Simultaneous Onset of Condensation of Molecules and Atoms in an Attractive Fermi Gas of Atoms

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The self-consistent equations for the order parameters of Bose-Einstein condensation (BEC) of molecules and Bardeen-Cooper-Schrieffer (BCS) condensation of atoms in a Fermi gas of atoms with an attractive two-body interaction between atoms have been derived within the Hartree-Fock-Bogoliubov approximation from the path integral representation of the grand partition function. We have found that the order parameters for BEC and BCS are proportional to each other, which implies that BEC and BCS onsets simultaneously. We have also found that the common critical temperature of BEC and BCS increases as the average number of molecules increases and that the atom-molecule coupling enhances the common critical temperature.

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The crossover regime \[1, 2, 3, 4, 5, 6, 7, 8\] of Bose-Einstein condensation (BEC) of molecules and Bardeen-Cooper-Schrieffer (BCS) condensation of atoms in a Fermi gas of atoms has recently been an active research field since it contains abundant information on the interplay of two kinds of quantum fluids (the Bose and Fermi quantum liquids) that exist in the nature. Progress in understanding of this crossover regime will certainly furnish significant implications and shed much light on our understanding of a plethora of macroscopic quantum phenomena including high temperature superconductivity. However, despite that great efforts have been put into it, the nature of condensation on either side of the crossover regime still remains an open question.

In this Letter, we report our results obtained in our study of Bose-Einstein condensation of molecules and BCS condensation of atoms on the BCS side in a Fermi gas of atoms with an attractive two-body interaction between atoms (an attractive Fermi gas of atoms). We will first derive a set of self-consistent equations for the order parameters of BEC and BCS in the Hartree-Fock-Bogoliubov approximation from the path integral representation of the grand partition function. Then, from the self-consistent equations we will draw the central conclusion in this Letter that BEC of molecules and BCS of atoms onset simultaneously in an attractive Fermi gas of atoms. We also calculate the common critical temperature of BEC and BCS and discuss its dependence on the fraction of atoms bound into molecules, on the two-body interaction between atoms, and on the atom-molecule coupling.

In the literature, the prime examples of Fermi gases of atoms are the gases of \(^{40}\text{K}\) and \(^{6}\text{Li}\) atoms, with the gas of \(^{40}\text{K}\) atoms most intensively studied so far. The magnetic-field Feshbach resonance [8, 9] is used to vary the sign and strength of the two-body interaction between atoms so that the BEC-BCS regime is conveniently accessed. In our present work, we are concerned with the BCS side in which the two-body interaction between atoms is attractive. On the BCS side, there exist an open channel and a closed channel, with bound states only in the closed channel. The bound-states in this case are referred to as unstable (unphysical) bound states. A resonance molecule refers to the entity formed by two atoms in such a bound state in real space. If the size of a bound state is small in real space, the bound state is then a conventional molecule. The size of a bound state can be varied by varying the strength of the two-body interaction between atoms through the Feshbach resonance. As its size increases, the bound state becomes better localized in momentum space and it can then be referred to as a preformed Cooper pair.

A Fermi gas of atoms with an attractive two-body interaction is described by the Hamiltonian [11]

\[
H = 2\Delta\nu \sum_p a_p^\dagger a_p + \sum_{k\sigma} (\epsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \frac{|U|}{N} \sum_{kk'p} c_{k+p,\uparrow}^\dagger c_{k'-p,\downarrow}^\dagger c_{k,\downarrow} c_{k,\uparrow} + \frac{g}{\sqrt{N}} \sum_{pk} a_{p}^\dagger c_{k} c_{p-k,\downarrow} + h.c.,
\]

where \(2\Delta\nu = 2(\nu - \mu)\) is the offset energy of a molecule relative to the chemical potential \(\mu\), \(a_p^\dagger\) and \(a_p\) are creation and annihilation operators of a molecule of momentum \(p\) and energy \(2\Delta\nu\), \(c_{k\sigma}^\dagger\) and \(c_{k\sigma}\) are creation and annihilation operators of a fermionic atom of momentum \(k\), spin \(\sigma\), and energy \(\epsilon_k = \hbar^2 k^2/2m, U < 0\) is the two-body interaction between atoms, \(g\) is the effective atom-molecule coupling constant, and \(N\) is the average number of single atoms.

Our starting point is the path integral representation [12, 13] of the grand partition function \(Z = Tr e^{-\beta H}\) with \(H\) given in Eq. (1). To obtain the path integral representation of the grand partition function, we introduce the complex variables \(\varphi_p^\dagger(\tau)\) and \(\varphi_p(\tau)\) for the creation and annihilation operators \(a_p^\dagger(\tau)\) and \(a_p(\tau)\) of molecules, and the Grassman variables \(\psi_{k\sigma}^\dagger(\tau)\) and \(\psi_{k\sigma}(\tau)\) for the...
creation and annihilation operators \( c^\dagger_{k\sigma}(\tau) \) and \( c_{k\sigma}(\tau) \) of atoms. Replacing \( a^\dagger_{\nu}(\tau) \), \( a_{\nu}(\tau) \) by \( \varphi^\dagger_\nu(\tau) \), \( \varphi_\nu(\tau) \) and \( c^\dagger_{k\sigma}(\tau) \), \( c_{k\sigma}(\tau) \) by \( \psi^*_k\sigma(\tau) \), \( \psi_{k\sigma}(\tau) \) in the Hamiltonian in Eq. (1) so that the Hamiltonian becomes a function of the above-introduced complex and Grassman variables and is denoted by \( H(\varphi, \psi) \), and then substituting \( H(\varphi, \psi) \) into

\[
Z = \int D[\varphi^*, \varphi; \psi^*, \psi] \exp\left\{-\int_0^\beta d\tau \left[ \varphi^*_\nu(\tau) \frac{\partial}{\partial \tau} \varphi_\nu(\tau) + \psi^*_k\sigma(\tau) \frac{\partial}{\partial \tau} \psi_{k\sigma}(\tau) - H(\varphi, \psi) \right] \right\}, \quad (2)
\]

we obtain the integral representation of the grand partition function. The integration measure in Eq. (2) is given by

\[
D[\varphi^*, \varphi; \psi^*, \psi] = \lim_{M \to \infty} \prod_{j=1}^M \prod_{k\sigma} d\psi_{k\sigma}(j\Delta \tau) d\psi^*_{k\sigma}(j\Delta \tau)
\]

\[
\times \prod_p \frac{d\varphi^*_p(j\Delta \tau) d\varphi_p(j\Delta \tau)}{2\pi i} \quad (3)
\]

with \( \Delta \tau = \beta/M \).

The complex variable \( \varphi^*_p(\tau) \) introduced above acts as the order parameter of Bose-Einstein condensation of molecules. To proceed further, we use Fourier transformations of \( \varphi^*_p(\tau) \) and \( \psi_{k\sigma}(\tau) \) given by \( \varphi^*_p(\tau) = \sum_{\omega_p} e^{-i\omega_p \tau} \varphi^*_p \) and \( \psi_{k\sigma}(\tau) = \sum_{\omega_{k\sigma}} e^{-i\omega_{k\sigma} \tau} \psi_{k\sigma} \) where \( \omega_p = 2m\pi/\beta \) and \( \omega_{k\sigma} = i(2n + 1)\pi / \beta \), with \( n \) and \( m \) being integers, are Matsubara imaginary frequencies for bosons and fermions, respectively, and \( p = (p, i\omega_{m}) \), \( k = (k, i\omega_n) \) to rewrite the path integral representation in imaginary frequency space. For the purpose of decoupling the two-body interaction between atoms through the Hubbard-Stratonovich transformation \[14, 15\], we rewrite it as

\[
\frac{1}{N} \sum_{kk'p} \psi^*_{k'p} \psi_{kp} \psi^*_{k'p} \psi_{kp}^\dagger = \sum_p \left[ \frac{1}{\sqrt{N}} \sum_k \psi^*_{kp} \psi_{kp} \right]^* \left[ \frac{1}{\sqrt{N}} \sum_k \psi^*_{kp} \psi_{kp} \right] \quad (4)
\]

The field introduced in implementing the Hubbard-Stratonovich transformation is denoted by \( \Delta_p \) and it corresponds to the order parameter of BCS condensation of atoms \[12\]. For discussion of Bose-Einstein condensation of molecules and BCS condensation of atoms, we need retain only zero bosonic momentum-frequency terms in the atom-molecule coupling and in the decoupled terms. Then all nonzero momentum-frequency order parameters can be integrated out, with only the order parameters of zero momentum and frequency [they are now simply denoted by \( \varphi \) and \( \Delta \), respectively] remaining in the path integral representation of the grand partition function.

The next algebraic manipulation to perform is to integrate out the Grassman variables. To integrate out the Grassman variables, we first bring the terms containing the Grassman variables as a whole into a diagonal form. This manipulation is similar to the diagonalization of the Hamiltonian of a system of fermions \[16\]. We found that it is convenient to introduce a column matrix of two Grassman variables and to write the concerned terms in a matrix form. Then we diagonalize the matrix appearing in the matrix form of the concerned terms. The transformation matrix that transforms the to-be-diagonalized matrix into a diagonal matrix is composed of the orthonormal eigenvectors of the to-be-diagonalized matrix. The new Grassman variables in terms of which the concerned terms are expressed in a diagonal form can be easily obtained by using the transformation matrix. It can be directly verified that the Jacobian of the change of variables from the old Grassman variables to the new Grassman variables is unity.

The final simplification we can do to the path integral representation of the grand partition function is to perform the summations over the imaginary frequencies \( \omega_m \) and \( \omega_n \). These summations can be easily performed by considering proper contour integrals \[17, 13\]. With the summations over \( \omega_m \) and \( \omega_n \) done, we obtain

\[
Z = N^2 \beta |U| \int \frac{d\varphi^* d\varphi d\Delta d\Delta^*}{2\pi i} |e^{-S}|, \quad (5)
\]

where

\[
S = \sum_{p \neq 0} \ln \left( \frac{\sinh(\beta \Delta \nu)}{\beta \Delta \nu} \right) - 2 \sum_k \ln \left[ 2 \cosh \left( \frac{\beta E_k}{2} \right) \right] + 2N \beta \Delta \nu |\varphi|^2 + N \beta |U| |\Delta|^2 \quad (6)
\]

with

\[
E_k = (\xi^2_k + |g\varphi + |U| |\Delta|^2)^{1/2}. \quad (7)
\]

Notice that the prefactor \( N^2 \beta |U| \) in Eq. (6) arises from the change of variables \( \varphi \rightarrow \sqrt{N} \varphi \) and \( \Delta \rightarrow \sqrt{N} \beta |U| \Delta \) before performing the summations over \( i\omega_m \) and \( i\omega_n \). The purpose of this change of variables is to make the order parameters \( \varphi \) and \( \Delta \) intensive.

An approximate explicit expression of \( Z \) can be obtained by making use of the steepest-descent method \[15\] in which \( S \) is expanded as a Taylor series in \( \varphi \) and \( \Delta \) about the stationary point of \( S \). As an approximation, this series is terminated at the second order. The integration over \( \varphi \) and \( \Delta \) can then be performed and an approximate explicit expression of \( Z \) is obtained. The stationary value of \( S \) is obtained by evaluating its value at the stationary point determined by the conditions that \( \partial S / \partial \varphi^* = 0 \) and \( \partial S / \partial \Delta^* = 0 \) and their complex conjugates. From the stationary conditions, we obtain the self-consistent equations for \( \varphi \) and \( \Delta \)

\[
\varphi = \frac{g}{4N\Delta^2} (g\varphi + |U| \Delta) \sum_k \frac{1}{E_k} \tanh \left( \frac{\beta E_k}{2} \right), \quad (8a)
\]

\[
\Delta = \frac{1}{2N} (g\varphi + |U| \Delta) \sum_k \frac{1}{E_k} \tanh \left( \frac{\beta E_k}{2} \right). \quad (8b)
\]
The self-consistent equations for the complex conjugates of \( \varphi \) and \( \Delta \) can be obtained simply by taking the complex conjugation of the above two equations.

From Eqs. (8), we immediately see that \( \varphi \) and \( \Delta \) are proportional to each other

\[
\varphi = \frac{g}{2 \Delta \nu} \Delta.
\]

(9)

The proportionality between \( \varphi \) and \( \Delta \) implies that they become nonzero at the same temperature as the temperature is lowered from a value higher than the critical temperature. In other words, Bose-Einstein condensation of molecules and BCS condensation of atoms occur simultaneously. This result is of great significance in that it reveals to us that both molecules and atoms condense in an attractive Fermi gas of atoms and furthermore that their condensation onsets at a common temperature. Physically, the simultaneity of condensation of molecules and atoms is due to the presence of the atom-molecule coupling.

We now turn to the evaluation of the common critical temperature of condensation of molecules and atoms. The common critical temperature \( T_c \) can be determined from any one of the two self-consistent equations in Eqs. (8) in conjunction with the relation in Eq. (9). Explicitly, we have

\[
1 = \left( \frac{g^2}{2 \Delta \nu} + |U| \right) \frac{1}{2N} \sum_{k} \frac{1}{\xi_k} \tanh \left( \frac{\xi_k}{2k_BT_c} \right).
\]

(10)

Notice that, since the chemical potential appears in \( \Delta \nu = \nu - \mu_c \), the chemical potential \( \mu_c \) has to be determined self-consistently. To determine \( \mu_c \), we set up a self-consistent equation for it by using the relation \( 2M = N = -\partial F/\partial \mu \) in which \( F \) is the Helmholtz free energy and \( M \) is the average number of molecules. This relation can be easily verified by using \( F = -\beta^{-1} \ln Z \) and \( Z = \text{Tr} e^{-\beta H} \) with \( H \) given in Eq. (1). With \( Z \) expressed as \( Z = e^{-S} \), the above relation can be written as \( 2M = N = -\beta^{-1} \partial S/\partial \mu \). In the Hartree-Fock-Bogoliubov approximation, it is satisfactory to approximate \( S \) with its stationary value. With the utilization of such an approximation to \( S \), we obtain the following self-consistent equation for the chemical potential \( \mu_c \) at \( T = T_c \)

\[
1 = \eta_m \left( \frac{1}{e^{\beta \Delta \nu} - 1} - \frac{1}{2 \Delta \nu} \right) + \frac{2\eta_a}{N} \sum_{k} \frac{e^{\beta \xi_k}}{\xi_k + 1},
\]

(11)

where \( \beta_c = 1/k_B T_c \), \( \eta_m \) is the ratio of the number of atoms bound into molecules to the total number of atoms, \( \eta_m = 2M/(2M + N) \), and \( \eta_a \) is the ratio of the number of single atoms to the total number of atoms, \( \eta_a = N/(2M + N) \). Notice that, in deriving the self-consistent equation for \( \mu_c \), the zero-point contributions must be omitted [20].

Before we proceed to solve for the common critical temperature \( T_c \) from Eqs. (10) and (11), we first specify values for several parameters. Firstly, an energy cutoff is required in Eq. (10). This cutoff indicates the energy range of atoms that participate in pairing. We take this energy cutoff to be the Fermi energy \( E_F \) since all atoms are allowed to participate in pairing. For a typical density of \( n = 10^{20} \text{ m}^{-3} \) [11], \( E_F \approx 1.25 \mu K \) for \(^{40}\text{K} \) atoms. Secondly, the range of the atom-molecule coupling \( g \) we will consider is between 0.1\( E_F \) and \( E_F \). Thirdly, for the two-body interaction between atoms, we use \( U = -0.2E_F \).

Lastly, for the molecular offset energy, we use \( \nu = E_F \). The above-quoted values of parameters are in consistency with the experiment [11] and with the previous theoretical analysis [11].

Shown in Fig. (a) [the solid line] is the dependence of the common critical temperature \( T_c \) on the fraction \( \eta_m \) of atoms bound into molecules, with the dependence on \( \eta_m \) of the chemical potential \( \mu_c \) at \( T_c \) shown in Fig. (b). It is seen that, as \( \eta_m \) increases, \( T_c \) increases almost linearly, with \( T_c \approx 0.12E_F \) at \( \eta_m = 0 \) and \( T_c \approx 0.63E_F \) at \( \eta_m = 0.25 \). We thus conclude that the presence of more molecules effectively raises the common critical temperature of condensation. The dependence of \( T_c \) on \( \eta_m \) can be well fitted with the power law \( k_BT_c/E_F = a + b\eta_m^\gamma \) [shown in Fig. (a) as a dashed-line] with \( a \approx 0.120 \), \( b \approx 1.569 \), and \( \gamma \approx 0.815 \). From Fig. (b), we can see that, as \( \eta_m \) increases, the value of the chemical potential \( \mu_c \) at \( T_c \) also increases, with the increase slowing down at large values of \( \eta_m \). The dashed-line in Fig. (b) is the fit to the power law \( k_BT_c/E_F = c + d\eta_m^\delta \) with \( c = 0.984 \), \( d = 1.824 \times 10^{-2} \), and \( \delta = 0.233 \).

![FIG. 1](image_url) The dependence of the common critical temperature \( T_c \) [(a)] and the chemical potential \( \mu_c \) at \( T_c \) [(b)] on the fraction of atoms bound into molecules for \( g = 0.1E_F \), \( U = -0.2E_F \), and \( \nu = E_F \). The dashed lines are power-law fits discussed in the text.

Both the two-body interaction between atoms and the atom-molecule coupling have significant influences on the common critical temperature \( T_c \) as shown in Fig. (a) for \( \eta_m = 0.15 \) and \( \nu = E_F \). At these values of \( \eta_m \) and \( \nu \), the values of \( T_c/E_F \) fall in the vicinity of 0.5\( E_F \) for values of
$|U|/E_F$ and $g/E_F$ within the range of $0.1 \sim 1.0$, which is in consistency with the experiment [1]. As $|U|$ or $g$ increases, $T_c$ increases monotonically. It has been found that both the $T_c$-versus-$|U|$ and $T_c$-versus-$g$ curves can be well fitted with a power law $k_B T_c/E_F = \alpha + \beta x^n$. For the $T_c$-versus-$|U|$ curve, $x = |U|/E_F$, $\alpha = 0.452$, $\beta = 7.85 \times 10^{-3}$, and $\rho = 2.410$; for the $T_c$-versus-$g$ curve, $x = g/E_F$, $\alpha = 0.435$, $\beta = 0.257$, and $\rho = 1.327$. These fits are shown in Figs. 2(a) and 2(b) as dashed lines. From Fig. 2, it can be seen that the influence on $T_c$ of the atom-molecule coupling is stronger than that of the two-body interaction between atoms. The reason for this behavior is the fact that $g$ appears in the quadratic form in the effective coupling constant ($g^2/2\Delta v + |U|$), while $|U|$ appears only in the linear form.

FIG. 2: The effects of the two-body interaction [(a)] and the atom-molecule coupling [(b)] on the common critical temperature $T_c$. The dashed lines are the power-law fits discussed in the text.

In encapsulation, in terms of the self-consistent equations for the order parameters derived from the path integral representation of the grand partition function, we have studied Bose-Einstein condensation of molecules and BCS condensation of atoms in an attractive Fermi gas of atoms as realized in experiments [1, 7, 21] by making use of the magnetic-field resonance. We have found that molecules and atoms start to condense at the same critical temperature, that the common critical temperature increases as the number of molecules increases, and that the atom-molecule coupling raises the common critical temperature.

Our findings have a number of important implications both to the BEC-BCS crossover in particular and to superfluidity (superconductivity) in general. The fact that both molecules and atoms condense and that they have the very same critical temperature resolves the controversy over the nature of condensation on the BCS side of the BEC-BCS crossover regime and manifests that the condensate in an attractive Fermi gas of atoms is actually composed of a Bose-Einstein condensate and a BCS condensate. The increase of the common critical temperature with the fraction of atoms bound into molecules indicates that high temperature (possibly room temperature) superfluidity (superconductivity) is likely to be achieved in a system in which Bose-Einstein condensation of bosons and BCS condensation of fermions can occur simultaneously. The enhancement of the common critical temperature by the atom-molecule coupling suggests that high temperature superfluidity (superconductivity) is likely to be discovered in a system with a strong boson-fermion interaction in addition to that both bosons and fermions in the system can undergo, respectively, Bose-Einstein and BCS condensations.

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