Proper treatment of the zero mode in quantum field theory for trapped Bose-Einstein condensation

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So far much theoretical consideration of experiments on the Bose-Einstein condensation (BEC) of alkali-metal atoms in harmonic traps is based on the Gross-Pitaevskii (GP) equation. In this paper, we attempt to formulate the BEC in the language of quantum field theory and to estimate the quantum and thermal fluctuation effects, which are neglected in the approximation using the GP equation. First, the formulation at zero temperature is developed, and then it is extended to the finite-temperature case by means of thermofield dynamics. We treat the zero-energy mode with care, so that the canonical commutation relations hold. As a result, an infrared divergence appears, but it can be renormalized into the observed condensate number. Numerical calculations are performed. For illustration, the corrections at one-loop level to the original GP equation are given. We also calculate numerically the effects of quantum and thermal fluctuations on the distribution of condensed atoms.

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I. INTRODUCTION

Since the first experiments on Bose-Einstein condensation (BEC) of alkali-metal atoms in harmonic traps succeeded in 1995 [1–3] and subsequent experiments were achieved in many laboratories all over the world, BEC phenomena have inspired various theoretical studies [4]. From the theoretical viewpoint, the BEC system is rather simple, i.e., the interaction is of the two-body contacting type and weak. The experiments are well controlled and are expected to give precise measurements under various experimental situations. In addition to future development of ''BEC technology'' and its potential applications, BEC can offer opportunities to confirm the foundations of quantum and statistical physics, or of the physics of quantum many-body system.

The behavior in BEC experiments has been treated consistently as the first step using the Gross-Pitaevskii (GP) equation [5]. The approach using the GP equation is considered as a mean-field approximation of quantum field theory (QFT) which is the most fundamental law of dynamics. The applicability of the GP equation is limited to cases where most of the trapped particles are condensed and the effects of noncondensed particles are very small. Actually, the GP equation explains the phenomena at rather low temperature observed in many experiments [4]. For future experiments in which physical quantities will be measured more accurately, or in which fluctuations (we mean both quantum and thermal fluctuations) will play an important role, one has to take those fluctuations into account. In a way they are estimated within the framework of the mean-field approximation [6].

Our purpose is to reconsider the BEC from the viewpoint of QFT beyond the GP equation. We want a theoretical formulation applicable to cases even with large fluctuations. For example, when the temperature approaches the critical one, the fluctuations are inevitably large. In this paper, we develop a formulation of the BEC problem from first principles; i.e., a quantum field theoretical one, and estimate the fluctuation effects.

In our approach, BEC is understood as a spontaneous breakdown of global phase symmetry. This mechanism gives an order parameter which behaves like a classical field. When a continuous symmetry is spontaneously broken, the Goldstone theorem implies the existence of a Nambu-Goldstone (NG) mode [7]. This gapless mode is the leading part, creating and maintaining the order. In a sense our discussions below emphasize the importance of the NG mode.

It should be pointed out that the spatial translational symmetry is broken explicitly for the BEC system due to the external trapping potential, while the systems treated in textbooks are usually invariant under the translation (although the symmetry may be spontaneously broken, e.g., when a lattice is formed). In the latter homogeneous cases the momentum is a good quantum number and the Goldstone mode usually belongs to a continuous spectrum as a zero-momentum mode. But, as will be seen later, the Goldstone mode in the present case is a discrete one. A discussion of the symmetry and the gapless mode is given in Ref. [6] within the mean-field formalism. There the symmetry and gapless mode are considered in the limit of homogeneous geometry; we do not take the homogeneous limit, but treat the inhomogeneous system directly.

The Ward-Takahashi (WT) relations [8] and the Goldstone theorem are derived solely from the canonical commutation relation, the Heisenberg equation of motion, and the transformation property for the Heisenberg operator. In this connection, we insist on preserving the canonical commutation relation, while the Bogoliubov prescription [9] violates it [10]. This problem has already been pointed out for the trapped BEC system [11]. For illustration, we will show that the WT relation holds at the tree level in our approach, which clarifies the important role of the NG mode for the existence of condensation.

The existence of the zero mode is also derived in [12,13], using a formalism slightly different from ours. There it is

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treated as a pair of collective coordinates, while we treat it as a particle mode. The point relevant to the discussions in this paper is that the two approaches correspond to choosing different vacua. When the choices of vacua are different in QFT, the physical results are different. The way to treat the zero mode and associated vacuum is not definite yet, and it is fair to say that it is still an open problem.

Once an operator representing the zero mode comes in as in our formulation, one expects that large fluctuation effects will appear, since it easily fluctuates due to gaplessness. In fact, it will be seen below that this fluctuation effect brings us an infrared divergence in the coefficient of the distribution function of the condensed particle and a finite deviation of the distribution function from that of the GP equation even at zero temperature. It is shown that the infrared divergence can be dealt with in a kind of renormalization prescription.

One has to take account of thermal fluctuations as well in order to compare theoretical results with experimental data. Formally, the formulation of QFT at zero temperature can be readily extended to include thermal effects, that is, to thermal field theories. We employ the formalism of thermofield dynamics (TFD) [14], because it is faithful to the concepts of QFT such as the particle picture, canonical properties, and so on, although any thermal theory for equilibrium would give us the same result as ours below within the one-loop calculation. According to the formulation of QFT at finite temperature, we can show in this paper that a finite deviation of the distribution function of condensed particles from that of the GP equation is predicted numerically.

The paper is organized as follows. In Sec. II, we give the formulation of quantum field theory for the trapped BEC system. The unperturbed Hamiltonian is diagonalized, so that one can obtain the unperturbed energy spectrum of noncondensate quasiparticles and the unperturbed propagator. There the canonical commutation relation is respected, which means a careful treatment of the zero mode. We develop one-loop calculations (tadpole diagram) including quantum and thermal fluctuations in Sec. III. There appears an infrared divergence as a result of the fluctuating zero mode. It is shown that the renormalization can deal with the divergence. In Sec. IV, we describe the method of numerical calculation and give numerical results for the distribution of condensed particles. Section V is devoted to a summary and conclusions. In the Appendix, we derive the WT identity at the tree level to indicate the role of the NG mode.

II. FORMULATION OF QUANTUM FIELD THEORY AND DIAGONALIZATION OF UNPERTURBED HAMILTONIAN

Let us start with the action given by

$$S=\int dtd^3x\left(\psi^\dagger(x)(T-K-V+\mu)\psi(x) - \frac{g}{2}\psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x)\right), \tag{1}$$

with the abbreviated notations of $T=i\hbar\partial/\partial t$, $K=-(\hbar^2/2m)\nabla^2$, and $V=\frac{1}{2}m\omega^2(x^2+y^2+z^2)$, where the trapping potential is assumed to be isotropic and ω is its frequency, and g is a coupling constant which is assumed to be small. We suppose that the system is cool and dilute enough to use this approximate interaction.

Note that the action above is invariant under the global phase transformation $\psi(x)\to e^{i\xi}\psi(x)$ and $\psi^\dagger(x)\to e^{-i\xi}\psi^\dagger(x)$, where ξ is an arbitrary constant phase.

In the terminology of the canonical operator formalism, the Heisenberg operator $\hat{\psi}_{\rm H}(x)$ is divided into c-number and operator parts as

$$\hat{\psi}_{\rm H}(x)=e^{i\theta}v(\boldsymbol{x})+\hat{\varphi}_{\rm H}(x), \tag{2}$$

where the c-number real function $v(\boldsymbol{x})$, whose square corresponds to the distribution function of the condensed particle, is unknown at the beginning and should be determined self-consistently. In what follows, $v(\boldsymbol{x})$ is assumed to be time independent, while θ is assumed to be real and time and space independent, meaning that there is no vortex. We require the condition

$$\langle\Omega|\hat{\psi}_{\rm H}(x)|\Omega\rangle=e^{i\theta}v(\boldsymbol{x}), \tag{3}$$

or equivalently

$$\langle\Omega|\hat{\varphi}_{\rm H}(x)|\Omega\rangle=0, \tag{4}$$

leading to an equation determining $v(\boldsymbol{x})$, where $|\Omega\rangle$ is the vacuum.

In order to tame the singular terms associated with the discrete NG mode, we introduce an artificial breaking term which is taken to be vanishing at the final stage of calculation, which is a conventional prescription for treating a system of spontaneous symmetry breakdown. Explicitly we add the following breaking term with an infinitesimal dimensionless parameter ε and a parameter $\bar{\epsilon}$, representing a typical energy scale of the system $\hbar\omega$:

$$\Delta S=\varepsilon\bar{\epsilon}\int dtd^3x[e^{-i\theta}v(\boldsymbol{x})\psi(x)+e^{i\theta}v(\boldsymbol{x})\psi^\dagger(x)] \tag{5}$$

to the original action (1),

$$S_\varepsilon=S+\Delta S, \tag{6}$$

but the suffix ε will be suppressed unless otherwise mentioned.

The expression in Eq. (2) is substituted into Eq. (6), which is rewritten in terms of $v(\boldsymbol{x})$, θ, and $\varphi(x)$ as follows:

$$S_\varepsilon=S_0+S_1+S_2+S_{3,4}, \tag{7}$$

where

$$S_0=\int dtd^3x\left(v(\boldsymbol{x})(-K-V+\mu+2\varepsilon\bar{\epsilon})v(\boldsymbol{x})-\frac{g}{2}v^4(\boldsymbol{x})\right), \tag{8a}$$

$$S_1=\int dtd^3x\{e^{-i\theta}v(\boldsymbol{x})[-K-V+\mu-gv^2(\boldsymbol{x})+\varepsilon\bar{\epsilon}]\varphi(x) + \varphi^\dagger(x)[-K-V+\mu-gv^2(\boldsymbol{x})+\varepsilon\bar{\epsilon}]e^{i\theta}v(\boldsymbol{x})\}, \tag{8b}$$

$$S_2=\int dtd^3x\Big\{\varphi^\dagger(x)[T-K-V+\mu]\varphi(x)-\frac{g}{2}v^2(\boldsymbol{x})\times[4\varphi^\dagger(x)\varphi(x)+e^{-2i\theta}\varphi^2(x)+e^{2i\theta}\varphi^{\dagger 2}(x)]\Big\}, \quad (8c)$$

$$S_{3,4}=\int dtd^3x\Big\{-gv(\boldsymbol{x})[e^{i\theta}\varphi^\dagger(x)\varphi^\dagger(x)\varphi(x)+e^{-i\theta}\varphi^\dagger(x)\varphi(x)\varphi(x)]-\frac{g}{2}\varphi^\dagger(x)\varphi^\dagger(x)\varphi(x)\varphi(x)\Big\}. \quad (8d)$$

As will be seen below, this ε prescription is crucial to control the symmetry breakdown and the infrared divergence appearing in higher-order loop.

As was emphasized, the role of the zero-energy mode is essential. We should adopt an approximate scheme in which the Goldstone theorem holds. The theorem can be derived from the WT identity. It is well known that the loop expansion respects the WT identity and that therefore the Goldstone theorem holds at each level of the loop. Thus, in what follows, we develop a loop expansion for the system of the action in Eq. (8d). It will be seen in the Appendix that the existence of the NG mode guarantees the WT relation at the tree (zero-loop) level.

First we investigate the system at the tree level, denoting $v(\boldsymbol{x})$ by $v_0(\boldsymbol{x})$. From Eq. (4) or from the condition $(\delta S/\delta\varphi)|_{\varphi=0}=0$ the classical equation of motion for v_0 is derived:

$$[K+V-\mu+gv_0^2(\boldsymbol{x})-\varepsilon\overline{\epsilon}]v_0(\boldsymbol{x})=0. \quad (9)$$

At the limit of vanishing ε, this equation is reduced to the GP equation: $[K+V-\mu+gv_0^2(\boldsymbol{x})]v_0(\boldsymbol{x})=0$. The integration of the square of v_0 is interpreted as the condensate particle number N_c,

$$N_c=\int d^3x v_0^2(\boldsymbol{x}). \quad (10)$$

Under the condition of Eq. (9), we have the Hamiltonian given by

$$\hat{H}=\hat{H}_0+\hat{H}_{\rm int}, \quad (11)$$

where

$$\hat{H}_0=\int d^3x\Big\{\hat{\varphi}^\dagger(x)(K+V-\mu)\hat{\varphi}(x)+\frac{g}{2}v_0^2(\boldsymbol{x})[4\hat{\varphi}^\dagger(x)\hat{\varphi}(x)+e^{-2i\theta}\hat{\varphi}^2(x)+e^{2i\theta}\hat{\varphi}^{\dagger 2}(x)]\Big\}, \quad (12a)$$

$$\hat{H}_{\rm int}=\int d^3x\Big\{gv_0(\boldsymbol{x})[e^{i\theta}\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x)\hat{\varphi}(x)+e^{-i\theta}\hat{\varphi}^\dagger(x)\hat{\varphi}(x)\hat{\varphi}(x)]+\frac{g}{2}\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x)\hat{\varphi}(x)\hat{\varphi}(x)\Big\}. \quad (12b)$$

We now turn to diagonalizing the unperturbed Hamiltonian (12a) and to establishing the quasiparticle picture at the tree level. Equation (9) suggests that it is adequate to expand the field $\hat{\varphi}(x)$ in terms of the complete orthonormal set $\{u_n(\boldsymbol{x})\}$ $(n=0,1,2,\ldots)$, whose eigenequations are

$$[K+V-\mu+gv_0^2(\boldsymbol{x})]u_n(\boldsymbol{x})=(\varepsilon_n+\varepsilon\overline{\epsilon})u_n(\boldsymbol{x}), \quad (13)$$

with

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

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

It is easily seen that $v_0(\boldsymbol{x})$ is proportional to $u_0(\boldsymbol{x})$ with $\varepsilon_0=0$:

$$v_0(\boldsymbol{x})=\sqrt{N_c}u_0(\boldsymbol{x}). \quad (16)$$

Let us expand $\hat{\varphi}(x)$ in terms of Eq. (13),

$$\hat{\varphi}(x)=\sum_{n=0}^{\infty}\hat{a}_n(t)u_n(\boldsymbol{x}). \quad (17)$$

The operators $\hat{a}_n$ and $\hat{a}_n^\dagger$ are subject to

$$[\hat{a}_n,\hat{a}_{n'}^\dagger]=\delta_{nn'}, \quad (18)$$

and $[\hat{a}_n,\hat{a}_{n'}]=[\hat{a}_n^\dagger,\hat{a}_{n'}^\dagger]=0$. These commutation relations with the completeness (15) are consistent with the canonical commutation relations

$$[\hat{\psi}(\boldsymbol{x},t),\hat{\psi}^\dagger(\boldsymbol{x}',t)]=[\hat{\varphi}(\boldsymbol{x},t),\hat{\varphi}^\dagger(\boldsymbol{x}',t)]=\delta^3(\boldsymbol{x}-\boldsymbol{x}') \quad (19)$$

and

$$\begin{aligned}[\hat{\psi}(\boldsymbol{x},t),\hat{\psi}(\boldsymbol{x}',t)]&=[\hat{\psi}^\dagger(\boldsymbol{x},t),\hat{\psi}^\dagger(\boldsymbol{x}',t)]\\&=[\hat{\varphi}(\boldsymbol{x},t),\hat{\varphi}(\boldsymbol{x}',t)]\\&=[\hat{\varphi}^\dagger(\boldsymbol{x},t),\hat{\varphi}^\dagger(\boldsymbol{x}',t)]\\&=0.\end{aligned} \quad (20)$$

Here the fact that $\hat{a}_0$ is included in the expansion (17) is essential, otherwise the canonical commutation relation would be violated. In the conventional Bogoliubov approach, $\hat{a}_0$ is excluded, or, more precisely, $v_0(\boldsymbol{x})+\hat{a}_0u_0(\boldsymbol{x})$ is replaced by a single c-number function $v_0(\boldsymbol{x})$. The difference between the conventional Bogoliubov approach and ours is a central subject in this paper.

The unperturbed Hamiltonian now reads

$$\hat{H}_0=\sum_{n=0}^{\infty}(\varepsilon_n+\varepsilon\overline{\epsilon})\hat{a}_n^\dagger\hat{a}_n+\sum_{n,n'=0}^{\infty}[2\hat{a}_n^\dagger U_{nn'}\hat{a}_{n'}+e^{-2i\theta}\hat{a}_nU_{nn'}\hat{a}_{n'}+e^{2i\theta}\hat{a}_n^\dagger U_{nn'}\hat{a}_{n'}^\dagger], \quad (21)$$

with the notation $U_{nn'}=\frac{1}{2}g\int d^3x v^2(\boldsymbol{x})u_n(\boldsymbol{x})u_{n'}(\boldsymbol{x})$. $\hat{H}_0$ is not diagonalized yet in terms of the $\hat{a}$ operators. Let us introduce the following operators:

$$\hat{q}_n=\sqrt{\frac{1}{2(\varepsilon_n+\varepsilon\bar{\epsilon})}}(e^{-i\theta}\hat{a}_n+e^{i\theta}\hat{a}_n^\dagger), \tag{22a}$$

$$\hat{p}_n=-i\sqrt{\frac{\varepsilon_n+\varepsilon\bar{\epsilon}}{2}}(e^{-i\theta}\hat{a}_n-e^{i\theta}\hat{a}_n^\dagger). \tag{22b}$$

These operators satisfy the canonical commutation relations $[\hat{q}_n,\hat{p}_{n'}]=i\delta_{nn'}$ and other commutations vanish. The Hamiltonian (21) is rewritten as

$$\hat{H}_0=\sum_{n=0}^{\infty}\frac{1}{2}\hat{p}_n^2+\sum_{n,n'=0}^{\infty}\frac{1}{2}\hat{q}_nW_{nn'}\hat{q}_{n'}-\sum_{n=0}^{\infty}\left[\frac{1}{2}(\varepsilon_n+\varepsilon\bar{\epsilon})+U_{nn}\right]. \tag{23}$$

Here the matrix W has a block structure,

$$W=\begin{pmatrix}4(\varepsilon\bar{\epsilon})U_{00}+O(\varepsilon^2) & \sqrt{\varepsilon\bar{\epsilon}}u'^{\mathrm{T}}+O(\varepsilon^{3/2})\\ \sqrt{\varepsilon\bar{\epsilon}}u'+O(\varepsilon^{3/2}) & W'+O(\varepsilon)\end{pmatrix}, \tag{24}$$

where

$$u'=\begin{pmatrix}4\sqrt{\varepsilon_1}U_{10}\\ 4\sqrt{\varepsilon_2}U_{20}\\ \vdots\end{pmatrix}, \tag{25}$$

$$u'^{T}=(4\sqrt{\varepsilon_1}U_{01},4\sqrt{\varepsilon_2}U_{02},\ldots), \tag{26}$$

$$W'_{nn'}=\varepsilon_n^2\delta_{nn'}+4\sqrt{\varepsilon_n}U_{nn'}\sqrt{\varepsilon_{n'}}\quad(n,n'=1,2,\ldots). \tag{27}$$

Then the symmetric matrix W can be diagonalized by an orthogonal matrix $\mathcal{O}$:

$$\sum_{m,m'=0}^{\infty}(\mathcal{O}_{nm}W_{mm'}\mathcal{O}_{n'm'})=E_n^2\delta_{nn'}. \tag{28}$$

It can be shown that the zeroth eigenvalue is

$$E_0=\sqrt{\varepsilon\bar{\epsilon}}(4U_{00}-u'^{\mathrm{T}}W'^{-1}u')^{1/2}+O(\varepsilon^{3/2}) \tag{29}$$

$$\equiv\sqrt{\varepsilon\bar{\epsilon}}\sqrt{\bar{E}_0}+O(\varepsilon^{3/2}), \tag{30}$$

and that the matrix $\mathcal{O}$ also has the form of

$$\mathcal{O}=\begin{pmatrix}1-\frac{1}{2}(\varepsilon\bar{\epsilon})u'^{\mathrm{T}}W'^{-2}u'+O(\varepsilon^2) & -\sqrt{\varepsilon\bar{\epsilon}}u'^{\mathrm{T}}W'^{-1}+O(\varepsilon^{3/2})\\ \sqrt{\varepsilon\bar{\epsilon}}\mathcal{O}'W'^{-1}u'+O(\varepsilon^{3/2}) & \mathcal{O}'+O(\varepsilon)\end{pmatrix}, \tag{31}$$

where $\mathcal{O}'$ satisfies

$$\mathcal{O}'W'\mathcal{O}'^{T}=E'^2, \tag{32}$$

with the diagonal matrix

$$E'_{nn'}=E_n\delta_{nn'}+O(\varepsilon^{1/2})\quad(n,n'=1,2,\ldots). \tag{33}$$

Using this $\mathcal{O}$ matrix, we introduce a new pair of canonical operators by

$$\hat{Q}_n=\sum_{m=0}^{\infty}\mathcal{O}_{nm}\hat{q}_m, \tag{34a}$$

$$\hat{P}_n=\sum_{m=0}^{\infty}\mathcal{O}_{nm}\hat{p}_m, \tag{34b}$$

where $[\hat{Q}_n,\hat{P}_{n'}]=i\delta_{nn'}$ and other commutation relations vanish. Finally, we have

$$\hat{H}_0=\sum_{n=0}^{\infty}\left[\frac{1}{2}\hat{P}_n^2+\frac{1}{2}E_n^2\hat{Q}_n^2-\frac{1}{2}(\varepsilon_n+\varepsilon\bar{\epsilon})-U_{nn}\right]=\sum_{n=0}^{\infty}\left[E_n\hat{b}_n^\dagger\hat{b}_n+\frac{1}{2}E_n-\frac{1}{2}(\varepsilon_n+\varepsilon\bar{\epsilon})-U_{nn}\right]. \tag{35}$$

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

$$\hat{Q}_n=\sqrt{\frac{1}{2E_n}}(\hat{b}_n+\hat{b}_n^\dagger), \tag{36a}$$

$$\hat{P}_n=-i\sqrt{\frac{E_n}{2}}(\hat{b}_n-\hat{b}_n^\dagger). \tag{36b}$$

In this way we have the generalized Bogoliubov transformation [11] with the zero mode

$$\hat{b}_n=\sum_{m=0}^{\infty}(e^{-i\theta}C_{nm}\hat{a}_m+e^{i\theta}S_{nm}\hat{a}_m^\dagger), \tag{37a}$$

$$\hat{b}_n^\dagger = \sum_{m=0}^{\infty} (e^{i\theta} C_{nm} \hat{a}_m^\dagger + e^{-i\theta} S_{nm} \hat{a}_m), \tag{37b}$$

where

$$C_{nm} = \frac{1}{2}\left(\sqrt{\frac{E_n}{\varepsilon_m + \varepsilon\epsilon}} + \sqrt{\frac{\varepsilon_m + \varepsilon\epsilon}{E_n}} \right) \mathcal{O}_{nm}, \tag{38a}$$

$$S_{nm} = \frac{1}{2}\left(\sqrt{\frac{E_n}{\varepsilon_m + \varepsilon\epsilon}} - \sqrt{\frac{\varepsilon_m + \varepsilon\epsilon}{E_n}} \right) \mathcal{O}_{nm}. \tag{38b}$$

The matrices C and S satisfy the following relations:

$$\sum_{m=0}^{\infty} (C_{nm} C_{n'm} - S_{nm} S_{n'm}) = \delta_{nn'}, \tag{39}$$

$$\sum_{m=0}^{\infty} (C_{nm} S_{n'm} - S_{nm} C_{n'm}) = 0. \tag{40}$$

We mention only the leading behaviors of elements of C and S with respect to ε: $C_{00}, S_{00} \sim \varepsilon^{-1/4}$, $C_{0n}, S_{0n} \sim \varepsilon^{1/4}$ $(n \neq 0)$, and C_{n0}, S_{n0}, and the other remaining elements $\sim \varepsilon^0$. It is remarked that the singular behavior in C and S comes from the mixing between the $\hat{a}_0$ and $\hat{a}_n$ $(n \neq 0)$. Although the mixing matrices are divergent as $\varepsilon \to 0$, the energy eigenvalues $\{E_n\}$ are finite.

We compare the quasiparticle picture in our theory with the one in the usual Bogoliubov theory, in which the zero mode is excluded in the expansion of Eq. (17). In our theory there are additional mixings between the operators with $n = 0$ and $n \neq 0$, but they do not affect the energy spectrum of noncondensate modes: the energy spectrum in our theory is given by $\{E_n\}$, while that in the Bogoliubov theory by $\{E_n'\}$. Equation (33) indicates that the former approaches the latter as $\varepsilon \to 0$ except for $n = 0$.

What is important here is that the energy spectrum of noncondensate quasiparticles is $\{E_n\}$, but not the "naive" energy parameter $\{\varepsilon_n\}$. The numerical difference between these two energies will be shown in Sec. IV.

Now that the unperturbed Hamiltonian is diagonalized in Eq. (33), the unperturbative vacuum $|\Omega_b\rangle$ is defined by

$$\hat{b}_n |\Omega_b\rangle = 0. \tag{41}$$

In terms of $\hat{b}_n$ and $\hat{b}_n^\dagger$, the field operators $\hat{\varphi}$ and $\hat{\varphi}^\dagger$ can be written as

$$\hat{\varphi}(x) = e^{i\theta} \sum_{m,n=0}^{\infty} [\hat{b}_n(t) C_{nm} u_m(\boldsymbol{x}) - \hat{b}_n^\dagger(t) S_{nm} u_m(\boldsymbol{x})], \tag{42a}$$

$$\hat{\varphi}^\dagger(x) = e^{-i\theta} \sum_{m,n=0}^{\infty} [\hat{b}_n^\dagger(t) C_{nm} u_m(\boldsymbol{x}) - \hat{b}_n(t) S_{nm} u_m(\boldsymbol{x})]. \tag{42b}$$

Here a crucial step is taken: We assume Eq. (41) even for $n = 0$, $\hat{b}_0 |\Omega_b\rangle = 0$. The authors in [12,13] suggest a vacuum different from ours, but could not propose a criterion to fix a single vacuum yet. In any case, their expression for the unperturbative propagator, if they calculated it, would differ from ours. One cannot apply the results of our loop expansion calculations naively to their approach.

We can easily construct the unperturbative propagators. Introduce the column notation as

$$\hat{\Phi}_i = \begin{cases} \hat{\varphi} & (\text{for } i = 1), \\ \hat{\varphi}^\dagger & (\text{for } i = 2), \end{cases} \tag{43a}$$

$$\hat{\Phi}_i^\dagger = \begin{cases} \hat{\varphi}^\dagger & (\text{for } i = 1), \\ \hat{\varphi} & (\text{for } i = 2), \end{cases} \tag{43b}$$

and define a 2×2 matrix propagator by

$$G_0(\boldsymbol{x}, \boldsymbol{x}'; t - t') \equiv \begin{pmatrix} G_{0,11}(\boldsymbol{x}, \boldsymbol{x}'; t - t') & G_{0,12}(\boldsymbol{x}, \boldsymbol{x}'; t - t') \\ G_{0,21}(\boldsymbol{x}, \boldsymbol{x}'; t - t') & G_{0,22}(\boldsymbol{x}, \boldsymbol{x}'; t - t') \end{pmatrix}, \tag{44}$$

where

$$G_{0,ij}(\boldsymbol{x}, \boldsymbol{x}'; t - t') \equiv -i \langle \Omega_b | T[\hat{\Phi}_i(\boldsymbol{x}, t) \hat{\Phi}_j^\dagger(\boldsymbol{x}', t')] | \Omega_b \rangle. \tag{45}$$

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. We give their Fourier transforms with respect to time,

$$\begin{aligned} G_0(\boldsymbol{x}, \boldsymbol{x}'; \omega) &\equiv \int d\tau e^{i\omega\tau} G_0(\boldsymbol{x}, \boldsymbol{x}'; \tau) \\ &= \sum_{\ell,m,n=0}^{\infty} \left\{ \left[\frac{1}{\omega - E_n + i\delta} \begin{pmatrix} C_{n\ell} C_{nm} & -C_{n\ell} S_{nm} \\ -S_{n\ell} C_{nm} & S_{n\ell} S_{nm} \end{pmatrix} \right. \right. \\ &\quad \left. \left. - \frac{1}{\omega + E_n - i\delta} \begin{pmatrix} S_{n\ell} S_{nm} & -S_{n\ell} C_{nm} \\ -C_{n\ell} S_{nm} & C_{n\ell} C_{nm} \end{pmatrix} \right] \right. \\ &\quad \left. \times u_\ell(\boldsymbol{x}) u_m(\boldsymbol{x}') \right\}, \end{aligned} \tag{46}$$

where δ is an infinitesimal constant.

III. ONE-LOOP CALCULATION

Next we proceed to the one-loop level. The field ψ is divided as

$$\psi(x) = e^{i\theta} v(\boldsymbol{x}) + \varphi(x), \tag{47}$$

where

$$v(\boldsymbol{x}) = v_0(\boldsymbol{x}) + \delta v(\boldsymbol{x}) \tag{48}$$

with an unknown function $\delta v(\boldsymbol{x})$ of the order of $\hbar$, while $v_0(\boldsymbol{x})$ is the one at the tree level, subject to Eq. (9). Because

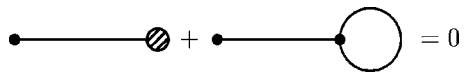

FIG. 1. Tadpole diagram.

the GP equation does not hold for this v due to the presence of δv, the term S_1 cannot be dropped. Thus the interaction Hamiltonian at the one-loop level should read as

$$\hat{H}_{\rm int}=\int d^3x\Big\{ e^{-i\theta}v(\boldsymbol{x})[K+V-\mu+gv^2(\boldsymbol{x})-\varepsilon\overline{\epsilon}]\hat{\varphi}(x) + \hat{\varphi}^\dagger(x)[K+V-\mu+gv^2(\boldsymbol{x})-\varepsilon\overline{\epsilon}]e^{i\theta}v(\boldsymbol{x}) + gv(\boldsymbol{x})[e^{i\theta}\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x)\hat{\varphi}(x)+e^{-i\theta}\hat{\varphi}^\dagger(x)\hat{\varphi}(x)\hat{\varphi}(x)] + \frac{g}{2}\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x)\hat{\varphi}(x)\hat{\varphi}(x)\Big\}. \tag{49}$$

Starting with v_0, we evaluate the quantum correction δv, using the unperturbed propagators in Eq. (46) and Feynman rules from the interaction Hamiltonian (49). Then the condition (4) up to the one-loop level amounts to calculating the tadpole diagram shown in Fig. 1, which leads to

$$[K+V-\mu+gv^2(\boldsymbol{x})]v(\boldsymbol{x}) + g\sum_{\ell,m,n=0}^{\infty}(2S_{n\ell}S_{nm}-C_{n\ell}S_{nm})u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v(\boldsymbol{x})=0. \tag{50}$$

Here a crucial observation is that the infrared divergence appears in the summation (tadpole contribution) as the divergence of $1/\sqrt{\varepsilon}$, but the divergent terms are limited to those with $\ell=m=0$. On the other hand, there are new finite quantum contributions. Within the approximation, one may rewrite Eq. (50) as

$$[K+V-\mu+3gv_0^2(\boldsymbol{x})]\delta v(\boldsymbol{x}) + g\sum_{\ell,m,n=0}^{\infty}(2S_{n\ell}S_{nm}-C_{n\ell}S_{nm})u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v_0(\boldsymbol{x})=0, \tag{51}$$

after the higher terms such as δv^3 and $\delta v^2 v_0$ are neglected and the equation for v_0, Eq. (9), is applied.

In order to isolate the infrared divergence, we express δv as a sum of two terms (one is infrared divergent, the other is finite),

$$\delta v(\boldsymbol{x})=\delta v^{(0)}(\boldsymbol{x})+\delta v^{(1)}(\boldsymbol{x}). \tag{52}$$

The $\delta v^{(0)}(\boldsymbol{x})$ is taken to be proportional to $u_0(\boldsymbol{x})$ and is subject to

$$2gv_0^2(\boldsymbol{x})\delta v^{(0)}(\boldsymbol{x})+g\sum_{n=0}^{\infty}(2S_{n0}^2-C_{n0}S_{n0})u_0^2(\boldsymbol{x})v_0(\boldsymbol{x})=0; \tag{53}$$

then $\delta v^{(1)}(\boldsymbol{x})$ is a solution of the equation

$$[K+V-\mu+3gv_0^2(\boldsymbol{x})]\delta v^{(1)}(\boldsymbol{x}) + g\sum_{\ell,m,n=0}^{\infty}{}'(2S_{n\ell}S_{nm}-C_{n\ell}S_{nm})u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v_0(\boldsymbol{x})=0, \tag{54}$$

where Σ' means a summation without $\ell=m=0$.

Although $(2S_{n0}^2-C_{n0}S_{n0})$ in Eq. (53) is divergent in the limit of $\varepsilon\to 0$, the solution can formally be found to be

$$\delta v^{(0)}(\boldsymbol{x})=-\frac{1}{2\sqrt{N_c}}\sum_{n=0}^{\infty}(2S_{n0}^2-C_{n0}S_{n0})u_0(\boldsymbol{x}). \tag{55}$$

The linear equation (54) is free from divergence and can be solved numerically. But when we expand $\delta v^{(1)}(\boldsymbol{x})$ in terms of the complete set $\{u_n(\boldsymbol{x})\}$, $\delta v^{(1)}(\boldsymbol{x})=\Sigma_{n=0}^{\infty}d_n u_n(\boldsymbol{x})$, the coefficient d_0 is not equal to zero in general. Thus $\delta v^{(0)}$ and $\delta v^{(1)}$ are not orthogonal to each other: $\int d^3x\,\delta v^{(0)}(\boldsymbol{x})\delta v^{(1)}(\boldsymbol{x})\neq 0$. Physically, one should redefine the two terms in δv as

$$\delta v(\boldsymbol{x})=\delta v_0(\boldsymbol{x})+\delta v_{\rm f}(\boldsymbol{x}), \tag{56}$$

where

$$\delta v_0(\boldsymbol{x})=\delta v^{(0)}(\boldsymbol{x})+d_0u_0(\boldsymbol{x}), \tag{57}$$

$$\delta v_{\rm f}(\boldsymbol{x})=\sum_{n=1}^{\infty}d_nu_n(\boldsymbol{x}). \tag{58}$$

In this way, while δv_0 is proportional to u_0, $\delta v_{\rm f}$ is orthogonal to δv_0, $\int d^3x\,\delta v_0(\boldsymbol{x})\delta v_{\rm f}(\boldsymbol{x})=0$. One cannot observe v_0, δv_0, and $\delta v_{\rm f}$ separately in experiments, but only a combination of $v_0+\delta v$. Therefore we should relate the condensate number, which we call $N_{\rm c,r}$, to the integration,

$$N_{\rm c,r}=\int d^3x[v_{0,\rm r}(\boldsymbol{x})+\delta v_{\rm f}(\boldsymbol{x})]^2\simeq\int d^3x v_{0,\rm r}^2(\boldsymbol{x}) \tag{59}$$

where the notation

$$v_{0,\rm r}(\boldsymbol{x})=v_0(\boldsymbol{x})+\delta v_0(\boldsymbol{x}) \tag{60}$$

is used, and $\delta v_{\rm f}^2$ has been dropped because it is of the order of $\hbar^2$. It should be noted that within the approximation v_0 can be replaced with the observable $v_{0,\rm r}$ in Eq. (54), which determines $\delta v_{\rm f}$.

Thus we isolate the infrared divergence and renormalize it into the observed condensate number $N_{\rm c,r}$. The explicit finite fluctuation effect can be observed in $\delta v_{\rm f}$ as a deviation from $v_{0,\rm r}$.

We can also evaluate the thermal correction, confining ourselves to equilibrium situations, to the condensate v_0. In order to include thermal fluctuations, we use TFD which is a real time formalism of thermal field theory. The above formulations in the zero-temperature case can straightforwardly be extended to the thermal situation in TFD, only with the doubling of each degree of freedom [14]. The doubling forces us to use a 4×4 matrix propagator instead of the

2×2 matrix in the zero-temperature case. But we comment that any conventional thermal field theory, e.g., the imaginary time formalism, closed-time path formalism, and so on [15], would give us the same result as in TFD for the quantities below.

After following all the same steps as at zero temperature above, we reach the following equation from calculating the one-loop tadpole diagram:

$$[K+V-\mu+gv^2(\boldsymbol{x})]v(\boldsymbol{x}) + g\sum_{\ell,m,n=0}^{\infty}(2S_{n\ell}S_{nm}-C_{n\ell}S_{nm})u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v(\boldsymbol{x}) + g\sum_{\ell,m,n=0}^{\infty}\frac{2}{\exp(\beta E_n)-1}(S_{n\ell}S_{nm}+C_{n\ell}C_{nm} - C_{n\ell}S_{nm})u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v(\boldsymbol{x})=0. \tag{61}$$

The corrected condensate part $v(\boldsymbol{x})$ is separated into the following three terms:

$$v(\boldsymbol{x})=v_0(\boldsymbol{x})+\delta v_\beta(\boldsymbol{x}), \tag{62}$$

$$\delta v_\beta(\boldsymbol{x})=\delta v_\beta^{(0)}(\boldsymbol{x})+\delta v_\beta^{(1)}(\boldsymbol{x}), \tag{63}$$

where $\delta v_\beta(\boldsymbol{x})$ represents all the corrections (thermal as well as quantum) and $\delta v_\beta^{(0)}(\boldsymbol{x})$ is proportional to $u_0(\boldsymbol{x})$ and is subject to

$$2gv_0^2(\boldsymbol{x})\delta v_\beta^{(0)}(\boldsymbol{x})+g\sum_{n=0}^{\infty}\left[(2S_{n0}^2-C_{n0}S_{n0}) + \frac{2}{\exp(\beta E_n)-1}(S_{n0}S_{n0}+C_{n0}C_{n0} - C_{n0}S_{n0})\right]u_0(\boldsymbol{x})u_0(\boldsymbol{x})v_0(\boldsymbol{x})=0. \tag{64}$$

This equation is infrared divergent again, but fortunately only with $\ell=m=0$ just as in Eq. (53). The finite correction term $\delta v_\beta^{(1)}$ is a solution of

$$[K+V-\mu+3gv_0^2(\boldsymbol{x})]\delta v_\beta^{(1)}(\boldsymbol{x})+g{\sum_{\ell,m,n=0}^{\infty}}'\left[(2S_{n\ell}S_{nm} - C_{n\ell}S_{nm})+\frac{2}{\exp(\beta E_n)-1}(S_{n\ell}S_{nm}+C_{n\ell}C_{nm} - C_{n\ell}S_{nm})\right]u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v_0(\boldsymbol{x})=0. \tag{65}$$

These results show that the infrared divergence appears at finite temperature in the same manner as at zero temperature and therefore that its isolation and renormalization can be performed quite similarly. Again, expanding as $\delta v_\beta^{(1)}(\boldsymbol{x}) = \Sigma_{n=0}^{\infty} d_{\beta,n}u_n(\boldsymbol{x})$, we redefine the two terms in δv_β as

$$\delta v_\beta(\boldsymbol{x})=\delta v_{\beta,0}(\boldsymbol{x})+\delta v_{\beta,\mathrm{f}}(\boldsymbol{x}), \tag{66}$$

where

$$\delta v_{\beta,0}(\boldsymbol{x})=\delta v_\beta^{(0)}(\boldsymbol{x})+d_{\beta,0}u_0(\boldsymbol{x}), \tag{67}$$

$$\delta v_{\beta,\mathrm{f}}(\boldsymbol{x})=\sum_{n=1}^{\infty}d_{\beta,n}u_n(\boldsymbol{x}). \tag{68}$$

The total corrected order parameter $v(\boldsymbol{x})$ is

$$v(\boldsymbol{x})=v_{\beta,0,\mathrm{r}}(\boldsymbol{x})+\delta v_{\beta,\mathrm{f}}(\boldsymbol{x}) \tag{69}$$

$$v_{\beta,0,\mathrm{r}}(\boldsymbol{x})=v_0(\boldsymbol{x})+\delta v_{\beta,0}(\boldsymbol{x}). \tag{70}$$

Before closing this section, we should compare our approach with others using QFT.

First, the quantum fluctuations to the condensate profile were calculated perturbatively by Braaten and Nieto [16]. The usual plane-wave expansion is used in their calculation because they focus on short-distance quantum fluctuations. Conversely, we respect low-lying modes, especially the zero mode, in calculating quantum and thermal fluctuations, then we use the complete orthonormal set (13) which fully includes the trapping potential, and diagonalize the unperturbed Hamiltonian. Although both the approaches deal with the same Feynman diagram (Fig. 1), the propagators are different from each other, as are the final results.

Next, we mention the difference between Hartree-Fock-Bogoliubov (HFB) theory and ours. Equations (50) and (61) at first sight seem to be equivalent to the generalized GP equation, derived by the HFB approximation [6]. However, the methods to evaluate the quantum and thermal fluctuations are different. The HFB theory is a variational method [17], but our calculation is based on the loop expansion, which enables us to improve the numerical results loop by loop.

Finally, we discuss the ultraviolet divergence arising from the contact type interaction, already discussed in several papers [16–18]. The contributions of $G_{0,12}(\boldsymbol{x},\boldsymbol{x};0)$ in the tadpole diagram, i.e., the $C_{n\ell}S_{nm}$ terms in Eqs. (50) and (61), correspond to the anomalous average in the HFB theory and give rise to UV divergences. The fact that the summations of the $C_{n\ell}S_{nm}$ terms there diverge roughly as the square root of the UV cutoff can be checked by the numerical method in the next section. In order to deal with the UV divergence, we adopt the renormalization procedure given in [18], which is to subtract the zero-temperature component of the anomalous average or to drop the zero-temperature component of the $C_{n\ell}S_{nm}$ terms in Eqs. (50) and (61). We have not formulated the whole renormalization scheme including the self-energy and vertices yet, but this procedure is considered legitimate within our one-loop calculation.

IV. NUMERICAL STUDY

Now let us perform numerical calculations regarding the quasiparticle picture and the effects of quantum and thermal fluctuations. The parameters that we use are as follows: the trapped atoms are ^{87}Rb, which has the mass $m=1.42\times 10^{-25}$ kg, the frequency of the trapping potential is

TABLE I. The energy spectra of ''naive'' and quasiparticles. (a) shows the energy spectrum with the number of condensate atoms $N_c=1000$ and (b) with $N_c=25\,000$.

(a) $N_c=1000$			(b) $N_c=25\,000$		
n	ε_n	E_n	n	ε_n	E_n
1	1.976	2.015	1	1.669	2.130
2	3.967	3.999	2	3.529	3.960
3	5.963	5.989	3	5.451	5.839
4	7.959	7.983	4	7.401	7.752
5	9.957	9.979	5	9.365	9.687
⋮	⋮	⋮	⋮	⋮	⋮
10	1.995×10	1.997×10	10	1.927×10	1.951×10
⋮	⋮	⋮	⋮	⋮	⋮
50	9.994×10	9.995×10	50	9.914×10	9.925×10
⋮	⋮	⋮	⋮	⋮	⋮

$\omega=200\times 2\pi$Hz, the coupling constant $g=0.03a_{\rm ho}$ ($a_{\rm ho}\equiv\sqrt{\hbar/2m\omega}\simeq 5.44\times 10^{-7}$ m), and the number of condensate atoms N_c is chosen as 1000 and 25 000. Here the value of g is taken to be small for the following technical reason, compared with the usual $g=4\pi\hbar^2 a_s/m$, where a_s is the s-wave scattering length of the ^{87}Rb atom. The situation of small g is realizable with Feshbach resonance [19]. The validity of the loop expansion is guaranteed under the choice of these parameters, since the parameters $g\sqrt{N_c}\simeq 0.095$ ($N_c=1000$) and 0.47 ($N_c=25\,000$), a factor appearing at each level of the loop, are small. In other words, a larger value for g would make loop expansion of lower orders unreliable.

First we investigate the unperturbed particle picture in this system. As was pointed out, our relevant energy spectrum is given by $\{E_n\}$ associated with the quasiparticle, but not by $\{\varepsilon_n\}$. We here compare the numerical values for these two energies. In order to know them, we solved the GP equation (9) by use of the Runge-Kutta method [20] as the first step, and then the eigenequation (13) with the solution of Eq. (9) as a potential and with 200 levels from the bottom and 400 eigenvalues of angular momentum for a spherical trap. The matrix elements of W in Eq. (27) are explicitly expressed by these solutions: $v_0(\boldsymbol{x})$ and $\{u_n(\boldsymbol{x})\}$. The matrix without zero mode W' is diagonalized as Eq. (32) [21]. Then we have $\{\varepsilon_n\}$, $\{\mathcal{O}_{nm}\}$, and $\{E_n\}$, with which the matrices C and S in Eq. (38) are given.

Table I shows the results with $N_c=1000$ and $N_c=25\,000$. The difference is rather small when the number of condensate atoms N_c is small [Table I(a)]. But when N_c is large, we are able to distinguish ε_n from E_n [Table I(b)]. We note that E_n is calculated at the tree level, but is not renormalized yet.

Next we evaluate the influences of quantum and thermal fluctuations on the spatial distribution of a condensate. The remaining parameter to calculate the effects is the temperature T. In the ideal Bose gas model ($g=0$) [4], one can derive the relation

$$\frac{T}{T_c}=\left(1-\frac{N_c}{N_{\rm tot}}\right)^{1/3}, \tag{71}$$

where T_c is the critical temperature and $N_{\rm tot}$ is the total number of particles (the sum of the numbers of condensate and noncondensate particles). But, in the interacting case ($g\neq 0$), we have neither such a simple relation nor T_c. We acquire the total number $N_{\rm tot}$ with the energy of the quasiparticle

$$N_{\rm tot}=N_c+\sum_{n=1}^{\infty}\frac{1}{\exp[\beta E_n]-1}. \tag{72}$$

Here the energy of the quasiparticle is defined in the unperturbed Hamiltonian of Eq. (35), in other words, at the tree level. We have the value of T/T_c which parametrizes our results.

Let us illustrate the steps to obtain $\delta v_f(\boldsymbol{x})$ in Eq. (58) numerically. We already have $v_0(\boldsymbol{x})$, $\{u_n(\boldsymbol{x})\}$, $\{\varepsilon_n\}$, $\{\mathcal{O}_{nm}\}$, $\{E_n\}$, $\{C_{nm}\}$, and $\{S_{nm}\}$. Put $\delta v^{(1)}(\boldsymbol{x})=\Sigma_{n=0}^{\infty}d_n u_n(\boldsymbol{x})$ into Eq. (54):

$$\sum_{n=0}^{\infty}[\varepsilon_n+2gv_0^2(\boldsymbol{x})]d_n u_n(\boldsymbol{x}) + g\sum_{\ell,m,n=0}^{\infty}{}' 2S_{n\ell}S_{nm}u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})v_0(\boldsymbol{x})=0, \tag{73}$$

multiply both sides of Eq. (73) by $u_{n'}(\boldsymbol{x})$, and integrate it over $\boldsymbol{x}$,

$$\sum_{n=0}^{\infty}\bar{W}_{n'n}d_n=-F_{n'}, \tag{74}$$

where

$$\bar{W}_{nn'}=\varepsilon_n\delta_{nn'}+2g\int d^3x[v_0^2(\boldsymbol{x})u_n(\boldsymbol{x})u_{n'}(\boldsymbol{x})], \tag{75}$$

$$F_{n'}=g\int d^3x\left[\sum_{\ell,m,n=0}^{\infty}{}' 2S_{n\ell}S_{nm}v_0(\boldsymbol{x})u_\ell(\boldsymbol{x})u_m(\boldsymbol{x})u_{n'}(\boldsymbol{x})\right]. \tag{76}$$

From this relation (74) the coefficients d_n are derived:

$$d_n=-\sum_{n'=0}^{\infty}\bar{W}^{-1}_{nn'}F_{n'}. \tag{77}$$

In this way we have the finite quantum correction $\delta v_f(\boldsymbol{x})$ in Eq. (58) numerically. As was mentioned in the last paragraph of Sec. III, we have dropped the UV divergent terms ($\Sigma C_{n\ell}S_{nm}$) in Eqs. (73) and (76).

At finite temperature the finite correction $\delta v_{\beta,f}(\boldsymbol{x})$ in Eq. (68), which represents the effects of both the quantum and thermal fluctuations, is obtained by the same procedure as above. As for the UV divergence, we subtract $\Sigma C_{n\ell}S_{nm}$ at zero temperature, keeping the temperature-dependent $C_{n\ell}S_{nm}$ terms.

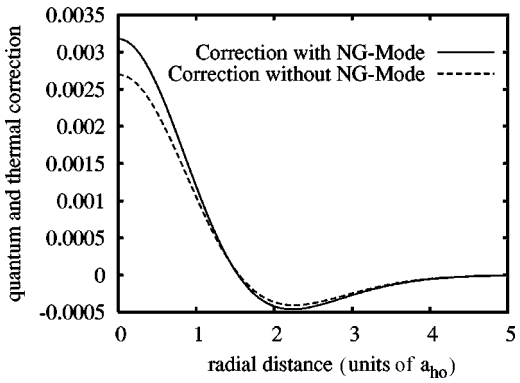

FIG. 2. This figure shows the radial distribution of $\delta v_{\beta,\mathrm{f}}(\boldsymbol{x})$ with and without zero mode with the parameters $N_{\mathrm{c}}=1000$ and $k_{\mathrm{B}}T=2\hbar\omega$. The solid line is the radial distribution of the correction calculated by our theory and the dotted line is the one by the Bogoliubov theory. We find that the zero mode has effects on the distribution of the correction.

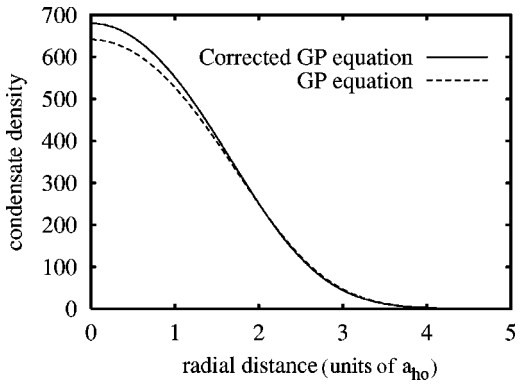

FIG. 3. The difference between corrected and uncorrected distributions with the parameters $N_{\mathrm{c}}=25\,000$ and $k_{\mathrm{B}}T=50\hbar\omega$ is shown in this figure. There is a small difference between the two at the center. The upper solid line is the corrected distribution, while the lower dashed line is the one without correction.

Now let us compare the result in our theory with the one in the usual Bogoliubov theory, which one can easily obtain just by suppressing all the quantities with suffix $n=0$ in Secs. II and III, and in which we see no infrared divergence in the loop calculation. For definiteness, we fix the parameters $N_{\mathrm{c}}=1000$ and $k_{\mathrm{B}}T=2\hbar\omega$ (k_{B} is the Boltzmann constant), which corresponds to the fraction of condensate $T/T_{\mathrm{c}}\simeq 0.275$ according to the relation (71). Figure 2 shows the corrections of the condensate profile, $\delta v_{\beta,\mathrm{f}}(\boldsymbol{x})$, with and without the zero mode (our theory and the usual Bogoliubov theory). We find that the existence of the zero mode makes a difference in the observable quantity.

Figure 2 may make us expect that quantum and thermal corrections give some contribution to the condensate. The corrections are too small to be measured with the parameters fixed.

However, the situation changes slightly when the number of condensate atoms is larger and the temperature of the system becomes higher. We calculate the corrected condensate density with $N_{\mathrm{c}}=25\,000$ and $k_{\mathrm{B}}T=50\hbar\omega$, keeping the other parameters the same. The fraction of temperature is given by $T/T_{\mathrm{c}}\simeq 0.949$ with these parameters. Figure 3 shows the radial corrected distribution of the condensate density $v^2(\boldsymbol{x})=[v_{\beta,0,\mathrm{r}}(\boldsymbol{x})+\delta v_{\beta,\mathrm{f}}(\boldsymbol{x})]^2$ and the solution of the GP equation without quantum and thermal corrections.

It is seen from Fig. 3 that the condensate density increases at the center of a trap from the distribution without the corrections. This can be explained as follows. The repulsive force between the condensate and noncondensate becomes substantial as the number of noncondensate particles increases, surrounding the condensate particles at the center. Consequently, the condensate density is pushed up to the center. The difference is too small to observe within the resolution of the present experiments. This result assures us that the GP equation is applicable to describe the condensate at rather high temperature. It is consistent with the present experiments which can be roughly explained by the solution of the GP equation.

V. SUMMARY AND CONCLUSION

We have given a formulation of QFT for a BEC system in a trap, which is a field theory in a finite region and without spatially translational invariance: the unperturbative representation is established under the assumption that the system is in a condensed stationary phase without a vortex. One can develop a loop expansion to include quantum fluctuation effects. The formulation can be extended straightforwardly to thermal field theory to include thermal fluctuation as well.

The BEC is considered as a spontaneous breakdown of a global phase symmetry in QFT. Then the existence of the NG mode, implied by the Goldstone theorem, is the most crucial to the behavior of the system. We respected the existence of the NG mode in this paper. To do this, we first introduced the zero-energy operator $\hat{a}_0$ in the expansion of the operator field $\hat{\varphi}$ in order to make the canonical commutation relation hold, since the canonical commutation relation is one of the indispensable relations, from which the Goldstone theorem is derived. Note that $\hat{a}_0$ is omitted in the usual Bogoliubov prescription. Next we utilized the loop expansion, because the WT relations, from which the Goldstone theorem follows, are preserved at each level of loop.

Thus our approach is more fundamental than the mean-field approximation (GP equation) and the Bogoliubov approach. One can check the validity of these approximate approaches from our fundamental one. In this paper we calculated only a single-point Green function at one loop (tadpole diagram) to estimate the condensate distribution, but found that the deviation from the result with the GP equation is too small to be observed at present experiments. So our study supports the applicability of GP equation to the present experiments. As a matter of fact, the GP approach is consistent with the experiments. According to our analysis, one can apply the GP equation, surprisingly, up to temperatures very close to the critical one. For our calculation of the one-loop expansion to be valid, we had to confine ourselves to small values of the parameter $g\sqrt{N_{\mathrm{c}}}$. Our analysis suggests that experiments with a rather large value of $g\sqrt{N_{\mathrm{c}}}$ will show

larger deviations, which may be observed at the present experimental resolution.

Although our formulation gives almost the same numerical results as the conventional approaches [22], the appearance of infrared divergence there is of great significance. The divergence certainly brings additional trouble, but is closely related to the presence of the zero-energy mode, without which the theory would not be consistent from the viewpoint of QFT. As was shown above, the divergence can be renormalized solely into the condensate number, and this is the main reason why our results are not different drastically from the others in spite of the divergence.

Our future task is to calculate the two-point Green function (self-energy diagram), which should be related to the one-point function through the WT relation. By doing this, we will be able to clarify more deeply the implication of the renormalization done in this paper, and to predict the energy spectrum of excited particles, affected by quantum and thermal fluctuations.

One interesting possibility is to consider the NG mode as collective coordinates as in [12,13]. Then the unperturbed propagator will be modified, as will our numerical results. A study along these lines will be reported in a future paper.

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APPENDIX: WARD-TAKAHASHI IDENTITY

First, we make a brief review of the derivation of the Ward-Takahashi identity for a general system [8,14]. Consider an infinitesimal transformation for a system of field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$,

$$\hat{\psi}(x) \to \hat{\psi}(x) + \xi \delta\hat{\psi}(x), \tag{A1}$$

where ξ is an infinitesimal parameter. For this transformation, one can find the Noether currents $(\hat{N}_0, \hat{\boldsymbol{N}})$ satisfying

$$\frac{\partial}{\partial t}\hat{N}_0(x) + \boldsymbol{\nabla}\cdot\hat{\boldsymbol{N}}(x) = \delta\hat{\mathcal{L}}(x), \tag{A2}$$

where $\delta\hat{\mathcal{L}}$ is the change of the Lagrangian density induced by the infinitesimal transformation above. The operator

$$\hat{N}(t) \equiv \int d^3x \hat{N}_0(x) \tag{A3}$$

generates the transformation as

$$[\hat{\psi}(x), \hat{N}(t')]\delta(t-t') = i\delta(t-t')\delta\hat{\psi}(x). \tag{A4}$$

It is easy to derive from Eqs. (A2), (A3), and (A4) that

$$\begin{aligned}
&\frac{\partial}{\partial t}\langle\Omega|T[\hat{N}(t)\hat{\psi}(x_1)\cdots\hat{\psi}(x_n)|\Omega\rangle \\
&= \sum_{a=1}^{n} \delta(t-t_a) \\
&\quad \times \langle\Omega|T[\hat{\psi}(x_1)\cdots[\hat{N}(t),\hat{\psi}(x_a)]\cdots\hat{\psi}(x_n)]|\Omega\rangle \\
&\quad + \langle\Omega|T\left[\left(\frac{\partial}{\partial t}\hat{N}(t)\right)\hat{\psi}(x_1)\cdots\hat{\psi}(x_n)\right]|\Omega\rangle \\
&= -i\sum_{a=1}^{n} \delta(t-t_a)\langle\Omega|T[\hat{\psi}(x_1)\cdots\delta\hat{\psi}(x_a)\cdots\hat{\psi}(x_n)|\Omega\rangle \\
&\quad + \int d^3x\langle\Omega|T[\delta\hat{\mathcal{L}}(x)\hat{\psi}(x_1)\cdots\hat{\psi}(x_n)]|\Omega\rangle.
\end{aligned} \tag{A5}$$

Integration with respect to t on both sides leads to

$$\begin{aligned}
&i\hbar\sum_{a=1}^{n}\langle\Omega|T[\hat{\psi}(x_1)\cdots\delta\hat{\psi}(x_a)\cdots\hat{\psi}(x_n)]|\Omega\rangle \\
&= \int d^4x\langle\Omega|T[\delta\hat{\mathcal{L}}(x)\hat{\psi}(x_1)\cdots\hat{\psi}(x_n)]|\Omega\rangle,
\end{aligned} \tag{A6}$$

which is called the Ward-Takahashi identity. Here it is remarked that the surface terms in the t integration vanish only when $\hat{N}$ and $\delta\hat{\mathcal{L}}$ are replaced by $\hat{N} - \langle\Omega|\hat{N}|\Omega\rangle$ and $\delta\hat{\mathcal{L}} - \langle\Omega|\delta\hat{\mathcal{L}}|\Omega\rangle$.

Let us consider the system in Eq. (1). The relevant transformation corresponding to Eq. (A1) is an infinitesimal global phase one, and we have

$$\delta\hat{\psi}(x) = i\hat{\psi}(x). \tag{A7}$$

Then we have the Noether currents from Eq. (A7) as follows:

$$\begin{aligned}
\hat{N}_0 &= -\hat{\psi}^\dagger(x)\hat{\psi}(x), \\
\hat{\boldsymbol{N}} &= \frac{i}{2m}\{[\boldsymbol{\nabla}\hat{\psi}^\dagger(x)]\hat{\psi}(x) - \hat{\psi}^\dagger(x)[\boldsymbol{\nabla}\hat{\psi}(x)]\},
\end{aligned} \tag{A8}$$

and $\delta\hat{\mathcal{L}} = 0$.

When the symmetry is broken spontaneously and therefore the Goldstone mode is present, we need a more subtle treatment. To do this, one intentionally introduces a breaking term in the Lagrangian density [14]. We introduced the explicit breaking term (5), which becomes in the notation of this appendix

$$\varepsilon\Xi(x) = \varepsilon\overline{\epsilon}[e^{-i\theta}v(\boldsymbol{x})\psi(x) + e^{i\theta}v(\boldsymbol{x})\psi^\dagger(x)], \tag{A9}$$

i.e., the Lagrangian density corresponding to S_ε in Eq. (6) is defined by

$$\mathcal{L}_\varepsilon(x) = \mathcal{L}(x) + \varepsilon\Xi(x). \tag{A10}$$

This Lagrangian is not invariant under the phase transformation due to the explicit breaking term (A9). The variation of the Lagrangian density $\mathcal{L}_\varepsilon$ is

$$\delta\hat{\mathcal{L}}_\varepsilon(x)=\varepsilon\,\delta\hat{\Xi}(x)=i[\hat{N}(t),\hat{\Xi}(x)]\neq 0. \tag{A11}$$

Now we can use the WT identity (A6) with Eq. (A11),

$$i\langle\Omega|\,\delta\delta\hat{\Xi}(x)|\Omega\rangle=\int d^4x'\langle\Omega|T[\,\varepsilon\,\delta\hat{\Xi}(x')\,\delta\hat{\Xi}(x)|\Omega\rangle. \tag{A12}$$

The quantities in Eq. (A12) are

$$\delta\hat{\Xi}(x)=i[\hat{N}(t),\hat{\Xi}(x)]=i\overline{\epsilon}[e^{-i\theta}v(\boldsymbol{x})\hat{\psi}(x)-e^{i\theta}v(\boldsymbol{x})\hat{\psi}^\dagger(x)], \tag{A13}$$

$$\begin{aligned}\delta\delta\hat{\Xi}(x)&=i[\hat{N}(t),\delta\hat{\Xi}(x)]\\&=-\overline{\epsilon}[e^{-i\theta}v(\boldsymbol{x})\hat{\psi}(x)+e^{i\theta}v(\boldsymbol{x})\hat{\psi}^\dagger(x)].\end{aligned} \tag{A14}$$

Then we have from Eq. (A12)

$$\begin{aligned}v(\boldsymbol{x})=\frac{i}{2}(\varepsilon\overline{\epsilon})\int d^4x'v(\boldsymbol{x}')[&\langle\Omega|T[\,\hat{\psi}(x)\hat{\psi}^\dagger(x')]|\Omega\rangle\\&+\langle\Omega|T[\,\hat{\psi}^\dagger(x)\hat{\psi}(x')]|\Omega\rangle\\&-e^{-2i\theta}\langle\Omega|T[\,\hat{\psi}(x)\hat{\psi}(x')]|\Omega\rangle\\&-e^{2i\theta}\langle\Omega|T[\,\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')]|\Omega\rangle].\end{aligned} \tag{A15}$$

Let us evaluate Eq. (A15) at the tree level. The field operator $\hat{\psi}$ is divided as follows:

$$\hat{\psi}(x)=e^{i\theta}v_0(\boldsymbol{x})+\hat{\varphi}(x). \tag{A16}$$

Put Eq. (A16) into Eq. (A15), we then get

$$\begin{aligned}v_0(\boldsymbol{x})=\frac{i}{2}(\varepsilon\overline{\epsilon})\int d^4x'v_0(\boldsymbol{x}')[&\langle\Omega_b|T[\,\hat{\varphi}(x)\hat{\varphi}^\dagger(x')]|\Omega_b\rangle+\langle\Omega_b|T[\,\hat{\varphi}^\dagger(x)\hat{\varphi}(x')]|\Omega_b\rangle-e^{-2i\theta}\langle\Omega_b|T[\,\hat{\varphi}(x)\hat{\varphi}(x')]|\Omega_b\rangle\\&-e^{2i\theta}\langle\Omega_b|T[\,\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x')]|\Omega_b\rangle]\\=-\frac{1}{2}(\varepsilon\overline{\epsilon})\int d^4x'v_0(\boldsymbol{x}')&[G_{0,11}(\boldsymbol{x},\boldsymbol{x}';t-t')+G_{0,22}(\boldsymbol{x},\boldsymbol{x}';t-t')-e^{-2i\theta}G_{0,12}(\boldsymbol{x},\boldsymbol{x}';t-t')-e^{2i\theta}G_{0,21}(\boldsymbol{x},\boldsymbol{x}';t-t')]\\=-\frac{1}{2}(\varepsilon\overline{\epsilon})\int\frac{d\omega}{2\pi}\int d^4x'v_0(\boldsymbol{x}')&[G_{0,11}(\boldsymbol{x},\boldsymbol{x}';\omega)+G_{0,22}(\boldsymbol{x},\boldsymbol{x}';\omega)-e^{-2i\theta}G_{0,12}(\boldsymbol{x},\boldsymbol{x}';\omega)-e^{2i\theta}G_{0,21}(\boldsymbol{x},\boldsymbol{x}';\omega)]e^{-i\omega(t-t')}\\=(\varepsilon\overline{\epsilon})\int d^3x'v_0(\boldsymbol{x}')&\sum_{\ell,m,n=0}^{\infty}\frac{1}{E_n}[C_{n\ell}C_{nm}+S_{n\ell}S_{nm}+C_{n\ell}S_{nm}+S_{n\ell}C_{nm}]u_\ell(\boldsymbol{x}')u_m(\boldsymbol{x}),\end{aligned} \tag{A17}$$

where we use Eqs. (44) and (46). At the tree level, v_0 is proportional to u_0:

$$v_0(\boldsymbol{x})=\sqrt{N_c}u_0(\boldsymbol{x}). \tag{A18}$$

Substituting Eq. (A18) into the right hand side of Eq. (A17), we derive

$$\begin{aligned}v_0(\boldsymbol{x})&=(\varepsilon\overline{\epsilon})\sqrt{N_c}\sum_{m,n=0}^{\infty}\frac{1}{E_n}[C_{n0}C_{nm}+S_{n0}S_{nm}+C_{n0}S_{nm}+S_{n0}C_{nm}]u_m(\boldsymbol{x})\\&=(\varepsilon\overline{\epsilon})\sqrt{N_c}\left[\frac{1}{E_0}(C_{00}C_{00}+S_{00}S_{00}+C_{00}S_{00}+S_{00}C_{00})u_0(\boldsymbol{x})+\sum_{m,n=0}^{\infty}{}'\ \frac{1}{E_n}(C_{n0}C_{nm}+S_{n0}S_{nm}+C_{n0}S_{nm}+S_{n0}C_{nm})u_m(\boldsymbol{x})\right]\\&=\sqrt{N_c}[u_0(\boldsymbol{x})+O(\varepsilon^{1/2})],\end{aligned} \tag{A19}$$

where Σ' means summation without $m=n=0$. Finally, we have the correct value for $v_0(\boldsymbol{x})$ in the limit of $\varepsilon\to 0$:

$$v_0(\boldsymbol{x})\to\sqrt{N_c}u_0(\boldsymbol{x})\quad(\text{for }\varepsilon\to 0). \tag{A20}$$

Thus it has been shown that the WT identity is satisfied at the tree level, as it should be. There the NG mode plays a critical role to keep the original symmetry.

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