{q}^\dagger (\tau) - (b_{q}^\dagger)] c_{p+q,\uparrow} c_{k+q,\downarrow} c_{p,\uparrow}^\dagger (\tau') \rangle \\
+ g \sum_{p} \{ \langle \hat{T} [b_{q}^\dagger (\tau) - (b_{q}^\dagger)] b_{p} c_{p-k,\uparrow} c_{k,\downarrow} (\tau') \rangle - \langle \hat{T} c_{q-p,\downarrow} (\tau) c_{p,\uparrow}^\dagger c_{q-k,\uparrow} (\tau) c_{k,\downarrow}^\dagger (\tau') \rangle \}. 
\]

(5)

At this stage we applied the decoupling between the fermion operators and boson operators. As before, we assumed the contribution of the interaction terms of eqs. (4) and (5) (the third and fourth lines) can be incorporated into the one-particle energies \( \xi_k \) and \( \nu \). The resulting forms will be comprehensible and easy to analyze. Thus, eqs. (4) and (5) became

\[
\left[ \frac{d}{d\tau} + (\omega_{q} + \nu') - \xi_{k+q}^\prime \right] \langle \hat{T} [b_{q}^\dagger (\tau) - (b_{q}^\dagger)] c_{k,\downarrow}^\dagger c_{k,\uparrow} (\tau') \rangle \simeq -(\omega_{q} + \nu') \langle b_{q}^\dagger (\tau') c_{k,\uparrow}^\dagger (\tau') \rangle \\
\left[ \frac{d}{d\tau} - (\omega_{q} + \nu') + \xi_{k+q} \right] \langle \hat{T} [b_{q}^\dagger (\tau) - (b_{q}^\dagger)] c_{k,\downarrow}^\dagger c_{k,\uparrow} (\tau') \rangle \simeq (\omega_{q} + \nu') \langle b_{q}^\dagger (\tau') c_{k,\uparrow}^\dagger (\tau') \rangle. 
\]

(6)

(7)

Taking Fourier transform of eqs. (2), (3), (6) and (7) and making substitutions, we obtained

\[
G_{k,\uparrow} (i\omega_{n}) = \frac{i\omega_{n} + \xi_{k}}{\psi (i\omega_{n}, k)},
\]

(8)

and

\[
F_{k,\uparrow}^* (i\omega_{n}) = -UF_{k,\uparrow}^* + g\phi (i\omega_{n} - \xi_{k}) / (i\omega_{n} + \nu' - \xi_{k}) \psi (i\omega_{n}, k)
\]

(9)

where \( \phi = \langle b_{0} \rangle \) and

\[
\psi (i\omega_{n}, k) = (i\omega_{n} + \xi_{k})(i\omega_{n} - \xi_{k}) - [UF_{k,\uparrow}^* - g\phi (i\omega_{n} - \xi_{k}) / (i\omega_{n} + \nu' - \xi_{k})] [UF_{k,\uparrow} - g\phi (i\omega_{n} + \xi_{k}) / (i\omega_{n} - \nu' + \xi_{k})] \\
= \left[ (i\omega_{n})^2 - E_{k,\uparrow}^2 \right] \left[ (i\omega_{n})^2 - E_{k,\uparrow}^2 \right] / \left[ (i\omega_{n})^2 - (\xi_{k} - \nu')^2 \right]
\]

(10)

with

\[
E_{k,\pm}^2 = B \pm \sqrt{B^2 - \xi_{k}^2 (\xi_{k} - \nu')^2 - U^2 F_{k,\uparrow}^* (\xi_{k} - \nu')^2 - g^2 \phi^2 \xi_{k}^2 + 2UF_{k,\uparrow}^* g\phi \xi_{k} (\xi_{k} - \nu')} \]

(11)

where \( B = [\xi_{k}^2 + (\xi_{k} - \nu')^2 + (UF_{k,\uparrow}^* - g\phi)^2] / 2 \). Clearly, the Green’s functions still possess the conventional form of BCS theory. However, we accounted for the most important ingredient: the coupling between \( F_{\alpha\beta}^* \) and \( \phi \), to insure that we
The parameters are the same as those in ref. 12, i.e.,

\[ N_0 = \mu \]

with eqs. (13-15) we can solve for three unknowns. Here, we have kept only the zeroth and first order terms. The relation

\[ \Omega = \sum_k \xi_k + (U F_{1\uparrow} - g \phi) F_{1\uparrow}^* - k_B T \sum_{n,k} \ln \psi(i \omega_n, k) + (\nu - 2 \mu) \phi^2 + k_B T \sum_q \{ 1 - e^{-[(\omega_n + \nu')]^2} \} \]

is also helpful. Now we take the variational approach.

\[ N = -\frac{\partial \Omega}{\partial \mu} = \sum_k \left[ 1 + \frac{\partial E_{+,k}}{\partial \mu} \tanh \frac{\beta E_{+,k}}{2} + \frac{\partial E_{-,k}}{\partial \mu} \tanh \frac{\beta E_{-,k}}{2} - \tanh \frac{\beta (\xi_k - \nu')}{2} \right] + 2 \phi^2 + 2 \sum_q n_B(\omega_q), \]

and

\[ \frac{\partial \Omega}{\partial \phi} = 2 \phi' - g F_{1\uparrow}^* - \sum_k \frac{\partial E_{+,k}}{\partial \phi} \tanh \frac{\beta E_{+,k}}{2} + \frac{\partial E_{-,k}}{\partial \phi} \tanh \frac{\beta E_{-,k}}{2} = 0 \]

where \( n_B(\omega_q) = 1/[e^{(\beta \omega_q + \nu') - 1}] \). Additionally, we have the gap equation

\[ F_{1\uparrow}^* = \sum_{n,k} F_{1\uparrow}^* (i \omega_n, k) = \sum_k \frac{U F_{1\uparrow}^*[E_{+,k}^2 - (\xi_k - \nu')^2] - g \phi [E_{+,k}^2 - \xi_k (\xi_k - \nu')]}{2 E_{+,k} (E_{+,k}^2 - E_{-,k}^2)} - \sum_k \frac{U F_{1\uparrow}^*[E_{-,k}^2 - (\xi_k - \nu')^2] - g \phi [E_{-,k}^2 - \xi_k (\xi_k - \nu')]}{2 E_{-,k} (E_{+,k}^2 - E_{-,k}^2)} \]

With eqs. (13-15) we can solve for three unknowns: \( \mu, \phi \) and \( F_{n\beta}^* \).

We showed the results in Figs. 1 by plotting \( \phi \) and \( F_{1\uparrow}^* \) versus temperature at detuned energies \( \nu = \pm 0.5 E_F \) in the solid and dashed lines respectively. The parameters are the same as those in ref. 12, i.e., \( g = -0.6 E_F, U = 0.3 E_F \) and a cutoff factor \( \exp[-(\xi_k/2 E_F)^2] \). In Fig. 2 the amplitudes of the states of phase coherence \( F_{1\uparrow}^* \) and \( \phi \) at \( k_B T = E_F/3 \) (in the dashed lines) and \( k_B T = E_F/6 \) (in the solid lines) are plotted against the detuned energy. It is remarkable that in Figs. 1 and 2 \( F_{1\uparrow}^* \) and \( \phi \) coexist in the whole range and vanish together. There is no crossover. In fact, similar results had been obtained by previous calculations[11,12] with the static approximation \( \langle h(\tau) \rangle = 0 \) and the resultant relation \( \phi = -g F_{1\uparrow}^*/(\nu - 2 \mu) \) and energy gap \( \Delta = |U + g^2/(\nu - 2 \mu)| F_{1\uparrow}^* \).

Note that one of the consequences of the approximation is that \( \phi \) and \( F_{1\uparrow}^* \) are proportional. However, our approach did not have the proportional relation \textit{a priori}. Therefore, we are able to conclude that the original concept of BEC-BCS crossover cannot be applied here.

In Fig. 3 we presented \( -\text{Im} F_{1\uparrow}^*(E) \) versus \( E/E_F \). On the BCS side (\( \nu > 0 \)), the feature of Cooper pair density of states is clearly shown. It gradually became
molecule-like when $\nu$ became negative. The reason, as pointed out by Leggett[2], is that when the chemical potential becomes negative, the divergence in the spectrum disappear. Note that in the whole range, the amplitude of BEC is greater than that of BCS due to the parameters we chose. Yet the spectrum underwent drastic change. Clearly, the shape of spectrum is not an indication of whether it is BEC or BCS state.

It should not be surprising that BEC persists deeply into the BCS side of Feshbach resonance. Although the detuned energy is positive, forming molecules can still be energetically favorable. It is because most atoms (fermions) have finite amount of kinetic energy. On the other hand, on the BEC side, it seems that molecule formation is advantageous. However, BCS state is helped by having the energy gap. The larger the gap, the lower the energy. For negative detuned energy, the chemical energy is also negative. As pointed out by Leggett[2], the gap under this situation is at least $\sqrt{\mu^2 + \Delta^2}$. The energy gain by forming Cooper pairs grows with the magnitude of the chemical potential and the detuned energy and thus, the coexistence. Furthermore, if we simplified our model by considering only the condensed bosons ($b_{\mathbf{q}} = 0$), then the Hamiltonian in eq. (1) would remind one of the Anderson model[17] or Fano resonance[18]. The eigenstate should be a mixture of localized state (condensed bosons) and continuum (fermions). This analogy, though not completely compatible, indicates that the states of phase coherence should have two components. In conclusion, we pointed out that either $\langle b(\tau) \rangle$ or $F_{\alpha\beta}^* (\tau, \tau)$ should be time-dependent and our calculation show that BCS state and BEC always coexist.

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Figure captions

Fig. 1 $F_{↑↓}^\ast$ and $\phi$ versus temperature at $\nu = 0.5E_F$ (solid lines) and $\nu = -0.5E_F$ (dashed lines).

Fig. 2 $F_{↑↓}^\ast$ and $\phi$ versus the detuned energy $\nu$ at temperature at $E_F/6$ (solid lines) and $E_F/3$ (dashed lines).

Fig. 3 $-\text{Im} F_{↑↓}^\ast(E)$, the spectrum function of Cooper pairs versus $E/E_F$ at different detuned energies.
Fig. 1

\[ \mu \]

\[ \phi \]

\[ k_B T/E_F \]

- \( \phi, F^*, \nu=-0.5E_F \)
- \( \phi, F^*, \nu=-0.5E_F \)
Fig. 3