Green's Function Theory on A Fluctuation of Condensed Particle Number in Bose-Einstein Condensed Systems

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***Abstract*: By using the Green's function theory, we studied the fluctuation of condensed particle number for Bose-Einstein condensed systems in the canonical ensemble. The expressions for the fluctuations can be expressed by the Green's functions. Our results are consistent with previous theories in Bogoliubov approximation. In addition, a single-particle and a pair condensation equally contribute to the mean-square fluctuation of the condensates.**

***Keywords*: Bose-Einstein condensation, the fluctuation of particle number, Green's function.**

1. Introduction

Bose-Einstein condensation exists in both free particle systems and an intereacting systems, but has certain differences in its macroscopic phenomena and mechanism. For example, there is no superfluidity in the free boson system, but the interacting Bose liquid has superfluidity due to the presence of an energy gap that explains the pair correlation [1, 2]. This phenomenon can also be seen in superconductivity, which is explained by the superfluid of electron gas, the Fermi particle.

Condensation in the interacting Bose system has two types, one is the single-particle condensation where the single particle has zero momentum, and a pair condensation with two particles of the same magnitude but opposite momentum. The anomalous Green's function is used to mathematically describe this pair condensation. When Bose-Einstein condensation exists, the interacting Bose liquid exhibits a superfluidity, with the density larger than the density of condensation.

In particular, Condensed particles account for about 10% of the total particle number, but the superfluid particles is close to the total particle number. The theoretical researches for these mechanisms have already been dealt with in the Ref. [2]. In this paper, the current density of the rotating frame was expressed as the Green's function of the rotating frame to calculate the superfluid density. According to these results, the single-particle condensation is a superfluid fraction, and some or all of the non-condensing particles becomes to the superfluid fraction according to the temperature. In superconductors, there is no the single-particle condensation, so there is only a pair correlation superfluid, which is the current of Cooper pairs. How this pair-correlation might affect the other properties of a Bose-Einstein condensate system is a very interesting question.

The fluctuation of condensed particle number is also present not only in the free Bose gas, but also in the interacting Bose gas [3, 4]. More recently, the fluctuation of condensed particle number is also discussed in Bose-Einstein condensed photons [5, 13]. In general, the fluctuation of the condensed particle number depends on the temperature T and particle number N, and the dependence on them will differ from each other in statistical ensemble [6, 7]. Christoph Weiss and Martin Wilkens presented the fluctuation of condensed particles in canonical ensemble. By using Maxwell's Demon ensemble, they accurately estimated the fluctuation for a box and trap potential in different spatial dimensions

For free Bose gas, the mean-square fluctuation on the condensate occupation becomes dependent in a form like $N^{\frac{4}{3}}\left(T/T_c\right)^2$ in canonical ensemble. Here T_c is a critical temperature of Bose-Einstein condensation. The fluctuation of the condensed particle number for the weakly interacting Bose gas in a box has studied by means of calculating the fluctuation of non-condensed part in canonical ensemble. Based on Bogoliubov transformation, the mean-square fluctuation of the condensate occupation are represented by Bogoliubov coefficients, thus the fluctuations of free Bose systems comply with Ref. [8]. In addition, it is obtained that the mean-square fluctuations of the condensate occupation of the weakly interacting boson systems are only half that of the free boson systems [9]. This is the clear evidence that pair correlation suppresses the fluctuation [10]. In this case we used Bogoliubov approximation, therefore the results on fluctuation conform to the first order correction of perturbation theory.

In order to study the fluctuation in detail, we developed the Green's function theory of the fluctuation from a microscopic point of view. According to these opinions, not only the higher order approximation of the perturbation expansion, but also the relation between the physical quantities related to the Green's function and the fluctuation can be revealed. Our discussion is carried out only in the canonical ensemble.

2. Green's Function Theory

In the canonical ensemble, the particle number of systems is constant, so that the fluctuation of the condensed part is related to the fluctuation of the non-condensed part.

$$N = N_0 + N' = < N_0 > + \Delta N_0 + < N' > - \Delta N' \tag{1}$$

Let N_0, N' are the particle numbers of the condensed part, non-condensed part. ΔN_0, $\Delta N'$ are their corresponding fluctuations. Because number of particles is conserved, $\Delta N_0 = \Delta N'$ is valid. Thus a mean-square fluctuation on the condensate occupation is given as the follow

$$< (\Delta N')^2 > = < N'^2 > - < N' >^2 . \tag{2}$$

the particle numbers of non-condensed part is given by $N' = \sum_{\mathbf{k} \neq 0} a_{\mathbf{k}}^{+} a_{\mathbf{k}}$, Eq (2) becomes to the following equation.

$$< (\Delta N')^2 > = \sum_{\mathbf{k},\mathbf{k}' \neq 0} (< a_{\mathbf{k}}^{+} a_{\mathbf{k}} a_{\mathbf{k}'}^{+} a_{\mathbf{k}'} > - < a_{\mathbf{k}}^{+} a_{\mathbf{k}} >< a_{\mathbf{k}'}^{+} a_{\mathbf{k}'} >) \tag{3}$$

In order to express Eq (3) by the Green's function, T-product is applied to the operators of Heisenberg picture

$$< a_{\mathbf{k}}^{+} a_{\mathbf{k}} a_{\mathbf{k}'}^{+} a_{\mathbf{k}'} > = \lim_{\tau_1 \to \tau_2 \to \tau_3 \to \tau_4} < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}}(\tau_2) a_{\mathbf{k}'}^{+}(\tau_3) a_{\mathbf{k}'}(\tau_4)] > . \tag{4}$$

Here $a_{\mathbf{k}}^{+}(\tau)$, $a_{\mathbf{k}}(\tau)$ are creation and annihilation operator on the particle in Heisenberg picture. Symbol T_τ means time order product, is called T-product. If Eq (4) is always valid, such a condition $\tau_1 > \tau_2 > \tau_3 > \tau_4$ must be satisfied. For convenience, we suppose that conditions $\tau_1 = \tau_2 + \delta,\ \tau_2 = \tau_3 + \delta, \tau_3 = \tau_4 + \delta$ are established without a loss of generality. Here the symbol δ is a positive infinitesimal. The right hand side of Eq (4) is expressed by two-particle Green's function, therefore it could be given by the perturbation theory of Bethe-Salpeter equation in general. Starting from our aim, We develop the fluctuation theory by using a single particle Green's function.

Wick's theorem could be available to the right-hand side of Eq (4) in weakly interacting Bose gas, i.e. the approximation $< \ldots\ldots > \approx < \ldots\ldots >_0$ is applied to statistical averages on physical quantities. Symbol $< \ldots\ldots >_0$ is for free particle systems. Thus the right hand side of Eq (4) is as follows

$$\begin{aligned} < a_{\mathbf{k}}^{+} a_{\mathbf{k}} a_{\mathbf{k}'}^{+} a_{\mathbf{k}'} > = \lim_{\delta \to 0} \{ & < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}}(\tau_2)] >< T_\tau [a_{\mathbf{k}'}^{+}(\tau_3) a_{\mathbf{k}'}(\tau_4)] > \\ & + < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}'}^{+}(\tau_3)] >< T_\tau [a_{\mathbf{k}}(\tau_2) a_{\mathbf{k}'}(\tau_4)] > \\ & + < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}'}(\tau_4)] >< T_\tau [a_{\mathbf{k}}(\tau_2) a_{\mathbf{k}'}^{+}(\tau_3)] > \} . \end{aligned} \tag{5}$$

The first term on the right side here is the same as the second term on the left side of Eq (3). when Eq (5) is inserted to Eq (3), the mean-square fluctuation on the condensate occupation is as follows

$$\begin{aligned} < (\Delta N')^2 > = \sum_{\mathbf{k},\mathbf{k}' \neq 0} \lim_{\delta \to 0} \{ & < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}'}^{+}(\tau_3)] >< T_\tau [a_{\mathbf{k}}(\tau_2) a_{\mathbf{k}'}(\tau_4)] > \\ & + < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}'}(\tau_4)] >< T_\tau [a_{\mathbf{k}}(\tau_2) a_{\mathbf{k}'}^{+}(\tau_3)] > \} . \end{aligned} \tag{6}$$

We only would like to illuminate the fluctuation mechanism; therefore, boundary condition could be neglected. Thus, it says, we also assume that the systems is spatially uniform. Eq (6) could become to the following equation

$$\begin{aligned} < (\Delta N')^2 > = \sum_{\mathbf{k} \neq 0} \lim_{\delta \to 0} \{ & < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{-\mathbf{k}}^{+}(\tau_3)] >< T_\tau [a_{\mathbf{k}}(\tau_2) a_{-\mathbf{k}}(\tau_4)] > \\ & + < T_\tau [a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}}(\tau_4)] >< T_\tau [a_{\mathbf{k}}(\tau_2) a_{\mathbf{k}}^{+}(\tau_3)] > \} . \end{aligned} \tag{7}$$

In order to calculate the second term of right hand side, we remove T-product in Eq (7). Thus Eq (7) is as follows

$$\begin{aligned} < (\Delta N')^2 > &= \sum_{\mathbf{k} \neq 0} \left(< a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+} >< a_{\mathbf{k}} a_{-\mathbf{k}} > + < a_{\mathbf{k}}^{+} a_{\mathbf{k}} >< a_{\mathbf{k}} a_{\mathbf{k}}^{+} > \right) \\ &= \sum_{\mathbf{k} \neq 0} < a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+} >< a_{\mathbf{k}} a_{-\mathbf{k}} > + < a_{\mathbf{k}}^{+} a_{\mathbf{k}} >< 1 + a_{\mathbf{k}}^{+} a_{\mathbf{k}} > \\ &= \sum_{\mathbf{k} \neq 0} < a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+} >< a_{\mathbf{k}} a_{-\mathbf{k}} > + < a_{\mathbf{k}}^{+} a_{\mathbf{k}} > + < a_{\mathbf{k}}^{+} a_{\mathbf{k}} >< a_{\mathbf{k}}^{+} a_{\mathbf{k}} > \\ &= < N' > + \sum_{\mathbf{k} \neq 0} < a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+} >< a_{\mathbf{k}} a_{-\mathbf{k}} > + < a_{\mathbf{k}}^{+} a_{\mathbf{k}} >< a_{\mathbf{k}}^{+} a_{\mathbf{k}} > \end{aligned} \tag{8}$$

We are going to give time again to the operators in expression (8) without losing generality in the same way as before. However, only the times of the operators included in the last statistical means of the right hand side of equation (7) must be substituted. Because Eq (8) can't be established for the condition $\tau_2 > \tau_3$.

$$\begin{aligned} < (\Delta N')^2 > = < N' > + \lim_{\delta \to 0} \sum_{\mathbf{k} \neq 0} [& < a_{\mathbf{k}}^{+}(\tau_1) a_{-\mathbf{k}}^{+}(\tau_3) >< a_{\mathbf{k}}(\tau_2) a_{-\mathbf{k}}(\tau_4) > \\ & + < a_{\mathbf{k}}^{+}(\tau_1) a_{\mathbf{k}}(\tau_4) >< a_{\mathbf{k}}^{+}(\tau_2) a_{\mathbf{k}}(\tau_3) >] \end{aligned} \tag{9}$$

Using the Green's function, Eq (9) becomes

$$<(\Delta N')^2>=<N'>+\lim_{\delta\to 0}\sum_{\mathbf{k}\neq 0}[F^+(\mathbf{k},\tau_1-\tau_3)F(\mathbf{k},\tau_2-\tau_4)+G(\mathbf{k},\tau_1-\tau_4)G(\mathbf{k},\tau_2-\tau_3)] \quad (10)$$

If we develop the Fourier transform of the normal and anomalous Green's functions $G(\mathbf{k},\tau)$, $F(\mathbf{k},\tau)$ in Eq (10) with respect to the imaginary time τ, the following equation is given.

$$<(\Delta N')^2>=<N'>+\lim_{\delta\to 0}\sum_{\mathbf{k}\neq 0}\left[\frac{1}{\beta}\sum_n F^+(\mathbf{k},i\omega_n)e^{i\omega_n 2\delta}\frac{1}{\beta}\sum_{n'}F(\mathbf{k},i\omega_{n'})e^{i\omega_{n'}2\delta}+\frac{1}{\beta}\sum_n G(\mathbf{k},i\omega_n)e^{i\omega_n 3\delta}\frac{1}{\beta}\sum_{n'}G(\mathbf{k},i\omega_{n'})e^{i\omega_{n'}\delta}\right] \quad (11)$$

Eq (11) is similar to the formula for superfluid density [2]. The mean-square fluctuation on the condensate occupation can be divided into two parts. One involves the first term and the third term of the right hand side of the equation (11) as the non-condensed part of a single particle. The other is the second term, which contains the product of the anomalous Green's functions. Here the anomalous Green's functions is interpreted as the wave function of the pair condensation. This exhibits that the pair condensation directly contributes to the fluctuation of condensation occupation. Here β is given as $\beta=1/k_BT$, $G(\mathbf{k},i\omega_n)$ and $F(\mathbf{k},i\omega_n)$ are normal, anomalous Green's functions that are defined by Eq (12) in a 4-momentum space[11]. the normal Green's function as well as anomalous Green's function are related to energy gap. We would like to use a new system of units where $k_B=1,\hbar=1$ is available.

$$G(\mathbf{r},\tau)=\frac{1}{\beta V}\sum_{\mathbf{k}}e^{i\mathbf{kr}}\sum_n e^{-i\omega_n\tau}G(\mathbf{k},i\omega_n),$$

$$F(\mathbf{r},\tau)=\frac{1}{\beta V}\sum_{\mathbf{k}}e^{i\mathbf{kr}}\sum_n e^{-i\omega_n\tau}F(\mathbf{k},i\omega_n) \quad (12)$$

Symbol ω_n is Matsubara frequency, satisfies the condition $\omega_n=2n\pi/\beta$. V is a volume of system. In order to calculate the sum with respect to frequencies in Eq (12), the Green's functions in the momentum space is required .

3. Bogoliubov Approximation

Because of the weak interaction, the Bogoliubov approximation is applied. The normal, anomalous Green's function is as follows

$$G(\mathbf{k},i\omega_n)=\frac{i\omega_n+e_{\mathbf{k}}}{(i\omega_n-E_{\mathbf{k}})(i\omega_n+E_{\mathbf{k}})},$$

$$F(\mathbf{k},i\omega_n)=\frac{-\Delta_{\mathbf{k}}}{(i\omega_n-E_{\mathbf{k}})(i\omega_n+E_{\mathbf{k}})}, \quad (13)$$

where $e_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ are given by the equations $e_{\mathbf{k}}=\varepsilon_{\mathbf{k}}+n_0\nu_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}=n_0\nu_{\mathbf{k}}$. $\Delta_{\mathbf{k}}$ is usually called energy gap. The kinetic energy of a free particle is given by the equation $\varepsilon_{\mathbf{k}}=\mathbf{k}^2/2m$. Here $\nu_{\mathbf{k}}$ is Fourier transformation on the interaction potential, the particle number density of condensed part n_0 is expressed by the equation $n_0=N_0/V$.

Inserting Eq (13) into Eq (11), the mean-square fluctuation is as follows

$$<(\Delta N')^2>_{\text{BBG}}=<N'>+\sum_{\mathbf{k}\neq 0}\left\{\left[\frac{\Delta_{\mathbf{k}}(1+e^{\beta E_{\mathbf{k}}})}{2E_{\mathbf{k}}(e^{\beta E_{\mathbf{k}}}-1)}\right]^2+\left[\frac{E_{\mathbf{k}}+e_{\mathbf{k}}-e^{\beta E_{\mathbf{k}}}(E_{\mathbf{k}}-e_{\mathbf{k}})}{2E_{\mathbf{k}}(e^{\beta E_{\mathbf{k}}}-1)}\right]^2\right\}. \quad (14)$$

Here $<(\Delta N')^2>_{\text{BBG}}$ is the fluctuation of condensed part for Bogoliubov Bose gas. For free particle systems, $\nu_{\mathbf{k}}=0$ is available, so that energy gap reduces to $\Delta_{\mathbf{k}}=0$. Therefore, the second term on the right side of Eq (14) disappears and the pair correlation fails to contribute to the fluctuation of condensed part. These are in accordance with the fact that there does not exist a pair condensation in the Bose-Einstein condensation of the free boson.

In the case of the free particle systems, $e_{\mathbf{k}}=E_{\mathbf{k}}=\varepsilon_{\mathbf{k}}$ are also available, Eq (14) reduces to the following equation

$$<(\Delta N')^2>_{\text{IBG}}=<N'>+\sum_{\mathbf{k}\neq 0}\left[\frac{1}{(e^{\beta\varepsilon_{\mathbf{k}}}-1)}\right]^2. \quad (15)$$

By using the Bose-Einstein distribution $b(\mathbf{k})=\frac{1}{e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}-1}$, the mean square of fluctuation is given as follows

$$<(\Delta N')^2>_{\text{IBG}}=\sum_{\mathbf{k}\neq 0}\frac{1}{4sh^2(\beta\varepsilon_{\mathbf{k}}/2)}, \quad (16)$$

where $<(\Delta N')^2>_{\text{IBG}}$ is for fluctuation of a free Bose gas. In addition we use that chemical potential of a free Bose gas is zero, i.e. $\mu=0$. Eq (16) is exactly consistent with the results of preliminaries. In the temperature region $\varepsilon_1<1/\beta$, Eq (16) is dominated by the discrete sum over the low momentum region $\beta\varepsilon_{\mathbf{k}}<<1$ [8]. Therefore Bose-Einstein distribution reduces to $2m\beta/\mathbf{k}^2$ in the low momentum region, Eq (16) is as follows

$$<(\Delta N')^2>_{\mathrm{IBG}}=T^2\left(\frac{L}{2\pi}\right)^4(2m)^2\sum_{\mathbf{n}\neq 0}\frac{1}{(n_1^2+n_2^2+n_3^2)^2}, \quad (17)$$

, where ε_1 is the first excited energy of quasi-particles. L means the length of one side of a cubic and a wave vector is given by $\mathbf{k}=(2n_1\pi/L, 2n_2\pi/L, 2n_3\pi/L)$. Because the non-condensed part is only discussed, condition $n_i(i=1,2,3)\neq 0$ is valid. In Eq (17), the momentum sum is given by Epstein zeta function $\zeta_d(s)=\sum_{\mathbf{n}\neq 0}(n_1^2+n_2^2+\cdots+n_d^2)^{-\frac{s}{2}}$ [12]. Eq (17) shows that the fluctuation of condensation in a free Bose gas is related to the particle number and temperature in the equation $<(\Delta N')^2>_{\mathrm{IBG}}=\frac{\zeta_3(2)}{\pi^2\zeta^4(3/2)}N^{\frac{4}{3}}\left(\frac{T}{T_c}\right)^2$, is consistent with the Ref. [8, 9, 10]. T_c is given by $T_c=\frac{2\pi}{m}\left(\frac{N}{\zeta(3/2)V}\right)^{\frac{2}{3}}$ as the transition temperature of the Bose-Einstein condensed system.

Unlike the free particle system, the condition $\Delta_{\mathbf{k}}\neq 0$ are established in the interacting systems, so the pair correlation contributes to the fluctuation of the condensates. As shown above, the fundamental contribution of the sum with respect to the wave vector for the high temperature lies in the momentum region of the phonon, i.e. the low-momentum region $\beta E_{\mathbf{k}}<<1$. The energy spectrum of phonon is given by $E_{\mathbf{k}}=uk$, an approximation $e^{\beta E_{\mathbf{k}}}\approx 1$ is available in the such region. u is given by $u=\sqrt{\frac{n_0\nu_0}{m}}$ as a sound velocity of phonon. Based on these results, the second term of right side in Eq (14) can be calculated as follows

$$\sum_{\mathbf{k}\neq 0}\left[\frac{\Delta_{\mathbf{k}}(1+e^{\beta E_{\mathbf{k}}})}{2E_{\mathbf{k}}(e^{\beta E_{\mathbf{k}}}-1)}\right]^2 \approx\sum_{\mathbf{k}\neq 0}\left[\frac{\Delta_{\mathbf{k}}}{uk(e^{\beta E_{\mathbf{k}}}-1)}\right]^2\approx\sum_{\mathbf{k}\neq 0}\left(\frac{mT}{k^2}\right)^2. \quad (18)$$

the first, third term of right hand side in Eq (14) are given by using a approximation $E_{\mathbf{k}}+e_{\mathbf{k}}-e^{\beta E_{\mathbf{k}}}(E_{\mathbf{k}}-e_{\mathbf{k}})\approx 2e_{\mathbf{k}}$, are as follows

$$<N'>+\sum_{\mathbf{k}\neq 0}\left[\frac{E_{\mathbf{k}}+e_{\mathbf{k}}-e^{\beta E_{\mathbf{k}}}(E_{\mathbf{k}}-e_{\mathbf{k}})}{2E_{\mathbf{k}}(e^{\beta E_{\mathbf{k}}}-1)}\right]^2=\sum_{\mathbf{k}\neq 0}\frac{4E_{\mathbf{k}}^2(e^{\beta E_{\mathbf{k}}}-1)+\left[E_{\mathbf{k}}+e_{\mathbf{k}}-e^{\beta E_{\mathbf{k}}}(E_{\mathbf{k}}-e_{\mathbf{k}})\right]^2}{\left[2E_{\mathbf{k}}(e^{\beta E_{\mathbf{k}}}-1)\right]^2}$$

$$\approx\sum_{\mathbf{k}\neq 0}\left[\frac{e_{\mathbf{k}}}{E_{\mathbf{k}}(e^{\beta E_{\mathbf{k}}}-1)}\right]^2\approx\sum_{\mathbf{k}\neq 0}\left[\frac{\Delta_{\mathbf{k}}}{uk(e^{\beta E_{\mathbf{k}}}-1)}\right]^2 =\sum_{\mathbf{k}\neq 0}\left(\frac{mT}{k^2}\right)^2. \quad (19)$$

Eq (18) is equal to Eq (19), the fluctuation of condensed systems can be evaluated by using the sum of them. The results are as follows

$$<(\Delta N')^2>_{\mathrm{BBG}}=\frac{1}{2}<(\Delta N')^2>_{\mathrm{IBG}}. \quad (20)$$

Eq (20) is also exactly consistent with the results of Ref. [9, 10]. As show above, the fluctuation of the condensation part is suppressed by the pair-correlation order in the canonical ensemble.

4. Conclusion

Our results provide a new method to consider the fluctuation of condensed particles. By expressing the fluctuation of condensed particles as the Green's function, it was possible to make an accurate evaluation of the factors contributing to them along with a deep analysis of the fluctuation of condensed particles. According to Equation (18) and Equation (19), in the Bogoliubov approximation, the fluctuations due to a single-particle and a pair condensation equally contribute to the mean-square fluctuation of the condensates, but their sum is only half of that of the free particle systems.

It is also possible to evaluate the roles of the self-consistent Bogoliubov-Hartree-Fock approximation, Popov approximation, and Beliaev approximation contribute to the fluctuation of condensed particles by using the different Green's functions.

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