Stability of the homogeneous Bose-Einstein condensate at large gas parameter

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The properties of the uniform Bose gas are studied within the optimized variational perturbation theory (Gaussian approximation) in a self-consistent way. It is shown that the atomic Bose-Einstein condensate with a repulsive interaction becomes unstable when the gas parameter $\gamma=\rho a^3$ exceeds a critical value $\gamma_{crit}\approx 0.01$. The quantum corrections beyond the Bogoliubov-Popov approximation to the energy density, chemical potential, and pressure in powers of $\sqrt{\gamma}$ expansions are presented.

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I. INTRODUCTION

The long wait after its prediction (more than 70 years) for realization of the Bose-Einstein condensate (BEC) is possibly related to the metastability of the initial Bose gas. In fact, we require first, that an atomic system would stay gaseous and metastable at a very low temperature all the way to the BEC transition, and second, development of cooling and trapping techniques to reach the required regimes of temperature and density [1]. Clearly, without a proper cooling technique, any ordinary atomic gas would transform into a liquid or a solid state at low temperatures, so a metastable state could be created only with low pressure and weak interaction between atoms.

Even once created, the condensate still remains as a fragile and subtle object [2]. The enemies of BEC such as crystallization, disassociation, and three-body recombination may easily destroy it within a very short time. When the sign of interaction (or equivalently of the s-wave scattering length a) is suddenly changed into a negative value, the BEC collapses and then undergoes an explosion in which a substantial fraction of the atoms were blown off (*Bosenova*) [3,4].

Due to the "bad collisions," even an atomic BEC with a repulsive interaction has a limited lifetime. Recently, Cornish *et al.* [5] carried out an ingenious experiment with spin polarized atomic ^{85}Rb. In the experiment, they showed that one could control the strength of interatomic interaction for the BEC by employing the Feshbach resonance method. A very large value of the scattering length ($a\approx 4500$ Å) has been achieved in this experiment, which corresponds to the gas parameter of the condensate to be approximately $\gamma_{\max}\approx 0.01$. This phenomenon has been recently studied by Yin [6] in random phase approximation. The author has shown that when γ exceeds a certain critical value, the molecular excitation energy becomes imaginary and, hence, the atomic BEC is dynamically unstable against molecular formation.

Note also that, the sound attenuation in the quantum spin system $TlCuCl_3$ in magnetic fields where the BEC of magnons take place has been recently observed experimentally by Sherman *et al.* [7].

It is well known that many of the basic properties of the condensate of dilute Bose gases in existing experiments can be described reasonably well using the mean field approximation (MFA), which reduces the problem to the classical Gross-Pitaevskii equation (GPE) [8]. However, fluctuations of the quantum field around the mean field provide corrections which become increasingly important as higher condensate densities (say large γ) are achieved. It is therefore important to understand the effects of quantum field fluctuations especially at large gas parameters.

In the present paper, we study the properties of a homogeneous atomic Bose gas using optimized Gaussian approximation [9]. It has been proven that the corresponding Gaussian effective potential contains one loop, a sum of all daisy and superdaisy graphs of perturbation theory [10] and leading order in $1/N$ expansion.

The first application of the Gaussian variational approach to a uniform BEC was done by Bijlsma and Stoof ten years ago [11]. However, it was pointed out in an excellent review by Andersen that [12] even a modified (by introducing a many body T matrix) Gaussian approximation of Ref. [11] does not satisfy the Hugenholtz-Pines (HP) theorem especially at very low temperatures. This is particularly caused by a long-standing problem encountered in the most of field theoretical approximations: it is impossible to satisfy the HP theorem, namely, making the theory gapless at the same time and maintaining the number of particles with the same value of the chemical potential. In other words, the chemical potential defined by the HP theorem does not coincide with the chemical potential found from the minimization of the thermodynamic potential with respect to the condensate density. Note that, even the T-matrix approximation cannot resolve this problem completely since in this case one gets a "mismatch of approximations," which makes the approach non-self-consistent.

One of the possible solutions of the above mentioned problem has been proposed recently by Yukalov and Kleinert [13]. They have shown that Hartree-Fock approximation (HFA) can be made both conserving and gapless by taking into account two normalization conditions instead of one. Hence, two chemical potentials each for the condensed fraction (μ_0) and the uncondensed fractions (μ_1) should be in-

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troduced to describe the BEC self-consistently.

In the present paper, we reformulate the field theoretical Gaussian approximation following their prescription, and apply this self-consistent approach to investigate the properties of a uniform BEC.

The paper is organized as follows. In Sec. II, we extend the field theoretical approach by implementing the Yukalov-Kleinert prescription. In Sec. III, we calculate the free energy in a Gaussian approximation, and also show its relation to the one-loop and Bogoliubov-Popov approximations (BPA). In the next two sections, we present the procedure of minimization of the free energy. The numerical results and their discussion are presented in Sec. VI. Section VII summarizes the paper.

II. QUANTUM FIELD FORMULATION WITH A YUKALOV-KLEINERT PRESCRIPTION

A grand canonical ensemble of Bose particles with a short range s-wave interaction is governed by the Euclidean action [[12,25]

$$S[\psi,\psi^*]=\int_0^\beta d\tau\int d\mathbf{r}\left\{\psi^*(\tau,\mathbf{r})\left[\partial_\tau-\frac{\nabla^2}{2m}-\mu\right]\psi(\tau,\mathbf{r})+\frac{g}{2}[\psi^*(\tau,\mathbf{r})\psi(\tau,\mathbf{r})]^2\right\}, \tag{1}$$

where $\psi^*(\tau,\mathbf{r})$ is a complex field operator that creates a boson at the position $\mathbf{r}$, μ the chemical potential, g the coupling constant given by $4\pi a/m$, m the atomic mass, and $\beta=1/T$ the inverse of temperature T. The free energy of the system can be determined as

$$\mathcal{F}(\mu)=-T\ln Z, \tag{2}$$

where Z is the functional integral,

$$Z=\int\mathcal{D}\psi\mathcal{D}\psi^*\exp\{-S[\psi,\psi^*]\}, \tag{3}$$

performed all over Bose fields ψ and ψ^* periodic in $\tau\in[0,\beta]$. When the temperature in a Bose system falls below the condensation temperature T_c, breaking of the global $U(1)$ symmetry may be taken into account by the Bogoliubov shift of the field operator,

$$\psi(\tau,\mathbf{r})=v(\tau,\mathbf{r})+\tilde{\psi}(\tau,\mathbf{r}), \tag{4}$$

where $v(\tau,\mathbf{r})$ is the condensate order parameter. In the uniform system $v(\tau,\mathbf{r})$ is a real constant $v(\tau,\mathbf{r})=v$, and $\tilde{\psi}(\tau,\mathbf{r})$ is the field operator of the uncondensed particles satisfying the same Bose commutation relation as $\psi(\tau,\mathbf{r})$. The conservation of particle numbers requires that $\tilde{\psi}(\tau,\mathbf{r})$ has a nonzero momentum component so that

$$\langle\tilde{\psi}\rangle=0, \tag{5}$$

and $\tilde{\psi}$ and v are orthogonal to each other,

$$\int d\mathbf{r}\,\tilde{\psi}(\mathbf{r})v(\mathbf{r})=0. \tag{6}$$

The conservation of quantum numbers (5) can be also rewritten as the quantum conservation condition

$$\langle\hat{\Lambda}\rangle=0 \tag{7}$$

for the self-adjoint operator

$$\hat{\Lambda}\equiv\int d\mathbf{r}[\Lambda(\tau,\mathbf{r})\tilde{\psi}^*(\tau,\mathbf{r})+\Lambda^*(\tau,\mathbf{r})\tilde{\psi}(\tau,\mathbf{r})], \tag{8}$$

where $\Lambda(\tau,\mathbf{r})$ is a complex function [14].

The condensate order parameter v defines the density of condensed particles while $\tilde{\psi}$ defines the density of uncondensed particles as follows:

$$\rho_0=v^2,\quad \rho_1=\langle\tilde{\psi}^*(r)\tilde{\psi}(r)\rangle. \tag{9}$$

Having performed the Bogoliubov shift, one may introduce the grand canonical thermodynamic potential of the system Ω as

$$\Omega(\mu,v)=\mathcal{F}(\mu,v)|_{v=\langle\psi\rangle}. \tag{10}$$

In a stable equilibrium, Ω attains the minimum as follows:

$$\frac{d\Omega(\mu,v)}{dv}=0,\quad \frac{d^2\Omega(\mu,v)}{d^2v}>0. \tag{11}$$

Apart from the HP theorem, the chemical potential should satisfy the normalization condition

$$N=\left\langle\int d\mathbf{r}\,\psi^*(\mathbf{r})\psi(\mathbf{r})\right\rangle, \tag{12}$$

where N is the total number of particles. However, as it was pointed out in the above, the chemical potential corresponding to the minimum of Ω may not correspond to the chemical potential μ determined from the normalization condition.

To overcome these difficulties, Yukalov and Kleinert [13,14] proposed to

(1) Introduce one more normalization condition $N_0=\rho_0 V$, so that for the uniform system

$$N_0+N_1=N,\quad N_1=\left\langle\int d\mathbf{r}\,\tilde{\psi}^*(\mathbf{r})\tilde{\psi}(\mathbf{r})\right\rangle, \tag{13}$$

which simply states that the total number of particles should be equal to the sum of the number of condensed and uncondensed particles.

(2) Introduce two chemical potentials μ_0 and μ_1, for the condensed and the uncondensed fractions, respectively, as well as a Lagrange multiplier Λ to satisfy Eq. (5). The total system chemical potential $\mu=-(\partial\Omega/\partial N)$, is given by

$$\mu=\frac{\mu_0N_0+\mu_1N_1}{N}. \tag{14}$$

These prescriptions lead to the following action:

$$S[\psi,\psi^*] = \int_0^\beta d\tau \int d\mathbf{r}\Big\{ \psi^*(\tau,\mathbf{r})\Big[\partial_\tau - \frac{\nabla^2}{2m}\Big]\psi(\tau,\mathbf{r}) - \mu_1 \tilde{\psi}^*(\tau,\mathbf{r})\tilde{\psi}(\tau,\mathbf{r}) - \mu_0 v^2 - \Lambda\tilde{\psi}(\tau,\mathbf{r}) - \Lambda^*\tilde{\psi}^*(\tau,\mathbf{r}) + \frac{g}{2}[\psi^*(\tau,\mathbf{r})\psi(\tau,\mathbf{r})]^2\Big\}, \tag{15}$$

which should be used in Eq. (3). Further, μ_0 can be determined from the minimum condition Eq. (11), while μ_1 can be determined itself by the requirement of the HP theorem

$$\mu_1 = \Sigma_{11} - \Sigma_{12}, \tag{16}$$

where Σ_{11} and Σ_{12} are the normal and the anomalous self-energies. As to the condensed fraction N_0, it could be found by solving the normalization Eq. (13) where the uncondensed fraction N_1 is given by

$$N_1 = -\left(\frac{\partial\Omega}{\partial\mu_1}\right). \tag{17}$$

III. GAUSSIAN, ONE-LOOP, AND BOGOLIUBOV-POPOV APPROXIMATIONS

In the present section, we show how this scheme can be realized in practice. Substituting Eq. (4) into Eq. (15), one may rewrite the action in powers of v and $\tilde{\psi}$,

$$S = S^{(0)} + S^{(1)} + S^{(2)} + S^{(3)} + S^{(4)},$$

$$S^{(0)} = \int_0^\beta d\tau \int d\mathbf{r}\Big\{ -v^2\mu_0 + \frac{gv^4}{2}\Big\},$$

$$S^{(1)} = \int_0^\beta d\tau \int d\mathbf{r}[gv^3 - \Lambda^* - \Lambda][\tilde{\psi}^* + \tilde{\psi}],$$

$$S^{(2)} = \int_0^\beta d\tau \int d\mathbf{r}\Big\{ \tilde{\psi}^*\Big[\partial_\tau - \frac{\nabla^2}{2m} - \mu_1\Big]\tilde{\psi} + \frac{gv^2}{2}[\tilde{\psi}^*\tilde{\psi}^* + 4\tilde{\psi}^*\tilde{\psi} + \tilde{\psi}\tilde{\psi}]\Big\},$$

$$S^{(3)} = g\int_0^\beta d\tau \int d\mathbf{r}\, v\{\tilde{\psi}^*\tilde{\psi}^*\tilde{\psi} + \tilde{\psi}^*\tilde{\psi}\tilde{\psi}\},$$

$$S^{(4)} = \frac{g}{2}\int_0^\beta d\tau \int d\mathbf{r}\,\tilde{\psi}^*\tilde{\psi}^*\tilde{\psi}\tilde{\psi}. \tag{18}$$

In the following, $S^{(1)}$ will be omitted, since it can be set to zero by an appropriate choice of Λ in order to satisfy Eq. (5).

Now, in accordance with the variational perturbation theory, we add and subtract the following term:

$$S^{(\Sigma)} = \int_0^\beta d\tau \int d\mathbf{r}\Big[\Sigma_{11}\tilde{\psi}^*\tilde{\psi} + \frac{1}{2}\Sigma_{12}(\tilde{\psi}^*\tilde{\psi}^* + \tilde{\psi}\tilde{\psi})\Big], \tag{19}$$

assuming Σ_{11} and Σ_{12} as real constants. Further, we write the quantum fluctuating field $\tilde{\psi}$ in terms of two real fields

$$\tilde{\psi} = \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2), \quad \tilde{\psi}^* = \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2). \tag{20}$$

After some algebraic manipulations [15,16], one can split the action into "classical," "free," and "interaction" parts as follows:

$$S = S_{\mathrm{clas}} + S_{\mathrm{free}} + S_{\mathrm{int}},$$

$$S_{\mathrm{clas}} = V\beta\Big(-v^2\mu_0 + \frac{gv^4}{2}\Big),$$

$$S_{\mathrm{free}} = \frac{1}{2}\int_0^\beta d\tau \int d\mathbf{r}\Big[i\epsilon_{ab}\psi_a\partial_\tau\psi_b + \psi_1\Big(-\frac{\nabla^2}{2m} + X_1\Big)\psi_1 + \psi_2\Big(-\frac{\nabla^2}{2m} + X_2\Big)\psi_2\Big]. \tag{21}$$

$$S_{\mathrm{int}} = S_{\mathrm{int}}^{(2)} + S_{\mathrm{int}}^{(3)} + S_{\mathrm{int}}^{(4)},$$

$$S_{\mathrm{int}}^{(2)} = \frac{1}{2}\int_0^\beta d\tau \int d\mathbf{r}[\psi_1^2(3gv^2 - \Pi_{11}) + \psi_2^2(gv^2 - \Pi_{22})],$$

$$S_{\mathrm{int}}^{(3)} = \frac{g}{\sqrt{2}}\int_0^\beta d\tau \int d\mathbf{r}\, v\psi_1(\psi_1^2 + \psi_2^2),$$

$$S_{\mathrm{int}}^{(4)} = \frac{g}{8}\int_0^\beta d\tau \int d\mathbf{r}(\psi_1^4 + 2\psi_1^2\psi_2^2 + \psi_2^4). \tag{22}$$

Here, $\epsilon_{ab}(a,b=1,2)$ is the antisymmetric tensor in two dimensions with $\epsilon_{12}=1$ and the following notations are introduced:

$$\Pi_{11} = \Sigma_{11} + \Sigma_{12}, \quad \Pi_{22} = \Sigma_{11} - \Sigma_{12},$$

$$X_1 = \Pi_{11} - \mu_1, \quad X_2 = \Pi_{22} - \mu_1. \tag{23}$$

In accordance with Refs. [12,17], Π_{ab} are the components of the 2×2 self-energy matrix.

The free part of the action, S_{free} in Eq. (22) gives rise to a propagator, which can be used in perturbative framework. In a momentum space,

$$\tilde{\psi}_a(\tau,\mathbf{r}) = \frac{1}{\sqrt{\beta V}}\sum_{n=-\infty}^{\infty}\sum_k \tilde{\psi}_a(\omega_n,\mathbf{k})\exp\{i\omega_n\tau + i\mathbf{k}\cdot\mathbf{r}\}, \tag{24}$$

where $\Sigma_k = V\int d\mathbf{k}/(2\pi)^3$, and $\omega_n = 2\pi nT$ is the Matsubara frequency. The propagator is given by

$$G(\omega_n,k)=\frac{1}{\omega_n^2+E_k^2}\begin{pmatrix}\varepsilon_k+X_2 & \omega_n\\ -\omega_n & \varepsilon_k+X_1\end{pmatrix}, \quad (25)$$

with the dispersion relation, $E_k^2=(\varepsilon_k+X_1)(\varepsilon_k+X_2)$ and $\varepsilon_k=k^2/2m$.

With this Green's function using Eqs. (2) and (3), and neglecting terms $S_{\rm int}^{(3)}$ and $S_{\rm int}^{(4)}$, one may get the thermodynamic potential in the one-loop approximation:

$$\Omega^{(1L)}(\mu_0,\mu_1,v)=V\left(-\mu_0v^2+\frac{gv^4}{2}\right)+\frac{1}{2}\sum_k E_k+T\sum_k \ln[1-e^{-\beta E_k}]+\frac{1}{2}[B(3gv^2-\Pi_{11})+A(gv^2-\Pi_{22})], \quad (26)$$

with $\Pi_{11}=3gv^2$ and $\Pi_{22}=gv^2$ (A and B will be given below), so that the last term in square brackets can be dropped. Note that, hereafter we perform explicit summation by Matsubara frequencies (see, e.g., [16]). As to the BPA, it can be obtained by introducing an auxiliary expansion parameter η_{1L} as it was shown by Kleinert [18].

Loop expansion of Ω may be organized by using the propagator $G(\omega_n,\mathbf{k})$ with constraints $X_1=2gv^2$ and $X_2=0$ as illustrated in Ref. [19]. To take into account higher order quantum fluctuations, one has to calculate $\langle S_{\rm int}^{(3)}\rangle$ and $\langle S_{\rm int}^{(4)}\rangle$. Although these quantities cannot be evaluated exactly, they may be estimated in the Gaussian approximation [26], where for the homogeneous system,

$$\langle S_{\rm int}^{(3)}\rangle=0,$$

$$\langle\psi_a^2\rangle= G_{aa}(r-r')|_{r\to r'}\equiv G_{aa}(0),$$

$$\langle\psi_1^2\psi_2^2\rangle=\langle\psi_1^2\rangle\langle\psi_2^2\rangle,\quad \langle\psi_a^4\rangle=3G_{aa}^2(0),$$

$$G_{11}(0)=\frac{1}{V\beta}\sum_{n=-\infty}^{\infty}\sum_k G_{11}(\omega_n,\mathbf{k})=V^{-1}B,$$

$$G_{22}(0)=V^{-1}A. \quad (27)$$

Finally, combining Eqs. (26) and (27), we get the following expressions for the thermodynamic potential:

$$\Omega(X_1,X_2,v,\mu_0,\mu_1)=V\left(-\mu_0v^2+\frac{gv^4}{2}\right)+\frac{1}{2}\sum_k E_k+T\sum_k \ln[1-e^{-\beta E_k}]+\frac{1}{2}[B(3gv^2-\Pi_{11})+A(gv^2-\Pi_{22})]+\frac{g\rho}{8N}[3(A^2+B^2)+2AB], \quad (28)$$

where

$$A\equiv\sum_k\frac{\varepsilon_k+X_1}{E_k}\left[\frac{1}{2}+\frac{1}{\exp(\beta E_k)-1}\right],$$

$$B\equiv\sum_k\frac{\varepsilon_k+X_2}{E_k}\left[\frac{1}{2}+\frac{1}{\exp(\beta E_k)-1}\right]. \quad (29)$$

The free energy in Eq. (28) is supposed to have all the information about the system. Particularly taking it's derivative with respect to μ_1, one gets the expression for the uncondensed fraction N_1 as follows:

$$N_1=-\left(\frac{\partial\Omega}{\partial\mu_1}\right)=\frac{1}{2}\left\{A+B-(3gv^2-\Pi_{11})B'-(gv^2-\Pi_{22})A'-\frac{g}{2V}[(3A+B)A'+(3B+A)B']\right\}, \quad (30)$$

where $A'=\partial A/\partial\mu_1$ and $B'=\partial B/\partial\mu_1$. Note that the same expression for the uncondensed fraction could be obtained in an alternative way as

$$\rho_1=\frac{N_1}{V}=\langle\tilde{\psi}^*\tilde{\psi}\rangle=\frac{1}{Z}\int\mathcal{D}\tilde{\psi}\mathcal{D}\tilde{\psi}^*\exp\{-S[\psi,\psi^*]\}\tilde{\psi}^*\tilde{\psi}. \quad (31)$$

IV. GAP EQUATIONS AND THE THERMODYNAMIC POTENTIAL AT $T=0$

In this section, the variational parameters Π_{11} and Π_{22} will be determined using the principle of minimal sensitivity [9]. From Eqs. (28) and (29), the gap equations may be found.

$$\frac{\partial\Omega(X_1,X_2,v,\mu_0,\mu_1)}{\partial X_1}=\frac{1}{2}\{A_1'[gv^2-\mu_1-X_2]+B_1'[3gv^2-\mu_1-X_1]+g[A_1'(3A+B)+B_1'(3B+A)]/2V\}=0, \quad (32)$$

and

$$\frac{\partial\Omega(X_1,X_2,v,\mu_0,\mu_1)}{\partial X_2}=\frac{1}{2}\{A_2'[gv^2-\mu_1-X_2]+B_2'[3gv^2-\mu_1-X_1]+g[A_2'(3A+B)+B_2'(3B+A)]/2V\}=0, \quad (33)$$

where

$$A_1' \equiv \frac{\partial A}{\partial X_1} = \frac{1}{4}\sum_k \frac{1}{E_k} = \frac{\partial B}{\partial X_2} \equiv B_2',$$

$$A_2' \equiv \frac{\partial A}{\partial X_2} = -\frac{1}{4}\sum_k \frac{(\varepsilon_k + X_1)^2}{E_k^3},$$

$$B_1' \equiv \frac{\partial B}{\partial X_1} = -\frac{1}{4}\sum_k \frac{(\varepsilon_k + X_2)^2}{E_k^3}. \tag{34}$$

Above, we have two equations (32) and (33) with respect to three unknown quantities $\{X_1, X_2, \mu_1\}$. An additional equation is supplied from the relation between the chemical potential and the self-energies given by the HP theorem; so, from Eqs. (16) and (23), one can immediately conclude $X_2 = 0$, and, hence, in the long wavelength limit $(k \to 0)$, the quasiparticle energy E_k behaves as ck (with $c = \sqrt{X_1/2m}$) thus being gapless, as expected. With this constraint, the gap equations may be simplified as

$$2X_1 + \mu_1 - 5gv^2 - \frac{11}{8}\frac{g}{V}I_{1,1}(X_1) = 0, \tag{35}$$

$$I_{0,1}(X_1)[3gv^2 - \mu_1 - X_1] - I_{-2,-1}(X_1)[gv^2 - \mu_1] + \frac{gI_{1,1}(X_1)}{8V}[5I_{0,1}(X_1) + I_{-2,-1}(X_1)] = 0, \tag{36}$$

and Eq. (30) as

$$N_1 = \frac{1}{8}I_{1,1}(X_1) + \frac{[I_{0,1}(X_1) - 2I_{-2,-1}(X_1)][8Vgv^2 - gI_{1,1}(X_1) - 8V\mu_1]}{128Vm}. \tag{37}$$

Here, the following dimensionless integral

$$I_{i,j}(X_1) = \sum_k \frac{\varepsilon_k^i m^{j-i}}{E_k^j} \tag{38}$$

is introduced. Their explicit expressions and the relations between them evaluated in dimensional regularization are presented in the Appendix of Ref. [12]. In particular,

$$I_{1,1}(X_1) = \frac{V(2mX_1)^{3/2}}{3\pi^2} = 2B|_{X_2=0} = -4A|_{X_2=0},$$

$$\frac{dI_{1,1}(X_1)}{dX_1} = -\frac{I_{0,1}(X_1)}{m}. \tag{39}$$

Note that Eqs. (36) and (37) include $I_{-2,-1}(X_1)$, which is infrared divergent, $I_{-2,-1}(X_1) \sim 1/\epsilon + \ln \kappa^2/mX_1$ (with $\epsilon \to 0$). Below we show that this integral will be canceled exactly. In fact, eliminating X_1 from Eq. (35) as

$$X_1 = -\frac{\mu_1}{2} + \frac{5gv^2}{2} + \frac{11gI_{1,1}(X_1)}{16V}, \tag{40}$$

and substituting it into Eq. (36), one observes that the latter is factorized as follows:

$$[I_{0,1}(X_1) - 2I_{-2,-1}(X_1)][gI_{1,1}(X_1) - 8Vgv^2 + 8V\mu_1] = 0. \tag{41}$$

Due to the cancellation of the integrals which are divergent in the infrared, the gap equations and the free energy include only ultraviolet divergent integrals. As it was shown by Braaten and Nieto [19], in such cases the explicit renormalization of chemical potentials and coupling constant is unnecessary within dimensional regularization.

Thus, from the last two equations, we find the formal solutions of the gap equations

$$X_1 = 2gv^2 + \frac{3g}{4V}I_{1,1}(X_1), \tag{42}$$

$$\mu_1 = gv^2 - \frac{g}{8V}I_{1,1}(X_1). \tag{43}$$

We denote these optimum values of X_1 and μ_1 by $\bar{X}_1$ and $\bar{\mu}_1$, respectively, which are explicitly dependent on v^2. Now, comparing Eqs. (37) and (41), one can easily see that only the first term in Eq. (37) survives.

$$N_1 = \frac{1}{8}I_{1,1}(X_1). \tag{44}$$

Now, inserting these formal solutions into Eq. (28) and using the relations between the integrals, Eq. (39), gives the following form for Ω:

$$\Omega(\bar{X}_1, v, \mu_0) = V\left(-\mu_0 v^2 + \frac{gv^4}{2}\right) + \frac{m}{2}I_{0,-1}(\bar{X}_1) - \frac{11gI_{1,1}^2(\bar{X}_1)}{128V}, \tag{45}$$

where

$$I_{0,-1}(\bar{X}_1) = \frac{1}{m}\sum_k \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + \bar{X}_1} = \frac{2\sqrt{2}V(m\bar{X}_1)^{5/2}}{15m^2\pi^2}. \tag{46}$$

In particular, neglecting in Eq. (45) the last term gives the one-loop result as follows:

$$\Omega(\bar{X}_1, v, \mu_0)|_{\bar{X}_1 = 2gv^2} = \Omega^{(1L)}(\mu_0, \mu_1, v)|_{\mu_1 = gv^2}, \tag{47}$$

presented in the previous section. In the stable equilibrium, the grand canonical potential reaches the global minimum as a function of v.

$$\frac{d\Omega(\bar{X}_1, v, \mu_0)}{dn_0} = V\rho(-\mu_0 + g\rho n_0) + \frac{X_1' I_{1,1}(\bar{X}_1)}{4}\left[1 + \frac{11gI_{0,1}(X_1)}{16Vm}\right] = 0, \tag{48}$$

where $n_0 = v^2/\rho = N_0/N$ and $X_1' = (d\bar{X}_1/dn_0)$. Note that the same equation could be obtained from the original Eq. (28) as

$$\frac{d\Omega(X_1,X_2,v,\mu_0,\mu_1)}{dn_0}=\frac{\partial\Omega}{\partial n_0}+\left(\frac{\partial\Omega}{\partial\mu_1}\right)\frac{\partial\mu_1}{\partial n_0}+\left(\frac{\partial\Omega}{\partial X_1}\right)\frac{\partial X_1}{\partial n_0}+\left(\frac{\partial\Omega}{\partial X_2}\right)\frac{\partial X_2}{\partial n_0}=0, \quad (49)$$

where the last two terms may be omitted due to the gap equations (32) and (33), and the factor in the second term is related to N_1 by Eq. (17).

Clearly, the optimal value of v^2, i.e., $\bar{v}^2$ defined by Eq. (48), should correspond to the normalization condition in Eq. (13) (constraint) as follows:

$$\bar{v}^2+\rho_1(\bar{X}_1)=\bar{v}^2+\frac{I_{1,1}(\bar{X}_1)}{8V}=\rho, \quad (50)$$

which may be considered as a nonlinear equation with respect to the c number $\bar{v}^2$ with a fixed ρ and $\bar{X}_1(\bar{v}^2)$.

Strictly speaking, $\bar{v}^2$ must be determined from Eq. (48) as a function of μ_0, and after substituting it into Eq. (50), the latter should be solved with respect to μ_0. However, this would be a rather complicated way, since Eq. (48) is a highly nonlinear equation. On the other hand, one may assume that $\bar{v}^2$ is known as a solution of Eq. (50) and μ_0 could be extracted from Eq. (48).

Following this strategy, we obtain

$$\bar{\mu}_0=g\rho\bar{n}_0+\frac{X_1' I_{1,1}(\bar{X}_1)}{4V\rho}\left[1+\frac{11gI_{0,1}(\bar{X}_1)}{16Vm}\right], \quad (51)$$

in particular, neglecting the second term in square brackets and taking into account $X_1^{1L}=2g\rho n_0$, we have μ_0 for the one-loop approximation

$$\mu_0^{1L}=g\rho\left[n_0+\frac{I_{1,1}(\bar{X}_1^{1L})}{2V\rho}\right]. \quad (52)$$

Further simplification, by introducing an auxiliary expansion parameter η_{1L} as in Ref. [18], gives μ_0 for the BPA

$$\mu_0^{BP}=g\rho\left[1-\frac{gI_{0,1}(X_1=2g\rho)}{2Vm}\right]. \quad (53)$$

As to the total system chemical potential μ, it follows from Eqs. (13) and (14) as

$$\mu=\bar{\mu}_1\bar{n}_1+\bar{\mu}_0\bar{n}_0, \quad (54)$$

where $\bar{n}_1=1-\bar{n}_0$, and $\bar{\mu}_1$ and $\bar{\mu}_0$ are given by Eqs. (43) and (51), respectively. Now, substituting Eq. (51) into Eq. (45), one may obtain the pressure as $P=-\Omega/V$.

$$P=\frac{1}{2}gn_0^2\rho^2+\frac{1}{4V}[n_0\bar{X}_1' I_{1,1}(\bar{X}_1)-2mI_{0,-1}(\bar{X}_1)]+\frac{11gI_{1,1}(\bar{X}_1)}{128mV^2}[2n_0\bar{X}_1' I_{0,1}(\bar{X}_1)+mI_{1,1}(\bar{X}_1)]. \quad (55)$$

The ground state energy density of the BEC, $\mathcal{E}$, may be obtained by a well known formula $\mathcal{E}=(\Omega+\mu N)/V$. This may be easily done by rewriting the term $\mu_0 v^2 V$ in Eq. (45) as $\mu_0 v^2 V=\mu N-\mu_1 n_1 N$ [which follows from Eq. (52)] and using Eq. (43) as follows:

$$\Omega(\bar{X}_1,\bar{v})=-\mu N+\frac{V\rho^2 g\bar{n}_0^2}{2}+\frac{m}{2}I_{0,-1}(\bar{X}_1)+\frac{\rho g\bar{n}_0}{8}I_{1,1}(\bar{X}_1)-\frac{13g}{128V}I_{1,1}^2(\bar{X}_1). \quad (56)$$

Now, one may immediately obtain

$$\mathcal{E}=\frac{g\bar{v}^4}{2}+\frac{m}{2V}I_{0,-1}(\bar{X}_1)+\frac{g\bar{v}^2}{8V}I_{1,1}(\bar{X}_1)-\frac{13g}{128V^2}I_{1,1}^2(\bar{X}_1), \quad (57)$$

and

$$\mathcal{E}^{BP}=\frac{g\rho^2}{2}+\left.\frac{m}{2V}I_{0,-1}(X_1)\right|_{X_1=2g\rho}, \quad (58)$$

for the Gaussian and Bogoliubov-Popov approximations, respectively.

It is well known that in the BPA, the normal (Σ_{11}) and the anomalous self-energies (Σ_{12}) are rather simple [18].

$$\Sigma_{11}^{BP}=2g\rho, \quad \Sigma_{12}^{BP}=g\rho. \quad (59)$$

In the Gaussian approximation using Eqs. (23), (42), and (43), one obtains

$$\Sigma_{11}=\frac{X_1}{2}+\mu_1=2gv^2+\frac{g}{4V}I_{1,1}(X_1),$$

$$\Sigma_{12}=\frac{X_1}{2}=gv^2+\frac{3g}{8V}I_{1,1}(X_1), \quad (60)$$

which can be further simplified at the stationary point as

$$\bar{\Sigma}_{11}=2g\rho,$$

$$\bar{\Sigma}_{12}=g\rho(1+2\bar{n}_1). \quad (61)$$

Clearly, neglecting the uncondensed fraction $\bar{n}_1$ in the last equation, we recover the Bogoliubov-Popov approximation, Eq. (59). The dimensionless sound velocity defined as $c=\lim_{k\to 0}E_k/k=\sqrt{\bar{X}_1/2m}$ is simply related to Σ_{12} as

$$c^2=\frac{\bar{\Sigma}_{12}}{m}. \quad (62)$$

V. SOLUTIONS TO THE GAP EQUATIONS

In this section, we analyze possible solutions to the gap equation (42), which can be written as

$$X_1=2gv^2+\frac{g(mX_1)^{(3/2)}}{\sqrt{2}\pi^2}. \quad (63)$$

Before solving this equation, we emphasize that in accordance with the general principle of the variational Gaussian

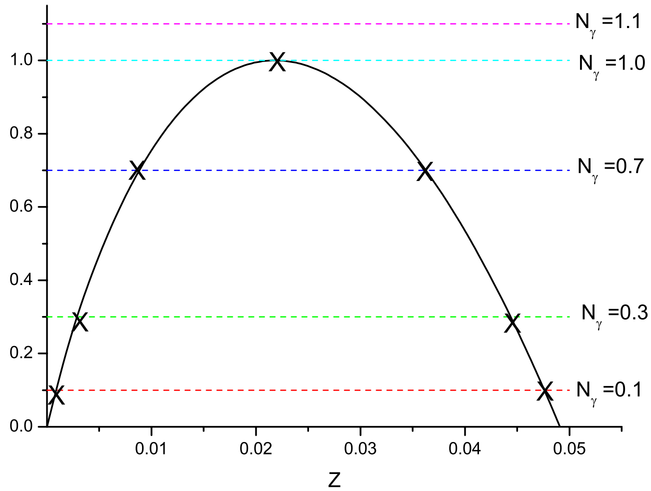

FIG. 1. (Color online) Graphical solution of the gap equation (64). The solid curve represents the right-hand side, and the dashed straight lines represent the left-hand side of the equation for N_γ=0.1;0.3;0.7;1.0;1.1 from the bottom to the top, respectively.

approximation, the constraint in Eq. (50) and the procedure of minimization of the free energy with respect to v^2 may be imposed only after finding an explicit expression for $X_1 \equiv X_1(v^2)$ as a function of v^2, which can be done by solving Eq. (63) analytically. Note that when the second term on the right-hand side of Eq. (63) is neglected, one obtains a well known result of the one-loop approximation, $X_1^{1L}=2gv^2$, and further, assuming here $v^2=\rho$ gives the self-energy for BPA, $X_1^{BP}=2\rho g$.

In general, Eq. (63) can be rewritten in a dimensionless form

$$N_\gamma = \frac{432Z}{\pi} - 3456\left(\frac{Z}{\pi}\right)^{3/2}, \tag{64}$$

where the following dimensionless quantities were introduced:

$$Z = \frac{\gamma X_1}{2g\rho}, \quad N_\gamma = \frac{432\gamma n_0}{\pi}, \tag{65}$$

with $\gamma=a^3\rho$ as the gas parameter. Analysis shows that Eq. (64) has no real positive solution when $N_\gamma > 1$. This is illustrated in Fig. 1 where the solid curve presents the right-hand side, and the dashed straight lines present the left-hand side of Eq. (64) for N_γ=0.1;0.3;0.7;1.0;1.1 from the bottom to the top, respectively. It is seen that when $N_\gamma < 1$, there are two different solutions (denoted as crosses in Fig. 1) which overlap at $N_\gamma=1$ and $Z=\pi/144=0.0218$, and then disappear. This is one of our main results confirming that there is a critical value of γ, or more exactly, a critical value of $N_0\gamma/N$, which controls the stability of the uniform Bose condensate at $T=0$. When $N_\gamma=432n_0\gamma/\pi$ exceeds unity, $(N_\gamma>1)$, X_1 and hence the self-energy becomes complex, and the BEC will be unstable.

Differentiating Eq. (64) by N_γ and solving with respect to dZ/dN_γ, one obtains

$$Z' \equiv \frac{dZ}{dN_\gamma} = \frac{\pi^{3/2}}{432(\sqrt{\pi}-12\sqrt{Z})}, \tag{66}$$

which is singular at $Z=\pi/144$, i.e., at $N_\gamma=1$. Thus, at the critical point, $N_\gamma=1$,

$$\lim_{N_\gamma\to 1} \frac{\partial X_1}{\partial n_0} = \infty, \tag{67}$$

and hence, at this point the chemical potential of the condensate μ_0 in Eq. (51), which is responsible for the thermodynamical stability of the system, has a singularity.

For $N_\gamma \le 1$, the solutions are given as [27]

$$Z_1 = \frac{\pi}{576}[2c_1\cos(c_2)+3] \approx \frac{\pi}{64} - \frac{\pi}{216}N_\gamma + O(N_\gamma^2), \tag{68}$$

$$Z_2 = \frac{\pi}{576}[-c_1\cos(c_2)+\sqrt{3}c_1\sin(c_2)+3] \tag{69}$$

$$\approx \frac{\pi N_\gamma}{432} + \frac{\sqrt{3}\pi N_\gamma^{3/2}}{1944} + \frac{\pi N_\gamma^2}{1944} + O(N_\gamma^{5/2}), \tag{70}$$

where $c_1=\sqrt{9-8N_\gamma}$, $c_2=\arccos\{[27-36N_\gamma+8N_\gamma^2]/c_1^3\}/3$.

It is understood that only the second solution, Z_2, is a physical one, since for the case of $Z=Z_1$ the self-energy X_1 is irregular at $\gamma\to 0$. Moreover, only $Z=Z_2$ corresponds to the minimum of the thermodynamic potential, $(\partial^2\Omega/\partial^2 X_1)|_{z=z_2} > 0$. Thus, we conclude, $\bar{X}_1=2g\rho Z/\gamma$ with $Z=Z_2$. In particular, taking into account the first term in the expansion of Z_2 in Eq. (70), one obtains $\bar{X}_1 \approx 2g\rho n_0 = \bar{X}_1^{1L}$ as expected.

VI. RESULTS AND DISCUSSIONS

Expansion for small γ. The starting point of our numerical calculations is Eq. (63), which can be rewritten as

$$1 - \bar{n}_0 - \frac{8Z^{3/2}(\bar{n}_0)}{3\gamma\sqrt{\pi}} = 0. \tag{71}$$

Before analyzing this nonlinear equation we note that the majority of experiments with ultracold trapped gases deal with weakly interacting atoms, so that γ is very small, i.e., $\gamma \sim 10^{-9},\ldots,10^{-4}$. Thus, to obtain a low-density expansion of physical quantities, one may search for the solutions of Eq. (71) in a power series of $\sqrt{\gamma}$ to get

$$\bar{n}_1 = 1 - \bar{n}_0 = \frac{8}{3}\left(\frac{\gamma}{\pi}\right)^{1/2} + \frac{64}{3}\frac{\gamma}{\pi} + \frac{1792}{9}\left(\frac{\gamma}{\pi}\right)^{3/2} + O(\gamma^2). \tag{72}$$

Clearly, the first term corresponds to the Bogoliubov approximation, while the others may be considered as quantum corrections to this approximation. Note also that the above expansion Eq. (72) is the same as the one obtained in the modified Hartree-Fock-Bogoliubov (HFB) approximation [13]. Now, using Eqs. (43), (51), (55), (57), (61), (62), and

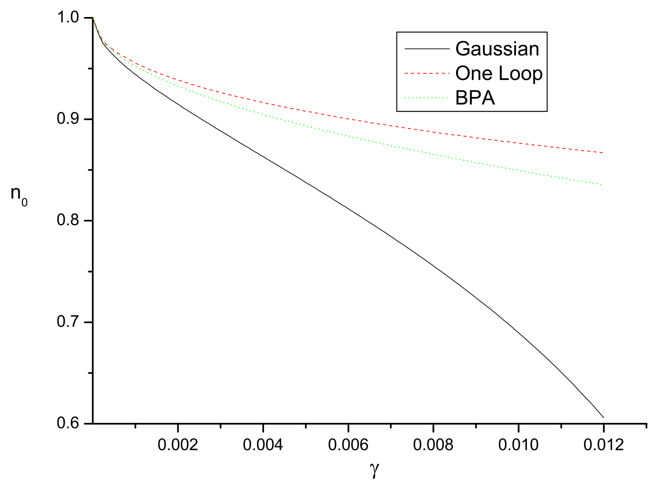

FIG. 2. (Color online) Condensate fraction $n_0 = n_0(\gamma)$ as a function of $\gamma = \rho a^3$. Solid (black), dashed (red), and dot-dashed (green) curves correspond to the Gaussian, the one-loop, and the Bogoliubov-Popov approximations.

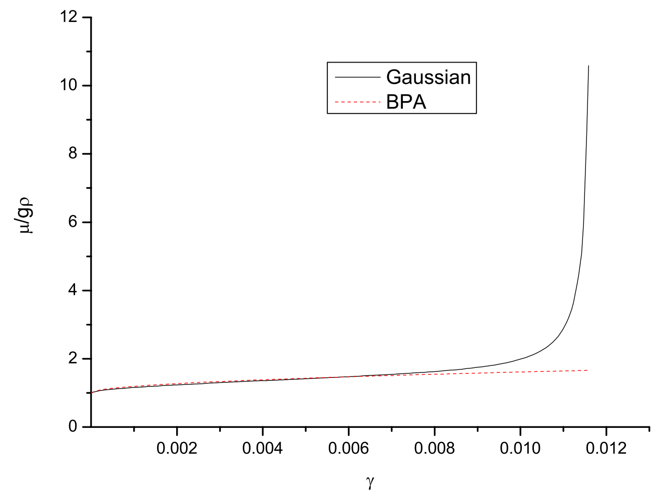

FIG. 3. (Color online) The chemical potential in the Gaussian (solid line, black) and Bogoliubov-Popov approximations (dashed line, red).

(72) we obtain the following low-density expansions for the energy density, chemical potentials, self energies, the sound velocity, and the pressure:

$$\mathcal{E} \approx g\rho^2 \left\{ 1 + \frac{128\sqrt{\gamma}}{\sqrt{\pi}} + \frac{128\gamma}{9\pi} \right\},$$

$$\mu_0 \approx g\rho \left\{ 1 + \frac{32\sqrt{\gamma}}{3\sqrt{\pi}} + \frac{224\gamma}{3\pi} \right\}, \tag{73}$$

$$\mu_1 \approx g\rho \left\{ 1 - \frac{16\sqrt{\gamma}}{3\sqrt{\pi}} - \frac{128\gamma}{3\pi} \right\},$$

$$\Sigma_{12} \approx g\rho \left\{ 1 + \frac{16\sqrt{\gamma}}{3\sqrt{\pi}} + \frac{128\gamma}{3\pi} \right\}, \tag{74}$$

$$c^2 \approx \frac{g\rho}{m} \left\{ 1 + \frac{16\sqrt{\gamma}}{3\sqrt{\pi}} + \frac{128\gamma}{3\pi} \right\},$$

$$P \approx \frac{g\rho^2}{2} \left\{ 1 + \frac{64\sqrt{\gamma}}{5\sqrt{\pi}} + \frac{64\gamma}{3\pi} \right\}, \tag{75}$$

which are in good agreement with BPA [20].

Critical density and exact solutions. In order to discuss exact solutions of Eq. (71), we first establish the boundary for γ, which is related to the critical value of N_γ found in the previous section. This may be evaluated directly by substituting $N_\gamma = 1$, $Z = \pi/144$ into Eq. (71), which immediately gives $\gamma_{\text{crit}} = 5\pi/1296 \approx 0.012120$. It is interesting to observe that when γ approaches this critical value, the condensed fraction remains still large, $\lim_{\gamma \to \gamma_{\text{crit}}} \bar{n}_0(\gamma) = \pi/432\gamma_{\text{crit}} = 3/5 = 0.6$, but the condensate as a whole becomes unstable.

Figure 2 presents the condensate fraction $\bar{n}_0(\gamma)$ in the Gaussian (solid line), the one-loop (dotted line), and the Bogoliubov-Popov approximations. It is seen that due to the quantum fluctuations the condensed fraction decreases faster (with increasing γ) in the Gaussian approximation than in BPA.

The chemical potential $\mu = \mu_0 n_0 + \mu_1 n_1$ is presented in Fig. 3. One may observe that, in the Gaussian approximation it varies slowly with increasing γ, almost coinciding with that for the BPA. However, when γ approaches the critical value $\gamma_{\text{crit}} = 0.012$ it starts to increase very fast since in this region, when $N_\gamma \to 1$, X_1' in Eq. (51) becomes very large and so does μ_0. Bearing in mind that the chemical potential is the energy needed to add (or extract) one more particle to (or from) the system, one may interpret this effect as a particle number saturation of the condensed particles. In other words, when γ (or more exactly N_γ) reaches the critical value, the number of condensed atoms N_0 cannot be further increased, since it will lead to a dynamical instability of the BEC. The pressure defined by Eq. (55) is positive in the region $\gamma < \gamma_{\text{crit}}$, but near the critical point $\gamma \sim \gamma_{\text{crit}}$ it becomes negative and small, as expected. Note that at this point the energy density, the self-energies, and the sound velocity remain finite, since corresponding expressions Eqs. (57)–(62) do not include X_1' explicitly.

Now we consider the possible origin of the instability found above. It is well known that [21] the BEC is an effect of the exchange coupling, which leads to an effective attraction between atoms forcing them to accumulate in a single state. However, when the density (or scattering length) reaches a critical value this effective attraction makes the condensate collapse.

Another possible reason is a three-body recombination of condensed atoms. Although there is no explicit three-body interaction in our starting Lagrangian, it was shown that [22], at $T \to 0$, the repulsive two-body interaction leads to a three-body recombination with the rate constant $\alpha_{\text{rec}} \propto a^4$ and, hence, the three-body recombination becomes very significant for a large scattering length, i.e., a large γ. This seems to be one of the main reasons for the fact that a stable condensate with a large gas parameter is inaccessible experimentally. When γ exceeds the critical value, the atoms start to combine into molecules and the condensate may undergo phase transition into a solid or a liquid state.

VII. SUMMARY

In conclusion, we have developed a new Bosonic self-consistent variational perturbation theory, which can be made the starting point for systematic expansion procedure [23]. We have shown that taking into account two normalization conditions at the same time solves the old outstanding problem of Bose systems making variational perturbation theory both conserving and gapless.

Studying the properties of a system of uniform Bose gas at zero temperature with repulsive interaction both analytically and numerically, we have found that in this system there is a dynamical parameter $N_\gamma \propto n_0 \rho a^3$ which controls the stability of the Bose condensate. When this parameter remains smaller than the critical value the phonon spectrum is purely real and the excitations have infinite lifetimes. On the contrary, when N_γ exceeds the critical value the condensate becomes unstable, in a similar fashion to the BEC with an attractive interaction. Note that this phenomena has not been be obtained in the loop expansion method before.

It would be quite interesting to study the dependence of critical N_γ on temperature. It was discovered long ago by Bethe [24] that the inelastic cross section, which tends to destroy the condensate, varies as $1/k$ (called the 1/velocity law), and hence the bad collisions can be surprisingly large near zero temperature. Thus, the temperature dependence of the critical N_γ seems not to be trivial. This work is in progress.

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[25] In the remainder of the paper, we set $\hbar = 1$ and $k_B = 1$ for convenience.
[26] The details of the calculations will be given in a separate paper.
[27] See, e.g., http://www.1728.com/cubic2.htm, about solving cubic equations for the case when Cardano's formula does not work.