Quantum Correction to the Gross–Pitaevskii Equation in a Bose–Eisntein Condensate

M. Okumura[1] and Y. Yamanaka[2]

[1] *Department of Physics, Waseda University, Tokyo 169-8555, Japan*
[2] *Waseda Univ. Senior High School, Kamishakujii, Nerima-ku, Tokyo 177-0044, Japan*

調和振動子型ポテンシャル中のアルカリ原子の Bose–Einstein 凝縮 (BEC) の実験に対する多くの理論的考察は Gross–Pitaevskii(GP) 方程式に基づいている．この報告書では，GP 方程式を超える試みとして，場の理論による定式化を行った．まず，零度で定式化し，それを Thermo Field Dynamics により有限温度に拡張する．非摂動的な定式化のために必要な数値計算も行い，例として，GP 方程式に対する 1-ループレベルの補正を計算した．また，凝縮相に対する量子・温度補正の影響も評価した．

So far many theoretical considerations for experiments of Bose–Einstein condensation (BEC) of alkali atoms in harmonic traps are based on the Gross–Pitaevskii (GP) equation . In this report, we attempt to formulate the BEC in the language of quantum field theory in order to go beyond the approximation of GP equation. First the formulation at zero-temperature is presented, and then it is extended to finite-temperature case by means of Thermo Field Dynamics. Numerical calculations, which are inevitable even in the unperturbative formulation of our approach, are performed. For illustration, the corrections at one-loop level to the original GP equation are given. We also calculate the effects of quantum and thermal fluctuations to the distribution of condensed atoms numerically.

1 Introdunction

Since the first experiments of Bose–Einstein condensation (BEC) [1, 2, 3], BEC of atomic gases trapped by a confining potential has attracted much attention among many experimental and theoretical physicists. Experiments of BEC are being performed in laboratories all over the world, and are giving us various interesting results. One can expect that the experiments will be improved further and that experimental results, more accurate and belonging to more wide ranges of physical parameters, will be acquired.

From the viewpoint of theoretical study, the BEC phenomena appearing at the present experiments is rather simple: The interaction between trapped atoms is weak and has a simple structure of two-body contact type, meaning that the potential can be described by a delta function. This situation is a contrast to other phenomena in condensed matter physics, e.g., superfluid. Our main concern is in the fact that the BEC offers us a clean field to check fundamental aspects of physics, i.e., the foundation of statistical physics, quantum field theory which is an ultimate one to deal with quantum many-body systems, and thermal field theory.

As the first approximation the approach using Gross–Pitaevskii equation (GP eq.) [4], which is a mean-field theory, explains the behaviors at the BEC experiments consistently. This is because the most part of trapped atoms are condensed and the effects of non-condensed (fluctuating) atoms are very small. But, as was pointed above, for future experiments in which physical quantities will be measured more accurately, or in which fluctuations (quantum as well as thermal) will play an important role, we will need more sophisticated theoretical considerations. For example, during the last few years, many attempts had been made to describe behaviors of the atomic system at finite-temperature in a trapping potential [5].

Our strategy is to start from an original quantum field theory, which is believed to be the most fundamental for description of quantum physics of many-body problems. We first formulate a quantum field theory for the BEC problem in this report. As will be shown below, we do not employ a plane wave expansion for the field operators, because the presence of trapping potential breaks space-translational invariance explicitly. Instead we expand the field operators by a complete set of appropriate wave functions, which can not be obtained analytically. We perform necessary numerical estimations to obtain physical results.

Our formulation above is limited to zero-temperature case. But, as is well-known, the formulation of quantum field theory can be readily extended to include thermal effects, that is, to thermal field theory. We will take Thermo Field Dynamics [6] for this purpose.

As an exemplar calculation we demonstrate one-loop correction to the GP eq. at zero-temperature and at finite-temperature cases. While the former involves only quantum corrections, the latter does thermal corrections as well as quantum ones. We also study the modification of the distribution function of condensate part numerically after fluctuation effects at one-loop level are taken account of.

2 Model and Notations

2.1 Action

We start with the following action for the self-interacting bosonic fields $\psi(\boldsymbol{x},t)$ and $\psi^\dagger(\boldsymbol{x},t)$ trapped by a confining potential $V(\boldsymbol{x})$,

$$S[\psi,\psi^\dagger] = \int dt d^3x \left[\psi^\dagger\left\{i\hbar\frac{\partial}{\partial t} - \left(-\frac{\hbar^2}{2m}\nabla^2\right) - V(\boldsymbol{x}) + \mu\right\}\psi - \frac{g}{2}\psi^\dagger\psi^\dagger\psi\psi\right] \tag{1}$$

where μ is the chemical potential, and the coupling constant g is given in terms of the scattering length a

$$g = \frac{4\pi\hbar^2 a}{m}. \tag{2}$$

In the recent experiments, the confining potential $V(\boldsymbol{x})$ is of harmonic-oscillator type:

$$V(\boldsymbol{x}) = \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right). \tag{3}$$

Let us consider a *stationary* situation in which Bose–Einstein condensation takes place. Then ψ is divided into two parts,

$$\psi(\boldsymbol{x},t) = v(\boldsymbol{x}) + \varphi(\boldsymbol{x},t), \tag{4}$$

where v and φ describe condensate and non-condensate (fluctuating) parts, respectively. In what follows, v is assumed to be real and time-independent. (This implies that the possible existence of vortex is neglected.) This expression is substituted into (1), and the action is rewritten in terms of v and φ as follows:

$$
\begin{aligned}
S &= S_0 + S_1 + S_2 + S_{\rm int} \\
S_0 &= \int dtd^3x \left[v \left\{ - \left(-\frac{\hbar^2}{2m}\nabla^2 \right) - V + \mu \right\} v - \frac{g}{2} v^4 \right] \\
S_1 &= \int dtd^3x \left[v \left\{ - \left(-\frac{\hbar^2}{2m}\nabla^2 \right) - V + \mu - gv^2 \right\} \varphi + \varphi^\dagger \left\{ - \left(-\frac{\hbar^2}{2m}\nabla^2 \right) - V + \mu - gv^2 \right\} v \right] \\
S_2 &= \int dtd^3x \left[\varphi^\dagger \left\{ i\hbar\frac{\partial}{\partial t} - \left(-\frac{\hbar^2}{2m}\nabla^2 \right) - V + \mu \right\} \varphi - \frac{gv^2}{2} \left(4\varphi^\dagger\varphi + \varphi^2 + \varphi^{\dagger 2} \right) \right] \\
S_{\rm int} &= \int dtd^3x \left[-gv \left(\varphi + \varphi^\dagger \right) \varphi^\dagger \varphi - \frac{g}{2} \left(\varphi^\dagger \varphi \right)^2 \right] .
\end{aligned} \tag{5}
$$

The S_1, linear in φ, is dropped if the equation for v holds,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) \right] v(\boldsymbol{x}) = 0 . \tag{6}$$

This is the GP equation [4].

The integration of the square of v is interpreted as the condensate particle number N_0,

$$N_0 = \int d^3x \, |v(\boldsymbol{x})|^2 . \tag{7}$$

2.2 Hamiltonian

Under the condition in (6), we have the Hamiltonian given by

$$\hat{H} = \hat{H}_0 + \hat{H}_{\rm int} \tag{8}$$

$$\hat{H}_0 = \int d^3x \left[\hat{\varphi}^\dagger \left(-\frac{\hbar^2}{2m}\nabla^2 + V - \mu \right) \varphi + \frac{gv^2}{2} \left(4\hat{\varphi}^\dagger\hat{\varphi} + \hat{\varphi}^2 + \hat{\varphi}^{\dagger 2} \right) \right] \tag{9}$$

$$\hat{H}_{\rm int} = g \int d^3x \left[v \left(\hat{\varphi} + \hat{\varphi}^\dagger \right) \hat{\varphi}^\dagger \hat{\varphi} + \frac{1}{2} \left(\hat{\varphi}^\dagger \hat{\varphi} \right)^2 \right] . \tag{10}$$

For the field operators in the Heisenberg picture, the equal-time canonical commutation relations are

$$\left[\hat{\varphi}(\boldsymbol{x}, t), \hat{\varphi}^\dagger(\boldsymbol{x}', t) \right] = \delta^3(\boldsymbol{x} - \boldsymbol{x}') \tag{11}$$

and $[\hat{\varphi}(\boldsymbol{x}, t), \hat{\varphi}(\boldsymbol{x}', t)] = [\hat{\varphi}^\dagger(\boldsymbol{x}, t), \hat{\varphi}^\dagger(\boldsymbol{x}', t)] = 0$.

Now we move to the interaction picture in which $\hat{H}_0$ and $\hat{H}_{\rm int}$ are considered as unperturbative and perturbative Hamiltonians, respectively. The $\hat{H}_{\rm int}$ may include possible renormalization counter terms, but they will be suppressed in this report.

2.3 Experimental Parameters

We list for later convenience the typical energy and length scales (Table 1) (for ^{87}Rb case) [7].

Table 1: Energy and Length Scale

Energy Scale		Length Scale	
harmonic oscillator level spacing $\hbar\omega$	6.59×10^{-32} [J]	oscillator length $a_{\mathrm{ho}} = \sqrt{\frac{\hbar}{2m\omega}}$	$6.47 \times 10[\mu\mathrm{m}]$
limiting temperature for S-wave scattering	1 [mK] $= 2.09 \times 10^5\hbar\omega$	scattering length a	5.77 [nm] $= 8.92 \times 10^{-3} a_{\mathrm{ho}}$
BEC transition temperature T_c	300 [nK] $= 6.28 \times 10\hbar\omega$	thermal de Broglie wavelength $\lambda_{\mathrm{dB}} = \sqrt{\frac{2\pi\hbar^2}{mk_{\mathrm{B}}T}}$	$5.94 \times 10[\mu\mathrm{m}]$ $= 0.919 a_{\mathrm{ho}}$

3 Formulation and Numerical Calculation of Unperturbative Part

3.1 Diagonalization of Unperturbative Hamiltonian

It is crucial in the formulation of the interaction picture to find an appropriate unperturbative vacuum. To do this, we expand the unperturbative field operators as

$$\begin{aligned} \hat{\varphi}(\boldsymbol{x}, t) &= \sum_{n=1}^{\infty} \hat{a}_n(t) u_n(\boldsymbol{x}) \\ \hat{\varphi}^\dagger(\boldsymbol{x}, t) &= \sum_{n=1}^{\infty} \hat{a}_n^\dagger(t) u_n(\boldsymbol{x}) \,. \end{aligned} \tag{12}$$

Here the orthonormal complete set $\{u_n\}$ $(n = 0, 1, 2, \cdots)$ are eigenfunctions of

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + g v^2(\boldsymbol{x})\right] u_n(\boldsymbol{x}) = \varepsilon_n u_n(\boldsymbol{x}) \,, \tag{13}$$

with

$$\int d^3x \, u_n(\boldsymbol{x}) u_{n'}(\boldsymbol{x}) = \delta_{nn'} \tag{14}$$

$$\sum_{n=0}^{\infty} u_n(\boldsymbol{x}) u_n(\boldsymbol{x}') = \delta^3(\boldsymbol{x} - \boldsymbol{x}') \,. \tag{15}$$

Note that the eigenfunctions are chosen to be real. The operators $\hat{a}_n$ and $\hat{a}_n^\dagger$ are subject to

$$\left[\hat{a}_n(t), \hat{a}_{n'}^\dagger(t)\right] = \delta_{nn'} \,, \tag{16}$$

and $[\hat{a}_n(t), \hat{a}_{n'}(t)] = [\hat{a}_n^\dagger(t), \hat{a}_{n'}^\dagger(t)] = 0$.

From (6) and (13), it is seen that v is proportional to u_0 with a vanishing eigenvalue

$$\varepsilon_0 = 0\,, \tag{17}$$

and from (7)

$$v(\boldsymbol{x}) = \sqrt{N_0}u_0(\boldsymbol{x})\,. \tag{18}$$

Put (12) into (9) and organize the expression :

$$\hat{H}_0 = \sum_{n=1}^{\infty} \varepsilon_n \hat{a}_n^\dagger \hat{a}_n + \sum_{n,n'=1}^{\infty} \left\{ 2\hat{a}_n^\dagger U_{nn'} \hat{a}_{n'} + \hat{a}_n U_{nn'} \hat{a}_{n'} + \hat{a}_n^\dagger U_{nn'} \hat{a}_{n'}^\dagger \right\}\,, \tag{19}$$

with the notation of

$$U_{nn'} = \frac{g}{2}\int d^3x\, v^2(\boldsymbol{x}) u_n(\boldsymbol{x}) u_{n'}(\boldsymbol{x})\,. \tag{20}$$

The unperturbed Hamiltonian is not diagonalized in terms of the $\hat{a}_n$-operators. As is done in [8] (see also [9]), we introduce the generalized Bogoliubov transformation

$$\begin{aligned} \hat{b}_n &= \sum_{m=1}^{\infty} \left[C_{nm}\hat{a}_m + S_{nm}\hat{a}_m^\dagger \right] \\ \hat{b}_n^\dagger &= \sum_{m=1}^{\infty} \left[C_{nm}\hat{a}_m^\dagger + S_{nm}\hat{a}_m \right]\,. \end{aligned} \tag{21}$$

The canonical commutation relations

$$\left[\hat{b}_n(t), \hat{b}_{n'}^\dagger(t) \right] = \delta_{nn'}\,, \tag{22}$$

and $[\hat{b}_n(t), \hat{b}_{n'}(t)] = [\hat{b}_n^\dagger(t), \hat{b}_{n'}^\dagger(t)] = 0$ require the relations among the coefficients C_{nm} and S_{nm},

$$\sum_{m=1}^{\infty} \left[C_{nm}C_{n'm} - S_{nm}S_{n'm} \right] = \delta_{nn'} \tag{23}$$

$$\sum_{m=1}^{\infty} \left[C_{nm}S_{n'm} - S_{nm}C_{n'm} \right] = 0\,. \tag{24}$$

To fix the C_{nm} and S_{nm}, let us define

$$\begin{aligned} \hat{q}_n &= \sqrt{\frac{1}{2\varepsilon_n}} \left(\hat{a}_n + \hat{a}_n^\dagger \right) \\ \hat{p}_n &= -i\sqrt{\frac{\varepsilon_n}{2}} \left(\hat{a}_n - \hat{a}_n^\dagger \right) \qquad (n \neq 0)\,, \end{aligned} \tag{25}$$

which satisfy the commutation relation

$$[\hat{q}_n, \hat{p}_{n'}] = i\delta_{nn'}\,. \tag{26}$$

The $\hat{H}_0$ is written in terms of $\hat{q}_n$ and $\hat{p}_n$ as

$$\hat{H}_0 = \sum_{n=1}^{\infty} \left(\frac{1}{2}\hat{p}_n^2 - \frac{1}{2}\varepsilon_n - U_{nn} \right) + \sum_{n,n'=1}^{\infty} \left(\hat{q}_n W_{nn'} \hat{q}_{n'} \right) \tag{27}$$

where

$$W_{nn'} = \varepsilon_n^2 \delta_{nn'} + \sqrt{2\varepsilon_n} U_{nn'} \sqrt{2\varepsilon_{n'}} \,. \tag{28}$$

The symmetric matrix $W_{nn'}$ can be diagonalized by an orthogonal matrix O :

$$\sum_{m,m'=1}^{\infty} (O_{nm} W_{mm'} O_{n'm'}) = E_n^2 \delta_{nn'} \,. \tag{29}$$

Using this O-matrix, we introduce a new pair of canonical operators by

$$\begin{aligned} \hat{Q}_n &= \sum_{n'=1}^{\infty} O_{nn'} \hat{q}_{n'} \\ \hat{P}_n &= \sum_{n'=1}^{\infty} O_{nn'} \hat{p}_{n'} \,, \end{aligned} \tag{30}$$

with $[\hat{Q}_n, \hat{P}_{n'}] = i\delta_{nn'}$. Thus we have

$$\begin{aligned} \hat{H}_0 &= \sum_{n=1}^{\infty} \left(\frac{1}{2}\hat{P}_n^2 + \frac{1}{2}E_n^2 \hat{Q}_n^2 - \frac{1}{2}\varepsilon_n - U_{nn} \right) \\ &= \sum_{n=1}^{\infty} \left[E_n \hat{b}_n^\dagger \hat{b}_n + \left(\frac{1}{2}E_n - \frac{1}{2}\varepsilon_n - U_{nn} \right) \right] . \end{aligned} \tag{31}$$

In the last equality, we have related $\{\hat{Q}, \hat{P}\}$ to $\{\hat{b}, \hat{b}^\dagger\}$ as

$$\begin{aligned} \hat{Q}_n &= \sqrt{\frac{1}{2E_n}} \left(\hat{b}_n + \hat{b}_n^\dagger \right) \\ \hat{P}_n &= -i\sqrt{\frac{E_n}{2}} \left(\hat{b}_n - \hat{b}_n^\dagger \right) . \end{aligned} \tag{32}$$

The manipulations above lead to

$$\begin{aligned} C_{nm} &= \frac{1}{2} \left(\sqrt{\frac{E_n}{\varepsilon_n}} + \sqrt{\frac{\varepsilon_n}{E_n}} \right) O_{nm} \\ S_{nm} &= \frac{1}{2} \left(\sqrt{\frac{E_n}{\varepsilon_n}} - \sqrt{\frac{\varepsilon_n}{E_n}} \right) O_{nm} \,. \end{aligned} \tag{33}$$

From these expressions, the relations in (21) can be inverted as

$$\begin{aligned} \hat{a}_n &= \sum_{m=1}^{\infty} \left[C_{mn} \hat{b}_m - S_{mn} \hat{b}_m^\dagger \right] \\ \hat{a}_n^\dagger &= \sum_{m=1}^{\infty} \left[C_{mn} \hat{b}_m^\dagger - S_{mn} \hat{b}_m \right] . \end{aligned} \tag{34}$$

The expression (31) is a digonalized one, so that the operator $\hat{b}$ can define the unperturbative vacuum, denoted by $|\Omega_b\rangle$:

$$\begin{aligned} \hat{b}_n |\Omega_b\rangle &= 0 \\ \langle \Omega_b | \hat{b}_n^\dagger &= 0 \,. \end{aligned} \tag{35}$$

We thus obtain field operators composed of $\hat{b}^\dagger$ and $\hat{b}$, which properly represent quasi particles in the situation of the BEC experiments,

$$\begin{aligned}
\hat{\varphi}(\boldsymbol{x},t) &= \sum_{n=1}^{\infty} \hat{a}_n(t)u_n(\boldsymbol{x}) \\
&= \sum_{m,n=1}^{\infty} \left[\hat{b}_m(t)C_{mn}u_n(\boldsymbol{x}) - \hat{b}_m^\dagger(t)S_{mn}u_n(\boldsymbol{x})\right] , \\
\hat{\varphi}^\dagger(\boldsymbol{x},t) &= \sum_{n=1}^{\infty} \hat{a}_n^\dagger(t)u_n(\boldsymbol{x}) \\
&= \sum_{m,n=1}^{\infty} \left[\hat{b}_m^\dagger(t)C_{mn}u_n(\boldsymbol{x}) - \hat{b}_m(t)S_{mn}u_n(\boldsymbol{x})\right] . \qquad (36)
\end{aligned}$$

3.2 Unperturbed Propagator

We now calculate the unperturbative propagator for the field operator $\hat{\varphi}$. Introduce the column notation as

$$\hat{\Phi}_i = \begin{cases} \hat{\varphi} & (\text{for } i=1) \\ \hat{\varphi}^\dagger & (\text{for } i=2) \end{cases} , \qquad (37)$$

$$\hat{\Phi}_i^\dagger = \begin{cases} \hat{\varphi}^\dagger & (\text{for } i=1) \\ \hat{\varphi} & (\text{for } i=2) \end{cases} , \qquad (38)$$

and define a 2×2-matrix propagator by

$$G_{0,ij}(\boldsymbol{x},\boldsymbol{x}';t-t') = -i\langle\Omega_b|\mathbf{T}[\hat{\Phi}_i(\boldsymbol{x},t)\hat{\Phi}_j^\dagger(\boldsymbol{x}',t')]|\Omega_b\rangle . \qquad (39)$$

Then we obtain the unperturbative propagators with the field operators (36) and the vacuum (35),

$$\begin{aligned}
G_{0,11}(\boldsymbol{x},\boldsymbol{x}';t-t') &= -i\langle\Omega_b|\mathbf{T}[\varphi(\boldsymbol{x},t)\varphi^\dagger(\boldsymbol{x}',t')]|\Omega_b\rangle \\
&= -i\theta(t-t')\sum_{l,m,n=1}^{\infty} C_{nl}C_{nm}u_l(\boldsymbol{x})u_m(\boldsymbol{x}')\mathrm{e}^{-\frac{i}{\hbar}E_n(t-t')} \\
&\quad - i\theta(t'-t)\sum_{l,m,n=1}^{\infty} S_{nl}S_{nm}u_l(\boldsymbol{x}')u_m(\boldsymbol{x})\mathrm{e}^{-\frac{i}{\hbar}E_n(t'-t)} \qquad (40) \\
&= G_{0,22}(\boldsymbol{x}',\boldsymbol{x};t'-t) , \qquad (41) \\
G_{0,12}(\boldsymbol{x},\boldsymbol{x}';t-t') &= -i\langle\Omega_b|\mathbf{T}[\varphi(\boldsymbol{x},t)\varphi(\boldsymbol{x}',t')]|\Omega_b\rangle \\
&= i\theta(t-t')\sum_{l,m,n=1}^{\infty} C_{nl}S_{nm}u_l(\boldsymbol{x})u_m(\boldsymbol{x}')\mathrm{e}^{-\frac{i}{\hbar}E_n(t-t')} \\
&\quad + i\theta(t'-t)\sum_{l,m,n=1}^{\infty} S_{nl}C_{nm}u_l(\boldsymbol{x}')u_m(\boldsymbol{x})\mathrm{e}^{-\frac{i}{\hbar}E_n(t'-t)} \qquad (42) \\
&= G_{0,21}(\boldsymbol{x},\boldsymbol{x}';t-t') . \qquad (43)
\end{aligned}$$

These propagators depend on $\boldsymbol{x}$ and $\boldsymbol{x}'$ separately due to the absence of space-translational invariance, but are functions of $t-t'$ since the stationary situation is under consideration.

3.3 Numerical Calculations in Perturbative Formulation

According to the unperturbative formulation in the previous subsections, we summarize the steps to numerically obtain all the parameters in the unperturbative formulation at zero-temperature.

1. Solve the nonlinear equation (6) numerically.
2. Relate the integration of the square of v to N_0. This relation determines μ as a function of N_0.
3. With the known v and μ, obtain u_n and ε_n.
4. Perform the integration in (20).
5. Obtain the orthogonal matrix together with E_n according to (29).
6. Calculate C_{nm} and S_{nm}.

The series of the steps demand troublesome numerical calculations. This price must be paid for precisely estimating physical quantities of our system which is very much complicated, nonlinear many-body one.

We have actually done the calculatinos for v, μ, u_n, ε_n, E_n, C_{nm} and S_{nm} with parameters: $m(^{87}\mathrm{Rb}) = 1.42 \times 10^{-25}$kg, the frequency of the spherical trap $\omega = 2\pi \times 200$Hz, S-wave scattering length $a = 5.77$nm, the number of atoms N_0=2000.

Our results for ε_n and E_n are given below (Table 2). Note that they are close to each other as n grow.

Table 2: ε_n and E_n

n	1	2	3	4	5	10	20	30	40	50
ε_n	1.14	2.68	4.40	6.22	8.08	17.73	37.48	57.36	77.30	97.25
E_n	1.83	3.39	5.07	6.84	8.66	18.16	37.78	57.61	77.51	97.49

We also have C_{nm} and S_{nm}, for example, 5×5 matrices are shown for 1 to 5 of n,m.

$$C = \begin{pmatrix} 0.996 & 0.250 & 4.82\times10^{-2} & -1.21\times10^{-3} & -2.88\times10^{-3} \\ -0.248 & 0.938 & 0.259 & -7.25\times10^{-2} & 1.15\times10^{-2} \\ 2.28\times10^{-2} & -0.270 & 0.929 & -0.248 & 8.38\times10^{-2} \\ 1.19\times10^{-2} & 3.32\times10^{-3} & -0.271 & -0.930 & 0.234 \\ 4.20\times10^{-4} & 1.39\times10^{-2} & -1.50\times10^{-2} & 0.263 & 0.935 \end{pmatrix}$$

$$S = \begin{pmatrix} 0.231 & 5.80\times10^{-2} & 1.12\times10^{-2} & -2.81\times10^{-4} & -6.69\times10^{-4} \\ -2.91\times10^{-2} & 0.110 & 3.04\times10^{-2} & -8.52\times10^{-3} & 1.35\times10^{-3} \\ 1.61\times10^{-3} & -1.91\times10^{-2} & 6.57\times10^{-2} & -1.75\times10^{-2} & 5.93\times10^{-3} \\ 5.64\times10^{-4} & 1.58\times10^{-4} & -1.29\times10^{-2} & -4.42\times10^{-2} & 1.11\times10^{-2} \\ 1.44\times10^{-5} & 4.75\times10^{-4} & -5.15\times10^{-4} & 9.04\times10^{-5} & 3.21\times10^{-2} \end{pmatrix}$$

The behavior at large n can be seen below (Table 3).
We have $C_{nn} \to 1$ and $S_{nn} \to 0$ with $n \to \infty$,as should be.

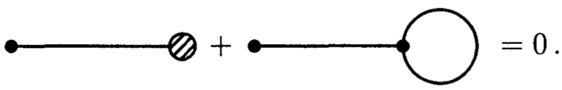
Table 3: C_{nn} and S_{nn}

n	C_{nn}	S_{nn}
1	0.996	0.232
10	-0.955	-1.14×10^{-2}
20	-0.973	-3.96×10^{-3}
30	-0.981	-2.13×10^{-3}
40	0.985	1.38×10^{-3}
50	0.992	1.21×10^{-3}

4 Quantum Correction

With the unpertubative formulation, we are now ready to develop Feynman diagram method as usual. Then the unperturbative propagators are 2×2-matrix ones $G_{0,ij}$ in (40) $\sim$ (43) and the interaction Hamiltonian is in (10). It should be remarked that the Feynman diagram method is formulated not in momentum space, but in configuration space, due to absence of space-translational invariance.

Let us demonstrate a loop calculation of quantum corrections to the GP eq. as an example of utilizing the Feynman diagram method. We calculate tadpole diagram at one-loop level: The Feynman diagrams to be evaluated are



The first diagram (at tree level) represents the propagator from $\boldsymbol{x}'$ to $\boldsymbol{x}$ with GP term at the end. The second diagram is the quantum correction. The sum of the contributions at tree and one-loop levels leads to

$$G_{0,ij}(\boldsymbol{x}', \boldsymbol{x}; t'-t)\,[\text{GP term}(\boldsymbol{x}) + \text{loop}(\boldsymbol{x})] = 0\,. \tag{44}$$

Since $\boldsymbol{x}'$ is arbitrary, this equation gives us

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) + igG_{0,ij}(\boldsymbol{x},\boldsymbol{x}) + 2igG_{0,ii}(\boldsymbol{x},\boldsymbol{x})\right] v(\boldsymbol{x}) = 0\,. \tag{45}$$

$G_{0,ii}(\boldsymbol{x},\boldsymbol{x})$ and $G_{0,ij}(\boldsymbol{x},\boldsymbol{x})$ are defined as

$$G_{0,ii}(\boldsymbol{x},\boldsymbol{x}) \equiv -\frac{i}{2}\sum_{l,m,n=1}^{\infty}\left[C_{nl}C_{nm} + S_{nl}S_{nm}\right]u_l(\boldsymbol{x})u_m(\boldsymbol{x})\,, \tag{46}$$

$$G_{0,ij}(\boldsymbol{x},\boldsymbol{x}) \equiv i\sum_{l,m,n=1}^{\infty} C_{nl}S_{nm}u_l(\boldsymbol{x})u_m(\boldsymbol{x})\,. \tag{47}$$

Put (46), (47) into (45), one can get

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) \right.$$
$$\left. + g\sum_{l,m,n}(C_{nl}C_{nm} - C_{nl}S_{nm} + S_{nl}S_{nm})u_l(\boldsymbol{x})u_m(\boldsymbol{x})\right] v(\boldsymbol{x}) = 0\,. \tag{48}$$

This way GP eq. (6) is modified, the last term in (48) being quantum correction. Our calculation is neither Hartree–Fock approximation nor Thomas–Fermi one.

We comment that this procedure above amounts to calculating quantum correction to the effective action, giving the one-loop order correction to the GP equation.

5 Finite Temperature Effect

Once the field-theoretical formulation at zero-temperature has been established, it is *formally straightforward* to extend it to thermal situations, in particular, to fineite-temperature case. (Here we use the expression "formally straightforward" with the reservation that the physical situation under consideration is not so different from that at zero-temperature that the same unperturbative formulation as at zero-temperature can be applied. If thermal effects are very large, then one has to reformulate the unperturbative formulation and the extension to thermal situation is never straightforward. In what follows, we restrict ourselves to the situation in which the unperturbative formulation is not so much influenced by thermal effects.) For the purpose to the extension from zero-temperature case to finite-temperature one, we take TFD formalism [6].

Details of TFD formalism can be found in [6], and is not repeated here. The essence of TFD is as follows : Each degree of freedom is doubled, an original operator called "non-tilde" one, and a new operator called "tilde one". Then "thermal Bogoliubov transformation" between non-tilde and tilde operators in the unperturbative formulation is introduced, so that "thermal vacuum" is defined without ambiguity. Physical thermal averages are given by the pure-state averages of non-tilde operators, sandwiched with the thermal vacua. Let us explicitly show the unperturbative propagators below.

5.1 Thermal Propagator

We introduce another column notation with respect to tilde and non-tilde field operators (Do not confuse this column notation with that in (37) and (38).);

$$\left\{ \begin{array}{lcl} \varphi^1 = \varphi & , & \varphi^2 = \tilde{\varphi}^\dagger \\ \bar{\varphi}^1 = \varphi^\dagger & , & \bar{\varphi}^2 = -\tilde{\varphi} \,. \end{array} \right. \tag{49}$$

In our present case, the zero-temperature propagators in (40) $\sim$ (43) form a 2×2-matrix, so at finite-temperature, we have 4×4-matrix propagator. The resultant unperturbative propagators become

$$G^{\mu\nu}_{\beta,ij}(\boldsymbol{x},\boldsymbol{x}';t-t') = \sum_n G^{\mu\nu}_{\beta,ij,n}(\boldsymbol{x},\boldsymbol{x}';t-t') \,, \tag{50}$$

where the sum of the energy level n is taken. Each component $G^{\mu\nu}_{0,ij,n}$ is given by

$$\begin{aligned} G^{\mu\nu}_{\beta,ij,n}(\boldsymbol{x},\boldsymbol{x}';t-t') &= B_n^{-1}(-\theta_n) G^{\mu\nu}_{0.ij,n}(\boldsymbol{x},\boldsymbol{x}';t-t') B_n(-\theta_n) \\ &= \begin{pmatrix} c(\theta_n) & -s(\theta_n) \\ -s(\theta_n) & c(\theta_n) \end{pmatrix} \begin{pmatrix} G^{11}_{0,ij,n} & 0 \\ 0 & G^{22}_{0,ij,n} \end{pmatrix} \begin{pmatrix} c(\theta_n) & s(\theta_n) \\ s(\theta_n) & c(\theta_n) \end{pmatrix} \\ &= \begin{pmatrix} c^2(\theta_n) G^{11}_{0,ij,n} - s^2(\theta_n) G^{22}_{0,ij,n} & c(\theta_n)s(\theta_n)\left(-G^{22}_{0,ij,n}\right) \\ c(\theta_n)s(\theta_n)\left(G^{11}_{0,ij,n} - G^{22}_{0,ij,n}\right) & -\left(s^2(\theta_n) G^{11}_{0,ij,n} - c^2(\theta_n) G^{22}_{0,ij,n}\right) \end{pmatrix} \end{aligned} \tag{51}$$

where the parameters in the thermal Bogoliubov transformation are

$$\begin{cases} c(\theta_n) = \cosh(\theta_n) = \frac{1}{\sqrt{1-\mathrm{e}^{-\beta E_n}}} \\ s(\theta_n) = \sinh(\theta_n) = \frac{\mathrm{e}^{-\beta E_n/2}}{\sqrt{1-\mathrm{e}^{-\beta E_n}}} \end{cases}, \tag{52}$$

and $G^{11}_{0,ij,n}$ and $G^{22}_{0,ij,n}$ are, for example,

$$\begin{aligned} G^{11}_{0,11,n}(\boldsymbol{x},\boldsymbol{x}';t-t') \equiv & -i\theta(t-t')\sum_{l,m=1}^{\infty} C_{nl}C_{nm}u_l(\boldsymbol{x})u_m(\boldsymbol{x}')\mathrm{e}^{-\frac{i}{\hbar}E_n(t-t')} \\ & - i\theta(t'-t)\sum_{l,m=1}^{\infty} S_{nl}S_{nm}u_l(\boldsymbol{x}')u_m(\boldsymbol{x})\mathrm{e}^{-\frac{i}{\hbar}E_n(t'-t)}, \end{aligned} \tag{53}$$

$$\begin{aligned} G^{22}_{0,11}(\boldsymbol{x},\boldsymbol{x}';t-t') \equiv & \, i\theta(t'-t)\sum_{l,m=1}^{\infty} C_{nl}C_{nm}u_l(\boldsymbol{x})u_m(\boldsymbol{x}')\mathrm{e}^{-\frac{i}{\hbar}E_n(t'-t)} \\ & + i\theta(t-t')\sum_{l,m=1}^{\infty} S_{nl}S_{nm}u_l(\boldsymbol{x})u_m(\boldsymbol{x}')\mathrm{e}^{-\frac{i}{\hbar}E_n(t-t')}. \end{aligned} \tag{54}$$

5.2 Evaluation of Thermal Fluctuation to the GP eq.

The unperturbative thermal propagators were calculated. Then in TFD the interaction Hamiltonian is given by $\hat{H}_{\text{int}} - \hat{\tilde{H}}_{\text{int}}$, where $\hat{H}_{\text{int}}$ is in (10) and $\hat{\tilde{H}}_{\text{int}}$ is obtained from replacing all the non-tilde operators with the corresponding tilde ones.

From the Feynman diagram method in TFD, we can now evaluate the effect of thermal fluctuation to the GP equation. The diagrams to be calculated is the same one in zero-temperature, except that the number of diagrams becomes larger because of the indices μ,ν. The result is

$$G^{\mu\nu}_{\beta,ij}(\boldsymbol{x}',\boldsymbol{x};t'-t)\left[\text{GP term}(\boldsymbol{x}) + igG^{\nu\nu}_{\beta,ij}(\boldsymbol{x},\boldsymbol{x}) + 2igG^{\nu\nu}_{\beta,ii}(\boldsymbol{x},\boldsymbol{x})\right] = 0\,. \tag{55}$$

Since $\boldsymbol{x}'$ is arbitrary, this implies

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) + igG^{\nu\nu}_{\beta,ij}(\boldsymbol{x},\boldsymbol{x}) + 2igG^{\nu\nu}_{\beta,ii}(\boldsymbol{x},\boldsymbol{x})\right]v(\boldsymbol{x}) = 0\,. \tag{56}$$

Put thermal propagators into (56), one can get

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) \right. \\ & \left. + g\sum_{l,m,n}\coth\left(\frac{\beta E_n}{2}\right)(C_{nl}C_{nm} - C_{nl}S_{nm} + S_{nl}S_{nm})u_l(\boldsymbol{x})u_m(\boldsymbol{x})\right]v(\boldsymbol{x}) = 0\,. \end{aligned} \tag{57}$$

Now we have the generalized GP eq. which contains quantum and thermal fluctuations, and we will consider about this equation a little more. In Sec. 3.3, the behaviors of matrix C_{nm} and S_{nm} are studied by numerical calculation, and we confirmed the asymptotic behavior of these matrices as

$$\begin{cases} C_{nm} \overset{n,m\to\infty}{\longrightarrow} \delta_{nm} \\ S_{nm} \overset{n,m\to\infty}{\longrightarrow} 0 \end{cases}. \tag{58}$$

We also see the asymptotic behavior of $\coth\left(\frac{\beta E_n}{2}\right)$:

$$\coth\left(\frac{\beta E_n}{2}\right) \xrightarrow{E_n\to\infty} 1\,. \tag{59}$$

If there is the number n' which satisfies asymptotic behavior (58) and (59), i.e., $C_{n'n'} \simeq 1$, $S_{n'n'} \simeq 0$ and $\coth(\frac{\beta E_{n'}}{2}) \simeq 1$, one can approximate (57) as

$$\begin{aligned}\Bigg[&-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) \\ &+g\sum_{n=1}^{n'}\sum_{l,m}\coth\left(\frac{\beta E_n}{2}\right)(C_{nl}C_{nm} - C_{nl}S_{nm} + S_{nl}S_{nm})u_l(\boldsymbol{x})u_m(\boldsymbol{x}) \\ &+g\sum_{n=n'}^{\infty} u_n(\boldsymbol{x})u_n(\boldsymbol{x})\Bigg]v(\boldsymbol{x}) = 0\,,\end{aligned} \tag{60}$$

or

$$\begin{aligned}\Bigg[&-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) \\ &+g\sum_{n=1}^{n'}\sum_{l,m}\coth\left(\frac{\beta E_n}{2}\right)(C_{nl}C_{nm} - C_{nl}S_{nm} + S_{nl}S_{nm})u_l(\boldsymbol{x})u_m(\boldsymbol{x}) \\ &+g\left\{\sum_{n=n'}^{\infty} u_n(\boldsymbol{x})u_n(\boldsymbol{x}) + \sum_{n=0}^{n'} u_n(\boldsymbol{x})u_n(\boldsymbol{x})\right\} - g\sum_{n=0}^{n'} u_n(\boldsymbol{x})u_n(\boldsymbol{x})\Bigg]v(\boldsymbol{x}) = 0\,.\end{aligned} \tag{61}$$

From relation (15),

$$\begin{aligned}\Bigg[&-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - \mu + gv^2(\boldsymbol{x}) \\ &+g\sum_{n=1}^{n'}\sum_{l,m}\coth\left(\frac{\beta E_n}{2}\right)(C_{nl}C_{nm} - C_{nl}S_{nm} + S_{nl}S_{nm})u_l(\boldsymbol{x})u_m(\boldsymbol{x}) \\ &+g\delta^3(\boldsymbol{x}) - g\sum_{n=0}^{n'} u_n(\boldsymbol{x})u_n(\boldsymbol{x})\Bigg]v(\boldsymbol{x}) = 0\,.\end{aligned} \tag{62}$$

This equation is different from Hartree–Fock–Bogoliubov (HFB) approximated equation [10, 9] at the following points: First, the HFB approximation contains only $\langle\varphi^\dagger(\boldsymbol{x})\varphi(\boldsymbol{x})\rangle$, $\langle\varphi(\boldsymbol{x})\varphi(\boldsymbol{x})\rangle$ terms, and doesn't have $\langle\varphi(\boldsymbol{x})\varphi^\dagger(\boldsymbol{x})\rangle$, $\langle\varphi^\dagger(\boldsymbol{x})\varphi^\dagger(\boldsymbol{x})\rangle$ terms. Second, (57) have a delta function proportional to the coupling constant g as $g\delta^3(\boldsymbol{x})$.

5.3 Numerical Evaluation of the Thermal Correction to the GP Eq.

We solved (62) using the following parameters: $m(^{87}\mathrm{Rb}) = 1.42 \times 10^{-25}$kg, the frequency of the spherical trap $\omega = 2\pi \times 200$Hz, S-wave scattering length $a = 5.77$nm, the number of atoms N_0=2000 and temperature $T = 100$nK (FIG. 1). These parameters are the same ones, used in [9].

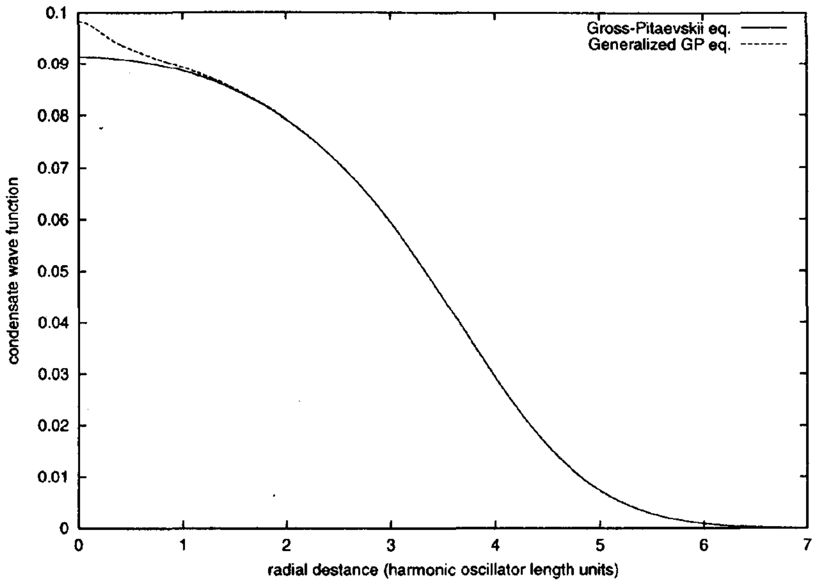


FIG. 1. This figure contains plots of the solution of the GP eq.(solid line) and generalized GP eq. (62)(dotted line).

6 Summary

We formulate a quantum field theory, at zero-temperature and finite-temperature for the BEC systems. In zero-temperature case it is essential to introduce the generalized Bogoliubov transformation.

In order to treat finite-temperature case, TFD formalism is applied.

For illustration, we performed necessary numerical calculations and obtained quantum corrections to the Gross–Pitaevskii equation at zero-temperature, and quantum and thermal corrections to it at finite-temperature.

References

[1] M.H. Anderson et al., Science **269**, 198 (1995).

[2] C.C. Bradley et al., Phys. Rev. Lett. **75**, 1687 (1995).

[3] K.B. Davis et al., Phys. Rev. Lett. **75**, 3969 (1995).

[4] E.P. Gross, Nuovo Cim. **20**, 454 (1961); J. Math. Phys. **4**, 195 (1963); L.P. Pitaevskii, Zh. Eksp. Teor. Fiz. **40**, 646 (1961) [Sov. Phys.-JETP **13**, 451 (1961)].

[5] F. Dalfo, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999)

[6] See for review, H. Umezawa, *Advanced Field Theory — Micro, Macro and Thermal Physics —*, (AIP, New York, 1993), and references therein.

[7] W. Ketterle, D.S. Durfee, and D.M. Stamper-Kurn, cond-mat/9904034

[8] H. Ezawa, K. Nakamura, K. Watanabe and Y. Yamanaka, *Fluctuation of the Bose-Einstein condensate in a trap*, preprint (1999).

[9] D.A.W. Hutchinson, E. Zaremba, and A. Griffin, Phys. Rev. Lett. **78**, 1842 (1997)

[10] A. Griffin, Phys. Rev. B **53**, 9341 (1996)