Conserving Gapless Mean-Field Theory for Bose-Einstein Condensates

Takafumi Kita

Division of Physics, Hokkaido University, Sapporo 060-0810, Japan

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We formulate a conserving gapless mean-field theory for Bose-Einstein condensates on the basis of a Luttinger-Ward thermodynamic functional. It is applied to a weakly interacting uniform gas with density $n$ and $s$-wave scattering length $a$ to clarify its fundamental thermodynamic properties. It is found that the condensation here occurs as a first-order transition. The shift of the transition temperature $\Delta T_c$ from the ideal-gas result $T_0$ is positive and given to the leading order by $\Delta T_c = 2.33a n^{1/3} T_0$, in agreement with a couple of previous estimates. The theory is expected to form a new theoretical basis for trapped Bose-Einstein condensates at finite temperatures.

KEYWORDS: Bose-Einstein condensation, mean-field theory, gapless excitation, conservation laws

Much effort has been devoted recently to calculating the leading-order correction $\Delta T_c = T_c - T_0$ to the transition temperature of a weakly interacting uniform Bose gas; see refs. 1 and 2 for an overview. However, the results differ substantially among different approaches, with $\Delta T_c$ ranging from negative to positive values. Unlike the quantities at $T = 0$, perturbational calculations are difficult for $\Delta T_c$. This situation also highlights the absence of an established mean-field theory for Bose-Einstein condensates (BEC), corresponding to the Bardeen-Cooper-Schrieffer theory of superconductivity, which has played an essential role in the pioneering perturbation theory of Bogoliubov; see refs. 1 and 2 for an overview. However, the unphysical energy gap in the excitation spectrum. Thus, as was reported by Hohenberg and Martin in 1965, there are a couple of previous estimates.

As was reported by Hohenberg and Martin in 1965 and emphasized recently by Griffin, there are a couple of key words that can be used in formulating a mean-field theory for BEC: “conserving” and “gapless.” Here, application of the conventional Wick-factorization procedure to the Hamiltonian of interacting Bose particles, known as the Hartree-Fock-Bogoliubov (HFB) theory, fails to satisfy the Hugenholtz-Pines theorem giving rise to an unphysical energy gap in the excitation spectrum. Thus, it has become customary to introduce a further approximation, now called the “Popov” approximation, of completely ignoring the anomalous quasiparticle pair correlation to recover a gapless excitation. However, when the same approximation is adopted for dynamics, it does not satisfy various conservation laws as required. Also, it is not clear whether it is permissible to neglect the pair correlation, which has played an essential role in the pioneering perturbation theory of Bogoliubov; see also refs. 3 and 4. Recently, Proukakis et al. have presented an improved gapless theory with the pair correlation. However, it still does not satisfy the conservation laws.

On the basis of these observations, we here formulate a new mean-field theory for BEC with the desired conserving gapless character. As first shown by Baym and discussed in detail by Hohenberg and Martin, the conservation laws are well satisfied in “$\Phi$-derivative approximations” where the self-energy $\Sigma$ is given as a derivative of some functional $\Phi = \Phi(\hat{G})$ with respect to Green's function $\hat{G}$. This relationship between $\hat{\Sigma}$ and $\hat{G}$ holds exactly for Fermi systems, as shown by Luttinger and Ward. Indeed, $\Phi$ was first introduced by Luttinger and Ward as a part of the exact thermodynamic functional $\Omega = \Omega(\hat{G})$. It was used later by Baym to give the criteria for obtaining dynamical equations with conservation laws. We hence ask the question here: Can we construct a Luttinger-Ward thermodynamic functional for BEC within a mean-field approximation that also satisfies the Hugenholtz-Pines theorem? This is indeed possible as will be shown below. The predictions of the resulting mean-field theory for the uniform system will be presented later with an expression for $\Delta T_c$. We put $\hbar = k_B = 1$ throughout.

As usual, we express the field operator $\psi(r)$ as a sum of the condensate wave function $\Psi(r)$ and the quasiparticle field $\phi(r)$. We also adopt Beliaev’s Green’s function approach and define our Matsubara Green’s function in Nambu space as

$$\hat{G}(r, r', \tau) \equiv -\tilde{\tau}_3 \langle \tau; \phi(r, \tau) \phi^\dagger(r') \rangle,$$

where $\tilde{\tau}_3$ is the third Pauli matrix and

$$\phi = \begin{bmatrix} \phi \\ \phi^\dagger \end{bmatrix}, \quad \phi^\dagger = [\phi^\dagger \phi].$$

The factor $\tilde{\tau}_3$ in eq. (1) is usually absent but essential for the present purpose. Indeed, the eigenvalue problem for $G^{-1}$ then becomes equivalent to the Bogoliubov-de Gennes equation for quasiparticles, as seen below in eqs. (6) and (11a), so that the logarithmic term in eq. (3) can be written entirely with respect to the quasiparticles.

Using the Fourier transform $\hat{G}(r, r', \omega_n)$ with $\omega_n$ being the Matsubara frequency, we write down our Luttinger-Ward functional $\Omega = \Omega(\Psi, \Psi^*, \hat{G})$ as

$$\Omega = \int \Psi^*(r) (H_0 - \mu) \Psi(r) \, dr$$

$$+ \frac{1}{2\beta} \sum_{n=-\infty}^{\infty} \text{Tr} \left[ \ln(H_0 + \hat{\Sigma} - \mu \tilde{\tau}_3 - i \omega_n \hat{1}) + \hat{G} \hat{\Sigma} \hat{G}^\dagger \right] \hat{1}(\omega_n)$$

$$+ \Phi .$$

(3)
Here, \( H_0 \) denotes the kinetic-energy operator plus the external potential, \( \mu \) is the chemical potential, \( \beta = T^{-1} \), \( \hat{1} \) is the unit matrix, and \( H_0 \) and \( \hat{1} (\omega_n) \) are defined by
\[
\hat{H}_0 = \begin{bmatrix} H_0 & 0 \\ 0 & -H_0 \end{bmatrix}, \quad \hat{1}(\omega_n) = \begin{bmatrix} e^{i\omega_n \hat{a}} & 0 \\ 0 & e^{-i\omega_n \hat{a}} \end{bmatrix},
\]
with \( \omega_n \) an infinitesimal positive constant. The symbol \( \text{Tr} \) in eq. (3) also includes an integration over space variables with multiplications of \( H_0, \hat{\tau}_3, \) and \( \hat{1} \) by the unit matrix \( \delta(r-r') \) implied. Finally, \( \Sigma \) is the irreducible self-energy matrix obtained from the functional \( \Phi = \Phi(\Psi, \Psi^*, \hat{G}) \) by
\[
\hat{\Sigma}(r, r', \omega_n) = -2 \delta \hat{\Phi}/\delta \hat{G}(r', r, \omega_n).
\]
With this relation, \( \Omega \) is stationary with respect to variation in \( \hat{G} \) satisfying Dyson’s equation:
\[
\hat{G}^{-1} = i\omega_n \hat{1} - \hat{H}_0 - \hat{\Sigma} + \mu \hat{\tau}_3.
\]
(6)

A key quantity in eq. (3) is \( \Phi \). We choose it so that the conservation laws and the Hugenholtz-Pines theorem are simultaneously satisfied. Explicitly, it is given by
\[
\Phi = \int dr \int dr' U(r-r') \left\{ \frac{1}{2} |\Psi(r)|^2 |\Psi(r')|^2 + \frac{1}{\beta} \sum_{n, n'} \left[ \frac{1}{2} \text{Tr} \hat{\tau}_3 \hat{G}(r, r', r, \omega_n) \hat{1}(\omega_n) + \frac{1}{2} \text{Tr} \hat{G}(r, r', \omega_n) \hat{1}(\omega_n) + \frac{1}{2} \text{Tr} \hat{G}(r, r', \omega_{n'}) \hat{1}(\omega_{n'}) \right] \right\} \delta(r-r'),
\]
(7)

where \( U \) denotes the interaction potential and \( \Psi, \Psi^\dagger \) are defined in the same way as eq. (2). The first and second terms in the two square brackets of eq. (7) are the Hartree and Fock terms in Nambu space, respectively. The difference between this theory and the HFB theory lies in the Fock terms. Indeed, the HFB equations satisfying both the Hugenholtz-Pines theorem and various conservation laws. Also, the pair correlation functions \( \langle \phi^\dagger \phi \rangle \) is adequately included in eqs. (9) and (11); neglecting this contribution yields the HFB-Popov theory. Finally, one can show by using the symmetry \( \hat{H} = -\hat{\tau}_1 \hat{H}^* \hat{\tau}_1 \) that the eigenstate of \( \hat{H} \) corresponding to \(-E_\nu \leq 0 \) is given by \((\nu, \nu, 0)^T \). Now, we can provide explicit expressions for \( \langle \phi^\dagger \phi \rangle \) as
\[
\langle \phi^\dagger \phi \rangle = \sum_\nu \left[ u_\nu(r) u_\nu^*(r') f_\nu + v_\nu(r) v_\nu^*(r') (1 + f_\nu) \right],
\]
(10a)
\[
\langle \phi \phi \rangle = \sum_\nu \left[ u_\nu(r) v_\nu(r') f_\nu + v_\nu(r) u_\nu(r') (0.5 + f_\nu) \right],
\]
(10b)
where \( f_\nu \equiv (e^{E_\nu/T} - 1)^{-1} \) is the Bose distribution function. In deriving eq. (12b), use has been made of the identity \( \sum_\nu u_\nu(r) v_\nu(r') = \sum_\nu v_\nu(r) u_\nu(r') \), as can be proved from the completeness of the eigenfunctions from eq. (11).

Equations (8)-(12) form a closed set of self-consistent equations satisfying both the Hugenholtz-Pines theorem and various conservation laws. Also, the pair correlation \( \langle \phi^\dagger \phi \rangle \) is adequately included in eqs. (9) and (11); neglecting this contribution yields the HFB-Popov theory.

Using eqs. (8)-(12) and the procedure in §6 of ref. 14, it is possible to transform eq. (3) in equilibrium into an expression without Green’s functions as
\[
\Omega_{eq} = T \sum_\nu \ln(1-e^{-E_\nu/T}) - \sum_\nu E_\nu \int \left| v_\nu(r) \right|^2 dr - \frac{1}{2} \int dr d r' \left\{ \Sigma(r, r') \left[ \Psi(r') \Psi^*(r) + \langle \phi^\dagger(r) \phi(r') \rangle \right] - \Delta^*(r, r') \left[ \Psi(r') \Psi(r) + \langle \phi(r) \phi^\dagger(r') \rangle \right] \right\},
\]
(13)
The expression for the entropy can be obtained from $S = -\partial \Omega / \partial T$ by differentiating eq. (3) in terms of the explicit $T$ dependences. It yields the well-known expression:

$$
S = \sum_{\nu} [(1 + f_{\nu}) \ln(1 + f_{\nu}) - f_{\nu} \ln f_{\nu}].
$$

(14)

This completes the formulation of our mean-field theory.

Now, let us apply eqs. (8)-(12) to a uniform system with no external potential and the interaction:

$$
U(r-r') = \frac{4\pi a}{m} \delta(r-r'),
$$

(15)

where $m$ is the particle mass and $a$ is the s-wave scattering length. We first expand quantities dependent on a single argument $r$ and two arguments $(r, r')$ in $V^{-1/2} e^{ik \cdot r}$ and $V^{-1} e^{i k \cdot (r-r')}$, respectively, with $V$ the volume. We then find from eq. (8) that the expansion coefficients $\Sigma_k$ and $\Delta_k$ are independent of $k$; we hence put $\Sigma_k \rightarrow \Sigma$ and $\Delta_k \rightarrow \Delta$ hereafter. Also, $\Psi = \sqrt{n_0}$ ($n_0$: condensate density) in eq. (9) so that the equation reduces to the Hugenholtz-Pines relation $\mu = \Sigma - \Delta$. Substituting these terms into eq. (11), we obtain $E_k = \sqrt{\xi_k (\epsilon_k + 2\Delta)}$, $u_k = \sqrt{\xi_k + E_k^2/2E_k}$, and $v_k = \sqrt{\xi_k (\epsilon_k - E_k)/2E_k}$ with $\epsilon_k = k^2/2m$ and $\xi_k = \epsilon_k + \Delta$. Putting these terms back into eqs. (8) and (10), we obtain $\Sigma = 8\pi a n a / m$ with $n = N/V$ and

$$
n = n_0 + \frac{1}{V} \sum_k \left( \frac{\xi_k - E_k}{2E_k} + \frac{\xi_k}{E_k} \frac{1}{e^{E_k/T} - 1} \right),
$$

(16a)

$$
\Delta = \frac{4\pi a}{m} \left[ n_0 + \frac{1}{V} \sum_k \frac{\Delta}{2E_k} \left( 1 + \frac{2}{e^{E_k/T} - 1} \right) \right].
$$

(16b)

The first term in the round brackets of eq. (16b) produces an ultraviolet divergence. In accordance with eq. (15) where the low-energy scattering length $a$ is used, we now introduce an energy cutoff $\epsilon_c$ to the integral in such a way that $T_0 \ll \epsilon_c \ll 1/ma^2$. Substituting $T_0 = 3.31n a^{1/3}/m$, the condition is transformed into $1 \ll \epsilon_c/T_0 \ll 0.3(\pi n a^{1/3})^{-2}$, which can be well satisfied for $an^{1/3} \ll 1$. Other summations in eq. (16) are convergent, and eq. (16) is now simplified into

$$
\frac{n_0}{n} = 1 - \left( \frac{T}{T_0} \right)^{3/2} g_1(\Delta/T),
$$

(17a)

$$
\left( 1 - \frac{8\pi a \epsilon_c}{\pi} \right) \frac{\Delta}{T_0} = 2\zeta(3/2)^{2/3} na^{1/3} \left[ \frac{n_0}{n} + \frac{\sqrt{2\pi a} \Delta}{\zeta(3/2)} \frac{T}{T_0}^3 g_2(\Delta/T) \right],
$$

(17b)

where $\zeta(3/2)$ is the Riemann $\zeta$ function, and

$$
g_1(x) = \frac{2\sqrt{2}}{\sqrt{\pi} \zeta(3/2)} \left( 2 \int_0^{\infty} \frac{\cosh 2t \sinh t}{e^{3t/2} - 1} dt + \frac{1}{3} \right)
$$

$$
\rightarrow 1 - \frac{2\sqrt{2}}{\zeta(3/2)} \sqrt{x} + O(x) \quad (x \rightarrow 0),
$$

(18a)

$$
g_2(x) = \frac{4}{x} \int_0^{\infty} \frac{\sinh t}{e^{3t/2} - 1} dt
$$

$$
\rightarrow 1 - 1.165\sqrt{x} + O(x) \quad (x \rightarrow 0).
$$

(18b)

Note that both $g_1$ and $g_2$ are given in powers of $\sqrt{x}$ for $x \rightarrow 0$, which causes anomalous behavior near $T_c$ in various thermodynamic quantities, as seen below. Equation (17) enables the complete determination of $n_0$ and $\Delta$, thereby fixing the thermodynamic equilibrium at a given temperature. The chemical potential is then obtained by the Hugenholtz-Pines relation $\mu = 8\pi a n a / m - \Delta$. Other quantities of interest are the entropy $S$ of eq. (14) and the superfluid density $\rho_s$ obtained by

$$
\rho_s = n \left[ 1 - \frac{1}{3mTV} \sum_k k^2 \frac{e^{E_k/T}}{(e^{E_k/T} - 1)^2} \right].
$$

(19)

The transition temperature corresponds to the point where $n_0 = 0$ in eq. (17). Solving the resulting coupled equations for $T_c$ and $\Delta(T_c)$ to the leading order in $\delta \equiv an^{1/3}$, we obtain

$$
\frac{T_c}{T_0} = 1 + \frac{8\pi}{3\zeta(3/2)^{4/3}} \delta = 1 + 2.33\delta,
$$

(20a)

$$
\frac{\Delta(T_c)}{T_0} = \frac{8\pi}{\zeta(3/2)^{2/3}} \delta^2 = 13.3\delta^2.
$$

(20b)

Thus, the transition is first order with $\Delta(T_c) > 0$; it is caused by the change in the low-energy quasiparticle dispersion through $T_c$. In contrast, $n_0$ is continuous at $T_c$ in the present theory. Note the differences from the HFB-Popov theory where $T_c = T_0$ and $n_0$ is discontinuous at $T_c$. Our expression for $\Delta T_c$ agrees with the analytic result by Baym et al. as well as the numerical one by Holzmann and Krauth. Quantities other than $n_0$ are discontinuous at $T_c$ as

$$
\Delta \mu(T_c) = \frac{2}{3} \frac{\Delta S(T_c)}{N} = \frac{4\pi}{\zeta(3/2)^{2/3}} \delta^2 = 6.63\delta^2,
$$

(20c)

$$
\frac{\Delta \rho_s(T_c)}{nm} = \frac{4\pi}{3\zeta(3/2)^{4/3}} \delta = 1.16\delta.
$$

(20d)

Singular behaviors are also seen around $T \lesssim T_c$ stemming from $g_1$ and $g_2$ in eq. (18). For example,

$$
\frac{n_0}{n} = \frac{\sqrt{6\pi}}{\zeta(3/2)^{2/3}} \delta^{1/2} (1 - T/T_c)^{1/2},
$$

(21a)

$$
\frac{\Delta T_0}{T_0} = \frac{\Delta(T_c)}{T_0} + \sqrt{96\pi \delta^{3/2}} (1 - T/T_c)^{1/2},
$$

(21b)

$$
\frac{S}{N} = \left( \frac{T}{T_0} \right)^{3/2} \left[ \frac{5\zeta(5/2)}{2\zeta(3/2)} - \frac{3\Delta}{2T} \right].
$$

(21c)

It follows from eqs. (21b) and (21c) that the specific heat $C = T (\partial S / \partial T)$ just below $T_c$ is divergent as $C/N \sim 13.0\delta^{3/2} (1 - T/T_c)^{-1/2}$.

Similar calculations at $T = 0$ lead to the following expressions in agreement with the Bogoliubov theory:

$$
\frac{n_0(0)}{n} = 1 - \frac{8}{3\sqrt{\pi}} \delta^{3/2} = 1 - 1.50\delta^{3/2},
$$

(22a)

$$
\frac{\mu(0)}{T_0} = \frac{\Delta(0)}{T_0} = 2\zeta(3/2)^{2/3} \delta = 3.79\delta.
$$

(22b)

Figures 1-3 show the overall temperature dependences of $C/N$, $n_0/n$, $\rho_s/nm$, and $\mu/T_0$ as functions of $T/T_c$. 
for a weakly interacting Bose gas with \( an^{1/3} = 0.05 \). For comparison, the corresponding results for the ideal gas \((a = 0; T_c = T_0)\) are also plotted. The curves for \( an^{1/3} = 0.05 \) satisfy the limiting behaviors derived above for \( T \to T_c \) and 0, although \( \Delta \rho_s(T_c) \) and \( 1 - n_0(0)/n \) are too small on the present scale to be seen clearly.

An important feature of the present mean-field theory is that the thermodynamic equilibrium is fixed by the coupled eq. (17) for \( n_0 \) and \( \Delta \). Thus, the pair correlation \( \langle \phi \phi \rangle \) also plays an essential role for \( T_c \). Now, one may ask: Are the results for the transition compatible with the second-order transition in superfluid \( ^4\text{He} \) with \( T_c < T_0 \)? It is expected that, as the interaction between particles is increased from zero, \( T_c \) initially increases towards a maximum, decreasing eventually below \( T_0 \), as rationalized by Grütter et al.\(^\text{18} \). Also, the transition may change its character during the course from first- to second-order.

We finally comment on our result \( \Delta T_c = 2.33an^{1/3}T_0 \) in connection with preceding numerical estimates. Among them, the path-integral approach by Holzmann and Krauth\(^\text{17} \) seems the most reliable, since they calculated \( \Delta T_c \) in terms of a correlation function in the noninteracting Bose gas derived by an expansion from \( a = 0 \). They thereby obtained the result \( \Delta T_c \sim 2.3an^{1/3}T_0 \) compatible with our analytical one. On the other hand, a different value \( \Delta T_c \sim 1.3an^{1/3}T_0 \) has been obtained from Monte Carlo calculations by Arnold and Moore\(^\text{1} \) and by Kashurnikov et al.\(^\text{19} \). However, they both adopted as a starting point an effective action with a finite interaction, where the effects from the pair correlation \( \langle \phi \phi \rangle \) may not have been included appropriately. Finally, it is worth mentioning that the higher-order corrections to eq. (20a) depend on the cut-off \( \epsilon_c \) and are hence model dependent.

In summary, we have derived new mean-field equations for BEC as eqs. (8)-(12), which are applicable to trapped atomic gases at finite temperatures. They have been applied to a uniform system to reveal its basic thermodynamic features, particularly around \( T_c \).

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