Conserving and Gapless Hartree-Fock-Bogoliubov theory for 3D dilute Bose gas

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The excitation spectrum for the three dimensional Bose gas in Bose-Einstein Condensation phase is calculated nonperturbatively with Modified Hartree-Fock-Bogoliubov theory, which is both conserving and gapless. From Improved $\Phi$-derivable theory, the diagrams needed to preserve Ward-Takahashi Identity are resummed in a systematic and nonperturbative way. It is valid up to the critical temperature where the dispersion relation of the low energy excitation spectrum changes from linear to quadratic. Because including the higher order fluctuation, the results show significant improvement on the calculation of the shift of critical temperature with other conserving and gapless theories.

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Since Einstein and Bose’s first proposal of Bose-Einstein Condensation (BEC) and experimental realization of it with alkali atoms[1,3], weakly interacting dilute Bose gas has attracted significant attentions[4].

The description of BEC at zero temperature began from Bogoliubov[5] and quantum loop corrections to energy density were calculated up to two loops [6-11] at low temperature. The self consistent Hartree-Fock-Bogoliubov (HFB) approximation was used but it gave a gapped spectrum[12–14], violating the Hugenholtz-Pines theorem[8] or the Goldstone theorem[15], which results from the spontaneous symmetry breaking of U(1). Popov theory neglects the anomalous average and gets a gapless spectrum[16]. But the anomalous average is not negligible at the Broken Phase. To correctly describe the BEC at high temperature, we need a theory to be both conserving (consistent with the conservation laws) and gapless[12, 14, 17]. The many-body T-matrix has been used to obtain an modified Popov approximation[18]. However, this approach yields the same critical temperature as that of ideal gas and the Hugenholtz-Pines theorem is not always satisfied (as noted in [4]). An improved Popov approximation based on many-body T-matrix approximation was developed[19,20] but its main application is in low dimensional systems. Conserving and gapless approximation has been developed by T.Kita with modified Luttinger-Ward functional[21] and F.Cooper et.al. with leading-order auxiliary field approximation[22]. However, their results are still mean field like with infinite quasiparticle lifetime.

It is a challenge to develop a conserving and gapless theory beyond mean field level. It has been shown that the critical temperature($T_c$) of weakly interacting Bose gas in 3 dimension is positively shifted from that of idea gas ($T_0$) proportional to the scattering length $a_{sc}$, $T_C/T_0 = ce^{1/3}$[23]. The accurate determination of $c$ by lattice simulations[24] and other analytical calculations from uncondensed phase[25] shows $c = 2.33[21,22]$. A non-perturbative theory beyond mean field level is needed to correctly describe the broken phase near $T_c$. Besides, when interaction is strong, the exact result may differ from mean field theory even at low temperature due to strong fluctuation effects.

In this work, we presents a modified Hartree-Fock-Bogoliubov (MHFB) approximation which is conserving and gapless and is beyond mean field level. We start from the gap equation of full HFB approximation by removing the divergence due to the double counting. Then the infinite series of diagrams are resummed to preserve the Ward-Takahashi Identity (WTI) are resummed. The approach in this paper is based on two particle irreducible(2PI) $\Phi$-derivable theory[26] and can be equivalently obtained from Schwinger-Dyson Equation approach[27]. The solution of the Broken Phase ends at the temperature where the dispersion of low energy excitation spectrum changes from linear to quadratic, which indicates a second order phase transition. The critical temperature shift coefficient is $c = 1.59$ and has significant improvement over Kita and Cooper’s result. And because the method incorporates the resummation of an infinite series of diagrams, the result differs from mean field theory even at low temperature.

For Bose gas, the grand-canonical partition function can be written with imaginary time path integral[4]:

$$Z[J, B] = \int D[\psi, \psi^\dagger] e^{-S[\psi^\dagger, \psi] - \int d(1) J_i \psi_i - \frac{1}{2} \int d(12) B_{ij} \psi_i \psi_j}$$

(1)

Where the action (in dimensionless unit) is

$$S[\psi, \psi^\dagger] = \int_0^\beta d\tau \int d^2x (\psi^\dagger \partial_\tau - \mu + \nabla^2) \psi + \frac{g}{2} \psi^\dagger \psi^\dagger \psi \psi$$

(2)

$$g = 8\pi a, \text{ where } a \text{ is the scattering length. } \beta = \frac{1}{T}, \psi_1, \psi_2 \text{ represent } \psi^\dagger, \psi. \text{ d(1) means } d\tau d^2x \text{ and J}_i, B_{ij} \text{ are auxiliary sources which will be set zero at last.}$$

The 2PI (two particle irreducible) functional $\Gamma[\varphi, G]$ is defined by the double Legendre transformation and can be written in the form:

$$\Gamma[\varphi, G] = S[\varphi] + \frac{1}{2} Tr\{D^{-1}(G-D)\} + \frac{1}{2} Tr \ln G^{-1} + \Phi[\varphi, G]$$

(3)
where $D^{-1}_{ij} = \frac{\partial^2 S[\varphi]}{\partial \varphi_i \partial \varphi_j}$ and $\varphi_i = \langle \psi_i \rangle$. $G_{ij}$ is the Green Function $G_{ij} = \langle \psi_i \psi_j \rangle_c = \langle \psi_i \psi_j \rangle - \langle \psi_i \rangle \langle \psi_j \rangle$. $\Phi[\varphi, G]$ is the sum of all 2PI vacuum diagrams.

$\Phi[\varphi, G]$ can be expanded to $n$ loop and we get $n$ loop $\Phi$-derivable approximation. Then we can get the truncated $\varphi$ and $G^{tr}$ by solve:

$$\frac{\delta \Gamma[\varphi, G^{tr}]}{\delta \varphi_i} = 0, \quad \frac{\delta \Gamma[\varphi, G^{tr}]}{\delta G^{tr}_{ij}} = 0$$

(4)

Including the simplest diagrams (Hartree Fock approximation),

$$\Phi[\varphi, G] = \frac{g}{2} \int d(1)[G_{11}(x,x)G_{22}(x,x)+2G_{12}(x,x)G_{21}(x,x)]$$

(5)

For Homogeneous gas, we define $\nu = \varphi_1 = \varphi_2$. Then $G_{ij}(x,y) = G_{ij}(x-y)$. $x$ means $(\tau, \vec{x})$.

Then from (4), we get the shift equation and gap equation:

$$\mu = g\nu^2 + gG^{tr}_{11}(0) + 2gG^{tr}_{12}(0)$$

(6)

$$\Gamma^{(2)}_{tr} = \left( \begin{array}{c} \Sigma^{tr}_{11} \omega_n - \mu + \Sigma^{tr}_{12} + k^2 \\ -i\omega_n \end{array} \right)$$

(7)

The equation is written after Fourier transformation $G_{ij}(x-y) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} k G_{ij}(\omega_n, \vec{k}) e^{-i\omega_n \tau + i\vec{k} \cdot (\vec{x} - \vec{y})}$; $\Gamma^{(2)}_{tr} = G^{tr-1}$. $\omega_n$ is the Matsubara frequency. $\omega_n = \frac{2\pi n}{\beta}$. And $\Sigma^{tr}_{11} = g\nu^2 + gG^{tr}_{11}(0)$, $\Sigma^{tr}_{12} = 2g\nu^2 + 2gG^{tr}_{12}(0)$. Due to the symmetry, we have $G^{tr}_{12}(0) = G^{tr}_{21}(0)$, $G^{tr}_{11}(0) = G^{tr}_{22}(0)$.

We define $\mu_R = \mu - \Sigma^{tr}_{12}$. $\mu_R, \Sigma^{tr}_{11}$ can be solved self-consistently with $G^{tr}$ which is the inverse of $\Gamma^{tr}$.

$$\Sigma^{tr}_{11} = g\nu^2 + \frac{g}{\sqrt{\beta}} \sum_{\omega_n, k} \frac{\Sigma^{tr}_{11}}{(\omega_n)^2 - \omega_k^2}$$

$$\mu_R = -2g\nu^2 + \Sigma^{tr}_{11}$$

(8)

where, $\omega_k = \sqrt{(k^2 - \mu_R)^2 - (\Sigma^{tr}_{12})^2}$.

In three dimension, $\omega_k = \sqrt{\frac{1}{2} \sum_{\omega_k} \left( \frac{1}{\omega_k e^{\beta \omega_k} - 1} + \frac{1}{2\omega_k} - \frac{1}{2k^2} \right)}$ has the ultraviolet divergence due to the double counting problem, which arises because we use the pseudopotential. The pseudopotential has already effectively incorporated in the first term of the Born series the information of the higher-order terms.$^{[28]}$

To avoid this problem, the vacuum terms should be subtracted: $\alpha_R = \alpha_0 + \frac{1}{\sqrt{\beta}} \sum_k \frac{1}{2k^2}$. The equation (8) after renormalization is:

$$\Sigma^{tr}_{11} = g\nu^2 - \frac{\Sigma^{tr}_{11}}{\sqrt{\beta}} \sum_k \left( \frac{1}{\omega_k e^{\beta \omega_k} - 1} + \frac{1}{2\omega_k} - \frac{1}{2k^2} \right)$$

(9)

The density $n = -\frac{1}{\sqrt{\beta}} \frac{\partial \alpha}{\partial \mu}$ can be calculated from (8):

$$n = \nu^2 + G^{tr}_{12}(0)$$

(10)

and

$$G^{tr}_{12}(0) = \frac{1}{V} \sum_k \left( \frac{k^2 + \Sigma^{tr}_{12}}{\omega_k} - \frac{1}{\omega_k} \right) \left( \frac{k^2 - k'^2 - \omega_k}{2\omega_k} \right)$$

(11)

We can get $\nu$ and $G^{tr}$ from $n$, $a$ and $T$ with equations $[8, 9, 10, 11]$.

WTI derived from 1PI formalism may be not preserved by $\Phi$-derivable approximations due to the missing of some diagrams. An improved $\Phi$-derivable theory was developed to systematically add the missing diagrams. We use $\Gamma[\varphi, G^{tr}]$ to approximate the 1PI effective action:

$$\Gamma[\varphi] = \Gamma[\varphi, G^{tr}(\varphi)]$$

(12)

with $G^{tr}(\varphi)$ defined by $\frac{\delta \Gamma[\varphi, G^{tr}]}{\delta G^{tr}_{ij}} = 0$.

Because $\Gamma[\varphi, G^{tr}(\varphi)]$ conserves the symmetry (as in $[3]$), the 1PI effective action remains unchanged under the transformation of $U(1)$ symmetry. The Green Function defined by the inverse of

$$\Gamma^{(2)} = \frac{\Gamma^{tr}[\varphi]}{\delta \varphi_i \delta \varphi_j}$$

(13)

will be gapless. It’s easy to show that

$$\Gamma^{(2)} = \frac{\delta \Gamma[\varphi, G^{tr}]}{\delta \varphi_i(x) \delta G^{tr}_{mn}(y)} \frac{\delta G^{tr}_{mn}}{\delta \varphi_i(y)}$$

(14)

$\frac{\delta G^{tr}_{mn}}{\delta \varphi_i(y)}$ can be got by taking the derivative of:

$$\int d(2') \Gamma^{(2)}_{tr, ij, jm} G^{tr}_{ij} = \delta_{ij}$$

(15)

By defining $\Lambda^{tr}_{jj, jm} = \frac{\delta G^{tr}_{jj}}{\delta \varphi_i}$, $\Gamma^{(3)} = \frac{\delta \Gamma^{tr}[\varphi]}{\delta \varphi_i \delta \varphi_j \delta \varphi_l};$ we get

$$\Lambda^{tr}_{jj, jm} = -\int \bar{d}(1', 2') \Gamma^{(3)}_{mj, m'j, jm} G^{tr}_{j1} G^{tr}_{1m'}$$

(16)

$\Gamma^{(3)}_{ij, jm}$ can be got by taking derivative of (16). These equations are actually the Bethe-Salpeter Equation to solve $\Lambda^{tr}_{jj, jm}$.

In the level of HFB, we can get Modified HFB approximation:

$$\Gamma^{(2)}_{11}(k) = \Sigma^{tr}_{11} + g\nu \Lambda^{tr}_{1122}(k) + 2g\nu \Lambda^{tr}_{1122}(k)$$

(17)

$$\Gamma^{(2)}_{12}(k) = -i\omega_n - \mu_R + k^2 + g\nu \Lambda^{tr}_{1222}(k) + 2g\nu \Lambda^{tr}_{1222}(k)$$

(18)

$$\Gamma^{(2)}_{21}(k) = i\omega_n - \mu_R + k^2 + g\nu \Lambda^{tr}_{1122}(k) + 2g\nu \Lambda^{tr}_{1122}(k)$$

(19)

$$\Gamma^{(2)}_{22}(k) = \Sigma^{tr}_{11} + g\nu \Lambda^{tr}_{1122}(k) + 2g\nu \Lambda^{tr}_{1122}(k)$$

(20)

Where $\Lambda^{tr}_{mn}(k)$ is the Fourier transformation of $\Lambda^{tr}_{mn}(x, y, \omega) = \frac{\delta G^{tr}_{mn}(x, x)}{\delta \varphi_i(y)}$. The latter can be solved by the Bethe-Salpeter Equation (16):

$$\Lambda^{tr}_{mn}(k) = \Lambda^{tr}_{m1}(k) I_{ml, in}(k) + \Lambda^{tr}_{m1}(k) I_{ml, in}(k)$$

$$+ \Lambda^{tr}_{m1}(k) (2I_{ml, in}(k) + 2I_{ml, in}(k))$$

$$+ 2( I_{ml, in}(k) + I_{ml, in}(k) + I_{ml, in}(k) )$$

(21)
where \( \bar{l} \) is defined as \( \delta_{\bar{l}l} = 0 \) and:

\[
I_{m,n,m',n'}(k) = -\frac{1}{V\beta} \sum_{\omega_{n1},k1} G^{tr}_{mn}(k_1 + k)G^{tr}_{m'n'}(k_1) \quad (19)
\]

Again due to the double counting, \( I_{12,21} \) and \( I_{21,12} \) have ultraviolet divergences. They should be renormalized by subtracting vacuum diagrams:

\[
I_{12,21}^{R} = -\left[ \frac{1}{V\beta} \sum_{\omega_{n1},k1} G^{tr}_{12}(k_1 + k)G^{tr}_{21}(k_1) - Vac \right]
V ac = \frac{1}{V} \sum_{k} \frac{1}{2k^2} \quad (20)
\]

Solve these linear equations and we can get the corrections to the self energy. The corrections are the resummation of the infinite series of diagrams (as shown in FIG.1).

The Green Function is the inverse of \( \Gamma^{(2)} \). By analytic continuation \( i\omega_n \to \Omega + i\varepsilon \), the retarded Green function \( G^R \) is got and the spectral weight function is:

\[
\rho(k,\Omega) = -2ImG^R(k,\Omega) \quad (21)
\]

We solve the gap equation numerically and the result is shown in FIG.2. The equation ceases to have a solution at \( T_c \), which is the end point of the Broken Phase and is actually the critical point of a second order phase transition. \( \nu^2 \) is not exactly equal to the condensation number \( n_0 \) and needs corrections to get the exact \( n_0 \) just like that \( G^{tr} \) needs corrections to get the exact Green function.

The spectral weight of quasi particle is plotted in FIG.3. The quasi particle peak is broadened and the quasi particle has finite lift time caused by the fluctuation effect.

At low temperature, the result of Modified HFB shows discrepancy with Popov theory and Cooper and Kita theory when interaction is strong, though it coincides with those theories at weakly interacting limit at low temperature. It has been shown that in one dimension, as interaction becomes large, the MHFB shows significant difference with Bogoliubov theory and is in very good agreement with the exact result at zero temperature[27].

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**FIG. 1.** The corrections to the self energy is the resummation of the infinite series of diagrams. The propagator in the diagrams are the gapped HFB ones but the final propagator after resummation is gapless.

**FIG. 2.** \( \nu^2 - T \) for HFB theory when \( n = 5, a = 0.005, T_0 = 19.3716, T_c = 19.635 \). At \( T_c, \nu^2 = 0.086 \).

**FIG. 3.** The spectral weight for \( k = 0.3, 0.6, 1 \) when \( n = 5, a = 0.005, T = 10 \); It is clear there is damping of quasiparticle.

**FIG. 4.** The excitation spectrum by Popov theory, Cooper-Kita theory and Modified HFB when \( n = 5, a = 0.005 \) for different temperature; \( T_0 = 19.3716, T_c = 19.635 \). Kita and Cooper’s theories get the same excitation spectrum. At \( T = 1 \), Cooper and Kita theory is very close to Popov theory.
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