Pairing Instability and Mechanical Collapse of a Bose Gas with an Attractive Interaction

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Abstract

We study the pairing instability and mechanical collapse of a dilute homogeneous bose gas with an attractive interaction. The pairing phase is found to be a saddle point and unstable against pairing fluctuations. This pairing saddle point exists above a critical temperature. Below this critical temperature, the system is totally unstable in the pairing channel. Thus the system could collapse in the pairing channel in addition to mechanical collapse. The critical temperatures of pairing instability and mechanical collapse are higher than the BEC temperature of an ideal bose gas with the same density. When fluctuations are taken into account, we find that the critical temperature of mechanical collapse is even higher. The difference between the collapse temperature and the BEC temperature is proportional to \((n|a_s|^3)^{2/9}\), where \(n\) is the density and \(a_s\) is the scattering length.
The system of Bose gas with attractive interaction has received a lot of attention recently due to the success in cooling $^7$Li [1] and $^{85}\text{Rb}$ [2] systems. In these trapped systems, Bose Einstein condensation can be realized at zero temperature if the number of atoms in the condensate is below a critical value [3], because of a finite size effect. In a $^7\text{Li}$ system, the condensate experiences repetitive growth and collapse as the system is cooled down [1]. In a $^{85}\text{Rb}$ system, the interaction can be varied from being repulsive to being attractive by tuning a Feshbach resonance. During this process, the system loses particles until the critical number is reached [2].

A homogeneous Bose gas with attractive interaction is generally unstable at zero temperature because the system can always lower energy by increasing density. At high temperatures entropy stabilizes the gaseous phase. There are several scenarios as to how the system becomes unstable when the temperature is lowered. The simplest picture is that the system collapses within the normal gaseous phase, which is supported by several theoretical studies [5]. This collapse is mechanical collapse, where the compressibility becomes negative and the system can lower energy by separating into a low density phase and a high density phase. Another possibility is that the system goes into the Bose-condensed phase and then collapses in the condensed phase. However the condensation transition temperature is found to be lower than that of mechanical collapse [5]. In addition to these scenarios, Evans and Imry proposed that there is a pairing phase similar to the BCS phase in superconductors at low temperature. However it was also concluded in the previous theoretical studies [5] that this pairing phase transition temperature is lower than the mechanical collapse temperature of the normal phase.

It was not fully addressed in the previous studies whether the pairing phase could exist as a metastable phase or not. In this paper, we examine its stability in detail. In addition, we go beyond the Hartree-Fock approximation to see how the temperature of mechanical collapse is affected by fluctuations.

The interaction between atoms is singular at short distances. However, as for other cases in condensed matter and elementary particle physics, at low energies the dilute Bose gas
system can be well described by the Hamiltonian with an effective contact interaction [6] with the coupling constant proportional to the scattering length $a_s$, up to a momentum transfer which is determined by the effective range of the interaction. The unphysical ultraviolet divergences in this approach can be subtracted by the pseudopotential method [6]. This renormalization scheme is justified in the case of a dilute Bose gas with weak interaction at zero temperature, where it can be shown that the divergences come from double counting of certain diagrams and the dominant perturbations come from the repetitive scatterings of two particles.

At finite temperature when there is no condensate, the medium effect becomes important and the coupling constant could depend on other quantities in addition to $a_s$. To avoid this complexity, here we use a simple model with a contact interaction which has coupling constant $g$ and an explicit cutoff $\Lambda$ in the wave-vector space. The Hamiltonian of the system is given by

$$H = \frac{\hbar^2}{2m} \nabla \psi^\dagger \cdot \nabla \psi + g\psi^\dagger \psi^2. \quad (1)$$

A length scale $a$ can be defined from the coupling constant, $a \equiv m/(4\pi\hbar^2 g)$, but $a$ is not the scattering length $a_s$. By solving the two-body scattering problem, we obtain the relation between $a$ and $a_s$, $a_s = a/(1 + 2a\Lambda/\pi)$. The cutoff $\Lambda$ is proportional to $1/\sqrt{|a_s|r_s}$, where $r_s$ is the effective range. Here we consider the case of a weakly attractive interaction with $a < 0$, $-2a\Lambda/\pi < 1$, and $|na^3| \ll 1$, where $n$ is the density.

To study this system, we use the Peierls variational method [7] which gives an upper bound for the free energy or grand thermodynamic potential of a quantum system. To discuss both the normal phase and the pairing phase, we assume the quasiparticles are superpositions of particles and holes, and they have certain occupation numbers at finite temperature. In momentum space, the density matrix is given by $\langle \psi_k^\dagger \psi_k \rangle = (f_k + 1/2) \cosh \theta_k - 1/2$, and $\langle \psi_k^\dagger \psi_{-k} \rangle = (f_k + 1/2) \sinh \theta_k$, where $\cosh \theta_k$ and $\sinh \theta_k$ are coherence factors and are chosen to be real. The occupation number is given by $f_k$.

Within this approach, the expectation value of the grand potential is given by
\[
\Omega(\{\theta_k\}, \{f_k\}) = \sum_k (\epsilon_k - \mu) [(f_k + 1/2) \cosh \theta_k - 1/2] + \frac{g}{2V} \{\sum_k (f_k + 1/2) \sinh \theta_k\}^2 \\
+ \frac{g}{V} \{\sum_k [(f_k + 1/2) \cosh \theta_k - 1/2]\}^2 - T \sum_k [(f_k + 1) \ln(f_k + 1) - f_k \ln f_k].
\]

The normal phase and the pairing phase are given by the saddle points of the variational space, \(\partial \Omega / \partial f_k = 0, \partial \Omega / \partial \theta_k = 0\). The saddle point equations can be further written as

\[
\tanh \theta_k = \frac{\Delta}{\epsilon_k - A - \mu}, \quad \tag{2}
\]

\[
f_k = \frac{1}{2} \coth \frac{E_k}{2T} - \frac{1}{2}, \quad \tag{3}
\]

where

\[
\Delta = -\frac{g}{V} \sum_k (f_k + 1/2) \sinh \theta_k,
\]

\[
A = -\frac{2g}{V} \sum_k [(f_k + 1/2) \cosh \theta_k - 1/2],
\]

\(E_k = \sqrt{\eta_k^2 - \Delta^2}\), and \(\eta_k = \epsilon_k - A - \mu\). The pairing phase corresponds to the solution with finite \(\Delta\) and the normal phase corresponds to the solution with \(\Delta = 0\). The transition from normal phase to pairing phase occurs when \(\Delta\) approaches zero.

To simplify the discussion without compromising the saddle point structure, we look at a more restricted variational space defined by Eq.(2) and Eq.(3) with \(\tilde{\Delta}\) and \(\tilde{A}\) as variational parameters. In terms of these new variational parameters, the grand potential is given by

\[
\Omega(\Delta, A) = \sum_k (\epsilon_k - \mu) \left[ \frac{\eta_k}{2E_k} \coth \frac{E_k}{2T} - \frac{1}{2} \right] + \frac{V \tilde{\Delta}^2}{2g} + \frac{V \tilde{A}^2}{4g} - \sum_k \frac{E_k}{2} \coth \frac{E_k}{2T} + T \sum_k \ln(2 \sinh \frac{E_k}{2T}), \quad \tag{4}
\]

where the parameters \(\tilde{\Delta}, \tilde{A}\) are defined by

\[
\tilde{\Delta}(\Delta, A) = -\frac{g}{V} \sum_k (f_k + 1/2) \sinh \theta_k = -\frac{g}{V} \sum_k \frac{\Delta}{2E_k} \coth \frac{E_k}{2T},
\]

and

\[
\tilde{A}(\Delta, A) = -2\frac{g}{V} \sum_k [(f_k + 1/2) \cosh \theta_k - 1/2] = -\frac{g}{V} \sum_k \frac{\eta_k}{E_k} \coth \frac{E_k}{2T} - 1].
\]

The new saddle point equations are given by \(\tilde{A} = A, \tilde{\Delta} = \Delta\).
The stable phases correspond to the local minimum points of the grand potential. If the pairing phase is stable, one of the necessary conditions is that it should be stable against fluctuations in pairing, which is given by

$$\frac{\partial^2 \Omega}{\partial \Delta^2} \bigg|_{\tilde{\Delta} = \Delta} > 0.$$  (5)

Since the transition into the pairing phase would be a second-order phase transition, at the critical temperature $T_P$,

$$\frac{\partial^2 \Omega}{\partial \Delta^2} \bigg|_{\tilde{\Delta} = \Delta} = 0,$$  (6)

and the stability condition Eq.(5) becomes

$$\frac{\partial^4 \Omega}{\partial \Delta^4} \bigg|_{\tilde{\Delta} = \Delta = 0} > 0.$$  (7)

However, we find that the opposite inequality holds

$$\frac{\partial^4 \Omega}{\partial \Delta^4} \bigg|_{\tilde{\Delta} = \Delta = 0} = \frac{3V}{2g} \left[ \frac{\partial^2 \tilde{A}}{\partial \Delta^2} \right]^2 - \sum_k \frac{3}{2 \eta_k} (1 + 2 f_k^2) < 0.$$  (8)

It clearly shows that the pairing phase is generally unstable. The instability of the pairing phase can also be illustrated by plotting the profile of the grand potential as shown in Fig.(1). The pairing phase is located at a saddle point and the normal phase is located at a minimum point. The pairing saddle point is a maximum in the direction of the normal phase and a minimum in the perpendicular direction.

This instability can be studied in more detail by constructing an effective Lagrangian near the critical temperature $T_P$ based on Landau’s theory of phase transitions

$$\mathcal{L}(\Delta) \equiv \Omega(\Delta, \tilde{A}) - \Omega(0, \tilde{A}) \approx \alpha \Delta^2 + \beta \Delta^4,$$  (9)

where $\alpha = \frac{\partial^2 \Omega}{\partial \Delta^2} \bigg|_{\tilde{\Delta} = \Delta = 0}$ and $\beta = \frac{\partial^4 \Omega}{\partial \Delta^4} \bigg|_{\tilde{\Delta} = \Delta = 0}$. $\beta < 0$ from Eq.(8). When $T > T_P$, $\alpha > 0$, there is a pairing saddle-point solution $\Delta^2 = -\alpha/(2\beta)$. When $T < T_P$, $\alpha < 0$, the normal phase becomes unstable in the pairing channel and there is no pairing saddle-point solution. It is clear that the system is unstable in the pairing channel when the temperature
is below $T_P$. Even above $T_P$, the normal phase can become unstable in the pairing channel by tunneling into the region beyond the pairing saddle point if any place in that region has lower energy than the normal phase. The pairing saddle point serves as an energy barrier in this case. However, in our limited numerical calculations, we have not been able to determine the condition for the normal phase to become metastable. When the temperature is far above $T_P$, the pairing saddle point disappears. In this case the effective Lagrangian description breaks down and a better method is needed to find the general expression of the critical temperature below which the pairing saddle point appears.

The critical temperature of pairing instability $T_P$ is given by the following equation

$$ 1 = -g \int \frac{d^3 k}{(2\pi)^3} \frac{1}{2\eta_k} \coth \frac{\eta_k}{2T_P}, \tag{10} $$

where $\eta_k = \epsilon_k + 2gn - \mu$. This equation has solution only when the temperature is close to the ideal BEC temperature $T_0$. In this case it can be further simplified,

$$ 1 + \frac{2a\Lambda}{\pi} \approx -g \int \frac{d^3 k}{(2\pi)^3} \frac{T_P}{\eta_k^2} \tag{11} $$

and

$$ 1 + \frac{2a\Lambda}{\pi} \approx -\frac{T_P a}{\hbar} \sqrt{\frac{2m}{\eta_0}}. \tag{12} $$

From the density equation, we obtain

$$ \eta_0 \approx \frac{9}{16\pi} \zeta^2 \left(\frac{3}{2}\right) T_0 \left(\frac{T}{T_0} - 1\right)^2, \tag{13} $$

where

$$ T_0 = \frac{2\pi\hbar^2}{m} \left(\frac{n}{\zeta(\frac{3}{2})}\right)^{\frac{\xi}{2}} $$

and $\zeta(x)$ is the Riemann-Zeta function. Therefore the solution of Eq.(10) is given by

$$ \frac{T_P}{T_0} - 1 \approx \frac{2\pi}{3\zeta^{\frac{3}{2}}(\frac{3}{2})} n^{\frac{\xi}{2}} |a| = \frac{8\pi}{3\zeta^{\frac{3}{2}}(\frac{3}{2})} n^{\frac{\xi}{2}} |a_s|. \tag{14} $$

In addition to the pairing instability, mechanical collapse can also occur in the normal phase as discussed in several references [5]. It is important to find out which instability
takes place first. The mechanical collapse happens when the compressibility goes to zero \( \partial \mu / \partial n = 0 \), which can be more explicitly written as

\[
-\frac{g}{2T_C} \int \frac{d^3k}{(2\pi)^3} \text{csch}^2 \frac{\eta_k}{2T_C} = 1,
\]

where \( T_C \) is the temperature of mechanical collapse. Similar to Eq.(10), Eq.(15) can only be satisfied when \( T_C \) is close to \( T_0 \), and can be simplified as

\[
1 \approx -g \int \frac{d^3k}{(2\pi)^3} \frac{2T_C}{\eta_k^2} 
\]

and

\[
1 \approx -\frac{2T_C a}{\hbar} \sqrt{\frac{2m}{\eta_0}}.
\]

The solution is given by

\[
\frac{T_C}{T_0} - 1 \approx \frac{16\pi}{3\zeta(3)} \eta_0 \frac{1}{a}.
\]

Similar results have been obtained in the previous studies [5].

By comparing the two critical temperatures Eq.(14) and Eq.(18), we find that when \(-4a\Lambda/\pi > 1\), \( T_P > T_C \); when \(-4a\Lambda/\pi < 1\), \( T_P < T_C \). However, this result is obtained within the variational approach, which is equivalent to the Hartree-Fock approximation. To obtain a better quantitative result, fluctuations need to be considered.

There are infrared divergences in all orders of perturbation at \( T_0 \). To obtain the correct renormalization near \( T_0 \), summing the leading divergent terms at each order is necessary, which can be effectively performed in a self-consistent approach. Here we consider the simplest one-loop renormalization with self consistency. In the Hartree-Fock approximation, the self-energy in the normal phase is simply given by \( 2gn \). When fluctuations are taken into account, the coupling constant \( g \) is renormalized. In one-loop order, \( g \) is renormalized by particle-particle scattering. It is well known that at zero temperature, such scatterings renormalize \( g \) to \( 4\pi\hbar^2\alpha_s/m \). In this approach, the renormalized coupling constant is given by the \( t \)-matrix.
\[ t(q, \Omega) = g - T \sum_\omega \int \frac{d^3k}{(2\pi)^3} g t(q, \Omega) G(k, \omega) G(q - k, \Omega - \omega), \] (19)

where \( G(k, \omega) = 1/(i\omega - \Sigma(k, \omega) - \epsilon_k + \mu) \) is the finite-temperature Green’s function. Under this approximation, the new self-energy is given by

\[ \Sigma(k, \omega) = 2T \sum_\Omega \int \frac{d^3q}{(2\pi)^3} t(q, \Omega) G(k - q, \omega - \Omega). \] (20)

The infrared behavior of the integrals in Eq.(19) and Eq.(20) is dominated by \( \Sigma(0, 0) - \mu \), which is small and finite at the collapse temperature. The \( k \)-dependence and \( \omega \)-dependence of \( \Sigma \) just provides a renormalization factor to the propagator in the leading order. So here we only consider only the constant part of self-energy,

\[ \Sigma \equiv \Sigma(0, 0) \approx 2t(0, 0)n, \]

and get

\[ \frac{g}{t(0, 0)} \approx 1 + g \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\eta'^k} \coth \frac{\eta'^k}{2T}, \] (21)

where \( \eta'_k = \epsilon_k + \Sigma - \mu \). Using the same technique in solving Eq.(10), we obtain \( t(0, 0) \) in terms of \( \Sigma \)

\[ t(0, 0) \approx \frac{g}{1 + \frac{2a\Lambda}{\pi} + \frac{T a}{\hbar} \sqrt{\frac{2m}{\Sigma - \mu}}}, \] (22)

Therefore the self-energy \( \Sigma \) is given by the self-consistent equation

\[ \Sigma \approx \frac{2gn}{1 + \frac{2a\Lambda}{\pi} + \frac{T a}{\hbar} \sqrt{\frac{2m}{\Sigma - \mu}}}. \] (23)

The condition of mechanical collapse \( \partial \mu / \partial n = 0 \) now leads to the following equation

\[ 1 = - \int \frac{d^3k}{(2\pi)^3} \frac{1}{4T} \frac{\partial \Sigma}{\partial n} \coth^2 \frac{\epsilon_k + \Sigma - \mu}{2T} \] (24)

\[ \approx - \frac{Tm}{4\pi \hbar^3} \frac{\partial \Sigma}{\partial n} \sqrt{\frac{2m}{\Sigma - \mu}}, \] (25)

where from Eq.(23) we obtain
\[
\frac{\partial \Sigma}{\partial n} \approx \frac{2g[1 + \frac{2a\Lambda}{\pi} + \frac{T\hbar}{\sqrt{2m}}(\Sigma - \mu)]}{[1 + \frac{2a\Lambda}{\pi} + \frac{T\hbar}{\sqrt{2m}}(\Sigma - \mu)]² - \frac{T\hbar}{\sqrt{2m}}gn\sqrt{2m/(\Sigma - \mu)}}. \quad (26)
\]

The solution of Eq.(25) is approximately given by

\[
(1 + \frac{2a\Lambda}{\pi})² \approx \frac{8\pi ha²nT}{\sqrt{2m(\Sigma - \mu)³}}. \quad (27)
\]

Close to \( T_0 \), the density equation yields

\[
\Sigma - \mu \approx \frac{9ζ²(\frac{3}{2})δT^2}{16πT_0}, \quad (28)
\]

where \( δT = T - T_0 \). Combining Eq.(27) with Eq.(28), we obtain the new critical temperature of mechanical collapse \( T_C' \)

\[
\frac{T_C'}{T_0} - 1 \approx 4\left(\frac{2π|a_s|n^{\frac{1}{3}}}{3ζ^{\frac{3}{2}}(\frac{3}{2})}\right)^\frac{3}{2}. \quad (29)
\]

The difference between \( T_C' \) and \( T_0 \) is now proportional to \((n|a_s|^3)^{2/9}\). In the weakly-interacting limit, it is much bigger than \( n^{1/3}|a_s| \) which is proportional to the temperature difference in Hartree-Fock approximation. The strong renormalization of the collapse temperature is a result of the enhancement of the Hartree-Fock attractive interaction due to fluctuations. In contrast, the critical temperature of pairing instability is not renormalized by the \( t \)-matrix. We have used the one-loop and constant self-energy approximations which may limit the accuracy of the numerical coefficient. Future works with better approximations may improve the numerical prefactor and provide an estimate of the next order term.

Our result shows that the collapse temperature is higher than the temperature of pairing instability. However the pairing saddle point exists above the temperature of pairing instability. The saddle point may still be important to collapse dynamics if it appears above the collapse temperature. In this case, if the normal phase is only a local minimum and not a global minimum of the grand potential, there is a finite probability for the system to pass the pairing saddle point and tunnel into the unstable region. Discussing the dynamical process of collapse is beyond the scope of this paper. However, within this variational
framework, the collapse process can probably be studied by the general method of analyzing the stability of metastable states [8] in the future.

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FIG. 1. Grand potential for $\mu = -400$, $T = 100$, and $\Lambda = 10$. Here the length and the energy are written in units of $|a|$ and $\hbar^2/2m|a|^2$, respectively.
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