Attractive Boson and the Gas-Liquid Condensation

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Abstract

We calculate a grand partition function of the attractive Bose gas in the infinite space within some approximations. Using the idea of the Yang-Lee zeros, it is proved that the gas-liquid condensation occurs before the conventional condition of the Bose-Einstein condensation is satisfied. Further, it is pointed out that Bosons with a zero momentum play a role of a trigger to this gas-liquid condensation. We discuss its implication to the trapped atomic gas.

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The study of the relationship between the Bose-Einstein condensation (BEC) and the gas-liquid condensation (GLC) is a long-standing problem [1]. Recently the experimental realization of BEC in dilute atomic vapors changed this academic problem to a realistic one [2]. Normally, the BEC, a condensation into a lowest energy level at low temperature and high density, is thought to be an essentially different phenomenon from the GLC in following points: (1) The BEC is caused by the Bose statistics, not by the interparticle interaction as in the GLC. (2) The BEC is sometimes described as a condensation in momentum space, while the GLC occurs in coordinate space.

An interesting point is that the reason by which we distinguish them is not so obvious as it looks. Both condensations have a similar thermodynamic manifestation as a first-order phase transition. Further, in two types of the quantum gas, the attractive Fermi gas and the attractive Bose gas, the relationship between the BEC and the GLC manifests itself quite differently.

For Fermions, the circumstance with low temperature and high density stabilizes the Cooper pairs: a BEC in a general sense [3]. Because of the Fermi statistics, however, two Fermions experience a strong repulsive force in the short distance. Hence, when the attractive force is increased within the Bardeen-Cooper-Schriefer (BCS) model, the GLC is impossible, a rigorous proof of which is given recently [4].

For Bosons, they remain in the gas state at high temperature and low density, because the quantum statistics plays a minor role. At low temperature, however, the Bosons have no large positive kinetic energy to stabilize the system behavior, especially in the BEC state. Thus, the attractive force plays a dominant role, so that the compressibility is no longer positive definite. The dilute Bose system will collapse into the dense one, leading to the GLC. Conversely, when the particle density increases by the GLC, an overlapping of the wave function is likely to cause the BEC.

There are some kinematical or thermodynamical evidences suggesting the instability of the attractive Bose gas.

(1) The Bogoliubov model says that if the interaction between the Bosons is attractive,
the velocity of sound propagating on the Bose-Einstein condensate would be imaginary, corresponding to a divergence of the density fluctuation and leading to a drastic change of the whole system.\(^5\)

\(2\) A variational argument of the many-Boson system shows that a many-body self-binding state (liquid) is more likely to be stable than a gas of the bound dimers.\(^6\)

\(3\) Recent stability analysis of the Gross-Pitaevskii equation in the trapped atomic gas with the attractive interaction indicates a collapse of the BEC at the thermal equilibrium.

These features suggest that an another type of relationship between the BEC and the GLC exists in the attractive Bose gas. The GLC in the classical imperfect gas is a long-standing and difficult problem.\(^7\) In the attractive Bose gas, however, there is a clear physical reason for the instability originated from the Bose statistics. In view of this, at least for the instability mechanism to the liquid, a model of the GLC in the attractive Bose gas would be simpler than that in the imperfect classical gas or in the attractive Fermi gas. With this in mind, it seems quite natural to consider the BEC and GLC on a common ground.

In this paper, we consider a spinless Bose gas with a repulsive core represented by \(H_{re}\) and a weak attractive s-wave pairing interaction \(g(<0)\):  

\[
H = \sum_k \epsilon_k a_k^\dagger a_k + H_{re} + \frac{g}{V} \sum_{k,k'} a_k^\dagger a_{-k}^\dagger a_{-k'} a_{k'}.
\]

(In Eq.(1), \(H_{re}\) is included only to assure universal natures of the many-body system, so that this paper does not deal with it explicitly.) We assume that the \(H_{re}\) and the attractive interaction makes an additive contribution to the free energy because of their different effective ranges, with a result that the grand partition function \(Z(\mu)\) is factorized as \(Z_0(\mu)Z_{re}(\mu)Z_{at}(\mu)\). Further we assume that diluteness of the system allows a contact interaction in \(g\) as a first approximation. What concerns us is a singularity induced by \(Z_{at}(\mu)\). We point out the following: (i) When the temperature decreases and the density increases, the grand partition function of the attractive Bose gas becomes zero at a negative critical value of the chemical potential \(\mu_c(<0)\). (ii) The Bosons with a zero momentum play a
special role in this instability.

The GLC can be considered as a singularity in the isothermal $p - V$ diagram. The pressure $p$ and the density $\rho$ are given by,

$$\frac{p}{kT} = \lim_{V \to \infty} \frac{\ln Z_V}{V},$$

(2)

$$\frac{\rho}{kT} = \lim_{V \to \infty} \frac{\partial}{\partial \mu} \left( \frac{\ln Z_V}{V} \right),$$

(3)

where $Z_V$ is the grand partition function in the volume $V$ and $\mu$ is a chemical potential. A zero of $Z(\mu)$ defines the GLC, giving the isothermal line a continuous but not differentiable point (Yang-Lee’s zero [9]). On the contrary, a pole of $Z(\mu)$ defines the BEC. Because of the logarithmic function in Eqs.(2) and (3), the pole gives the isotherm near the BEC point a similar shape to that by the zero. In contrast to the GLC, however, the isotherm is not only continuous but also differentiable at the BEC point of the free Bose gas.

The $Z(\mu)$ which explains the GLC should have a following feature. Generally in the condensed matter, local changes induced by an external perturbation, or local interactions responsible for the thermodynamic quantities in the normal phase are well described by a sum of the disconnected ring diagram like Fig.1(a). To describe a macroscopic change like the GLC, however, it is essential to include much greater networks of the interaction extending to all particles which consist of the system. As the particle number increases, a variety of such globally connected diagrams increases rapidly. Further, this connected networks is necessary for satisfying the quantum statistics correctly. When two particles having a same momentum and belonging to different ring diagrams are exchanged, a connected graph is produced as a result (for Fig.1(a), 1(b) is produced). Hence, to include a symmetrized or antisymmetrized state into calculation, the sum of the disconnected ring diagrams must be supplemented by the corresponding connected diagram. Summing up all these diagrams for $Z(\mu)$ is an essential step to describe the macroscopic change caused by the quantum statistics such as the GLC in the quantum system. (This viewpoint was originally formulated in the case of the attractive Fermi gas: superconductivity [10] [11].)
For completeness, we repeat the formalism in Ref. [10] [11] in a simplified form, and apply it to the Boson system. The connected diagram like Fig.1(b) is made of a combination of elementary diagrams like Fig.1(c) consisting of 2s particle lines. Since each graph in Fig.1(c) consists of Boson lines with a single \((l, p)\), a sum over \((l, p)\),

\[ K_s = \frac{1}{V} \sum_{l,p} \left( -\frac{1}{\sqrt{\beta}} \frac{1}{(\epsilon_p - \mu)^2 + (\frac{\gamma l}{\beta})^2} \right)^s, \quad (4) \]

is an elementary unit [12]. (Since each interaction line is connected to two \(K_s\), each \(K_s\) has \((g/V)^s\).) Only after summing the \(K_s\)’s over all ways of connecting them by the interaction lines, we get an expected \(Z(\mu)\).

Consider a connected diagram like Fig.1(b) where the \(K_s\) appears \(\nu_s\) times as in \(\{\nu_s\} = (\nu_1, \nu_2, \ldots)\) (In Fig.1(b), \(\{\nu_s\} = (3, 3, 0, \ldots)\)), and the \(K_s\)’s are connected to each other by \(n\) interaction lines.

1. There are \(\nu_s!\) ways of rearrangement which leaves the diagram invariant. 2. Since there are a number of ways of distributing frequency \(l\) and momentum \(p\) to each \(K_s\), each interaction line connecting the \(K_s\)’s has an individuality characterized by \((l, p)\) and \((l', p')\) of particles which enter or emerge at both ends. This allows us \(n!\) ways of rearrangements which produce different diagrams.

With this in mind, we get,

\[ \frac{Z(\mu)}{Z_0 Z_{re}} = \sum_{\{\nu_s\}} n! \prod_s \frac{1}{\nu_s!} \left( \frac{-K_s}{2s} \right)^{\nu_s}, \quad (5) \]

where \(2s\) in the denominator is a number of rotations which leave the \(K_s\) invariant. If the sum over \(\nu_s\) can be carried out independently to \(n\), we simply obtain \(\frac{Z(\mu)}{Z_0 Z_{re}} = n! \prod_s \exp(-\frac{K_s}{2s})\), but in reality they are related to each other by \(n = \sum_s s \nu_s\). To include this constraint in the summation, and to transform \(n!\) to a more tractable form, an identity

\[ n! = V \int_0^\infty dt (Vt)^n e^{-Vt}, \quad (6) \]

is used, and \(n\) in \((Vt)^n\) is replaced by \(\sum_s s \nu_s\). Using Eqs.(4) and (6) in Eq.(5), we can combine \(K_s^{\nu_s}\) with \((Vt)^n\). Summing it over \(\nu_s\), we get,
\[
\frac{Z(\mu)}{Z_0 Z_{re}} = V \int_0^\infty dt \exp(-V t - \sum_s \frac{1}{2s} K'_s(t)),
\]

where \(K'_s(t)\) is a redefinition of the \(K_s\) by replacing \(1/V\) by \(t\) in the right-hand side of Eq.(4). Summing \(K'_s(t)/s\) over an integer \(s\) from 1 to \(\infty\) using an identity,

\[
\ln(1 + x) = -\sum_{m=1}^\infty \frac{(-x)^m}{m},
\]

and carrying out the summation in \(K'_s(t)\) over an even integer \(l\) including zero (Bose statistics) by the use of an identity,

\[
\prod_{m=1}^\infty \left(1 + \frac{z^2}{(2m)^2}\right) = \frac{2}{\pi z} \sinh \frac{\pi z}{2},
\]

we obtain a final form,

\[
Z(\mu) = Z_0 Z_{re} \int_0^\infty dt \exp(-V t) \prod_{p=0}^\infty \left(1 + \frac{gt}{\beta (\epsilon_p - \mu)^2}\right) \times \left(\frac{\sinh \beta \sqrt{(\epsilon_p - \mu)^2 + \frac{gt}{\beta}}}{\sinh \beta (\epsilon_p - \mu)} \frac{(\epsilon_p - \mu)}{\sqrt{(\epsilon_p - \mu)^2 + \frac{gt}{\beta}}^2}\right).
\]

In view of Eq.(10), the interaction does not produce a new pole in \(Z(\mu)\), the conventional definition of the BEC. Instead, we obtain a new insight on the zero of \(Z(\mu)\), the definition of the GLC.

To extract qualitative features of \(Z(\mu)\) from Eq.(10), a most important part of the integrand is \(\left(1 + \frac{gt}{\beta (\epsilon_p - \mu)^2}\right)\), which comes from \(l = 0\), and, because of \((\epsilon_p - \mu)^2 > \mu^2\), especially important is its least term \(\left(1 + \frac{gt}{\beta \mu^2}\right)\) coming from a zero momentum. When the negative \(\mu\) increases, this term approaches zero first among many terms in the product because of \(g < 0\). Hence, at a critical value \(\mu_c(< 0)\), the zero of \(Z(\mu)\) is realized by a cancellation of two integrals which are obtained by dividing the integrand into two parts at this term. Generally the density \(\rho\) derived by Eq.(3) is a monotonic increasing function of \(\mu\), to which function the zero of this \(Z(\mu)\) adds a discontinuity at \(\mu = \mu_c\). Equations (2) and (3) together give the isotherm exhibiting the GLC.
It must be noted that the Bosons with the zero momentum play a role of a trigger to the GLC. The negative divergence of its $\rho$ in Eq.(3) implies that the Bosons with the zero momentum escape from the dilute gas, thereby making a droplet. This high density assembly of the zero momentum Bosons is in favor of the BEC.

Let us estimate a condition of this GLC for a weak attractive force. As a first approximation, we can estimate $\mu_c$ by,

$$\int_0^\infty dt \exp(-Vt) \left(1 + \frac{gt}{\beta \mu^2} \right) = 0,$$

and get a condition $\mu_c \cong -\sqrt{|g| k_B T/V}$. Further, for $\mu(T)$, we use the formula in the free Bose gas: $\mu(T) = -(g_{3/2}(1)/2\sqrt{\pi})^2 k_B T_{BEC}([T/T_{BEC}]^{3/2} - 1)^2$, where $g_{3/2}(x) = \sum m x^m / m^{3/2}$. Solving $-\sqrt{|g| k_B T/V} \cong \mu(T)$, we get,

$$\mu_c \cong -\left(\frac{2\sqrt{\pi} k_B T_{BEC}}{g_{3/2}(1)}\right)^{2/5} \left(\frac{|g|}{V}\right)^{3/5},$$

which shows non existence of the threshold strength of the attractive force: Under an infinite small attractive force, the GLC occurs before the chemical potential reaches zero.

For a weak attractive force, we extend $n\lambda^3 = g_{3/2}(1)$, the well known condition of the BEC, to a general condition of the instability caused by $Z(\mu)$. ($n$ is a number density and $\lambda = (2\pi m k_B T/h^2)^{-1/2}$, a thermal wave length [13].) Thus we replace $\mu = 0$ by $\mu_c$ such that $n\lambda^3 = g_{3/2}(e^{\beta \mu_c})$. Because of $e^{\beta \mu_c} < 1$, $T_{GLC} > T_{BEC}$ for a constant $n$, and $n_{GLC} < n_{BEC}$ for a constant $T$. Figure 2 illustrates the condition of the GLC by a solid curve for $g/V = -5nK$ and by a dotted curve for $g/V = -5\mu K$ with $T(nK) = 30\lambda^{-2}(\mu m)$ in Rb atom. (The shaded area represents the BEC phase of the free Bose gas: $n\lambda^3 \geq g_{3/2}(1)$.) When the temperature decreases and the density increases, the GLC occurs before the conventional BEC condition is satisfied. Under the same strength of the attractive force, it manifests itself more evidently in the lower temperature region. As the strength increases, its position in the phase diagram moves to the higher temperature and lower density region, a more realizable environment. Note that the GLC is very sensitive to $g/V$ due to its cooperative nature.

The trapped atomic gas is the Boson system in the harmonic potential. The BEC in
the confined space has been studied theoretically from old days. Although some differences from that in the infinite space were reported, they do not change the essential features of the BEC. Hence, for the trapped Bosons as well, we can expect an essentially similar phase diagram [14].

The BEC with the attractive interaction was first observed in $^7$Li gas as a metastable state [15]. A peculiar feature of the atomic gas is that we can control the sign of the interaction between the atoms using so-called “Feshbach resonance”. Using this technique, the condensate over a wide range of interaction strength is realized. By a sudden switching of the interaction from the repulsive to the attractive one, a collapse of the BEC gas to a high density spot was predicted. Recently such a phenomenon was really observed in $^{85}$Rb [16]. When such an experiment is performed in the region of $n\lambda^3 < g_{3/2}(1)$ (the normal phase of the free Bose gas) with the number of the atoms large enough to reach the thermal equilibrium, this type of experiment will provide us a method for finding the GLC line predicted in Fig.2.

In the attractive Bose gas, a possibility of the Boson pair has been explored by many people in analogy with the Cooper pair [17]. In view of the result of this paper, however, the attractive force responsible for such a Boson pair must have a property such that there is no residual attractive interaction between different Boson pairs. When such a residual force is there, the GLC must occur instead of the Boson pair formation. Forbidding the residual force, however, should impose a somewhat artificial constraint on the attractive interaction.

This paper deals with only an initial stage of the instability. Once the Bose gas changes to the liquid, the short range repulsive force due to $H_{re}$ plays a dominant role. (When the Bosons are in a high density gas state at high temperature, the situation is similar.) This makes Fig.2 a more complex phase diagram: The critical point $(n_c, \lambda_c)$ will appear on the GLC line, and the line below the $(n_c, \lambda_c)$ must be replaced by the gas-liquid coexisting region. Inclusion of the repulsive force will reveal a more complex nature of the later stage of this instability. To understand whether the formation of the droplet immediately leads to the BEC or not, we must get the $Z(\mu)$ which includes the $H_{re}$ explicitly. The later stage
of this instability is an open problem.

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FIGURES

FIG. 1. (a) A sum of the ring diagram which represents local changes. (b) A corresponding connected diagram which represents macroscopic changes. (c) Examples of building block $K_s(s = 1, 2, 3, 4)$ of the connected diagram, which are classified by $s$ where $2s$ is a number of particle lines.

FIG. 2. $(n, \lambda)$ phase diagram of the attractive Bosons, where $n$ is a number density and $\lambda = (2\pi mk_B T/h^2)^{-1/2}$. A solid curve is a GLC line defined by $n\lambda^3 = g_{3/2}(e^{\beta\mu c})$ for $g/V = -5nK$, and a dotted curve for $g/V = -5\mu K$ with $T(nK) = 30\lambda^{-2}(\mu m)$ in Rb atom. Shaded area is the BEC phase of the free Bose gas defined by $n\lambda^3 \geq g_{3/2}(1)$.