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

Abdulla Rakhimov\textsuperscript{a,b}, Chul Koo Kim\textsuperscript{c}, Sang-Hoon Kim\textsuperscript{d} and Jae Hyung Yee\textsuperscript{e}

\textsuperscript{a} Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, R.O. Korea
\textsuperscript{b} Institute of Nuclear Physics, Tashkent 702132, Uzbekistan
\textsuperscript{c} Division of Liberal Arts and Sciences, Mokpo National Maritime University, Mokpo 530-729, R.O. Korea

The properties of the uniform Bose gas is studied within the optimized variational perturbation theory (Gaussian approximation) in a self-consistent way. It is shown that the atomic BEC with a repulsive interaction becomes unstable when the gas parameter \(\gamma = \rho a_s^3\) exceeds a critical value \(\gamma_{\text{crit}} \approx 0.01\). 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 it's prediction (more than 70 years) for realization of the Bose-Einstein condensate (BEC) is possibly related to the meta-stability of the initial Bose gas. In fact, we require first, an atomic system would stay gaseous and meta-stable at very low temperature all the way to the BEC transition, and secondly, 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 undergo into a liquid or a solid state at low temperatures, so a meta-stable 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 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 \([\text{Bosenova}\ ] [3, 4]\).

Due to the "bad collisions", even an atomic BEC with a repulsive interaction has a limited life time. Recently, Cornish \emph{et. al.} \([5]\) carried out an ingenious experiment with spin polarized atomic \(^{85}\text{Rb}\). 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 \((a \approx 4500\text{A})\) has been achieved in this experiment, which corresponds to the gas parameter of the condensate to be about \(\gamma_{\text{max}} \approx 0.01\). This phenomenon has been recently studied by Yin \([6]\) in Random Phase Approximation. The author has shown that when \(\gamma\) exceeds a certain critical value the molecular excitation energy becomes imaginary and, hence, the atomic BEC is dynamically unstable against molecular formation.

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) \([7]\). However, fluctuations of the quantum field around the mean field provide corrections which become increasingly important as higher condensate densities (say large \(\gamma\)) 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 \([8]\). It has been proven that the corresponding Gaussian effective potential contains one loop, sum of all daisy and superdaisy graphs of perturbation theory \([9]\) 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 \([10]\). However, it was pointed out in excellent review by Andersen that even a modified (by introducing many body T-matrix) Gaussian approximation of Ref. \([10]\) does not satisfy the Hugenholtz-Pines (H-P) 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 H-P 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 H-P 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 "mismatch of approximations" which makes the approach as non self-consistent.

One of the possible solutions of the above mentioned problem has been proposed recently by Yukalov \([12]\). He has shown that Hartree-Fock approximation (HFA) can be made both conserving and gapless by taking into ac-
II. QUANTUM FIELD FORMULATION WITH YUKALOV PRESCRIPTION

A grand canonical ensemble of Bose particles with a short range s-wave interaction is governed by the Euclidan action \[ S[\psi, \psi^*] = \int_0^\beta d\tau \int d\vec{r} \{ \psi^*(\tau, r)[\partial_\tau - \frac{\nabla^2}{2m} - \mu] \psi(\tau, r) + \frac{g}{2}[\psi^*(\tau, r)\psi(\tau, r)]^2 \} , \] where \( \psi^*(\tau, r) \) is a complex field operator that creates a boson at the position \( \vec{r} \), \( \mu \) 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 \[ F(\mu) = -T \ln Z, \] where \( Z \) is the functional integral, \[ Z = \int D\psi D\psi^* \exp\{-S[\psi, \psi^*]\}, \] performed all over Bose fields \( \psi \) and \( \psi^* \) periodic in \( \tau \in [0, \beta] \). When the temperature in a Bose system falls below the condensation temperature \( T_c \), breaking of the \( U(1) \) gauge symmetry may be taken into account by the Bogoliubov shift of the field operator, \[ \psi(\tau, r) = v(\tau, r) + \tilde{\psi}(\tau, r), \] where \( v(\tau, r) \) is the condensate order parameter. In the uniform system \( v(\tau, r) \) is a real constant, \( v(\tau, r) = v \), \( \tilde{\psi}(\tau, r) \) is the field operator of the uncondensed particles satisfying the same Bose commutation relation as \( \psi(\tau, r) \). The conservation of particle numbers requires that \( \tilde{\psi}(\tau, r) \) has non-zero momentum component so that \[ \langle \tilde{\psi} \rangle = 0, \] and \( \tilde{\psi} \) and \( v \) are orthogonal each other \[ \int d\vec{r} \tilde{\psi}(r)v(r) = 0. \] The condensate order parameter \( v \) defines the density of condensed particles while \( \tilde{\psi} \) defines the density of uncondensed particles: \[ \rho_0 = v^2, \quad \rho_1 = \langle \tilde{\psi}^*(r)\tilde{\psi}(r) \rangle. \] Having performed the Bogoliubov shift, one may introduce the grand canonical thermodynamic potential of the system \( \Omega \) as \[ \Omega(\mu, v) = F(\mu, \nu)|_{\nu=\langle \psi \rangle}. \] In a stable equilibrium, \( \Omega \) attains the minimum: \[ \frac{d\Omega(\mu, v)}{dv} = 0, \quad \frac{d^2\Omega(\mu, v)}{dv^2} > 0. \] Apart from the H-P theorem, the chemical potential should satisfy the normalization condition \[ N = \langle \int d\vec{r} \tilde{\psi}^*(r)\tilde{\psi}(r) \rangle, \] 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 \( \Omega \) may not correspond to the chemical potential \( \mu \) determined from the normalization condition.

To overcome these difficulties, Yukalov [12] proposed to

- Introduce one more normalization condition \( N_0 = \rho_0 V \). So that for the uniform system \[ N_0 + N_1 = N, \quad N_1 = \langle \int d\vec{r} \tilde{\psi}^*(r)\tilde{\psi}(r) \rangle, \] which simply states that the total number of particles should be equal to the sum of the number of condensed and uncondensed particles.
- Introduce two chemical potentials \( \mu_0 \) and \( \mu_1 \), for the condensed and the uncondensed fractions respectively as well as a Lagrange multiplier \( \Lambda \) to satisfy the Eq. \[ \mu = \frac{\mu_0 N_0 + \mu_1 N_1}{N}. \] These prescriptions lead to the following action, \[ S[\psi, \psi^*] = \int_0^\beta d\tau \int d\vec{r} \{ \psi^*(\tau, r)[\partial_\tau - \frac{\nabla^2}{2m}] \psi(\tau, r) - \mu_1 \tilde{\psi}^*(\tau, r)\tilde{\psi}(\tau, r) - \frac{\mu_0 v^2}{2} - \Lambda \tilde{\psi}(\tau, r) - \Lambda^* \tilde{\psi}^*(\tau, r) + \frac{g}{2}[\psi^*(\tau, r)\psi(\tau, r)]^2 \}, \] which should be used in Eq. \[ \psi \]. Further, \( \mu_0 \) can be determined from the minimum condition Eq. \[ \Omega \], while \( \mu_1 \) itself by the requirement of H-P theorem \[ \mu_1 = \Sigma_{11} - \Sigma_{12}, \]
where \( \Sigma_{11} \) and \( \Sigma_{12} \) are the normal and the anomalous self-energies. As to the condensed fraction \( N_0 \), it could be found by solving the normalization Eq. 11 where the uncondensed fraction \( N_1 \) is given by

\[
N_1 = -\left( \frac{\partial\Omega}{\partial\mu_1} \right). \tag{15}
\]

### III. Gaussian, One-Loop and Bogoliubov-Popov Approximations

In the present section, we show how this scheme can be realized in practice. Substituting Eq. 11 into Eq. 13, one may rewrite the action in powers of \( v \) and \( \tilde{\psi} \),

\[
S = S^{(0)} + S^{(1)} + S^{(2)} + S^{(3)} + S^{(4)}.
\]

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

\[
S^{(1)} = \int_0^\beta d\tau \int d\vec{r}\{[\psi^* - \nabla^2/2m - \mu_1]\tilde{\psi}
+ \frac{gv^2}{2}[\psi^* \tilde{\psi}^* + 4\tilde{\psi}^* \tilde{\psi} + \tilde{\psi} \psi]\},
\]

\[
S^{(2)} = g \int_0^\beta d\tau \int d\vec{r}\{\psi^* \tilde{\psi}^* \tilde{\psi} + \psi \tilde{\psi} \psi^*\},
\]

\[
S^{(3)} = \frac{g}{2} \int_0^\beta d\tau \int d\vec{r}\tilde{\psi} \psi \tilde{\psi} \psi^*.
\]

\[
S^{(4)} = \frac{g}{2} \int_0^\beta d\tau \int d\vec{r}\tilde{\psi} \psi \tilde{\psi} \psi^* \tilde{\psi} \psi^*.
\]

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

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

\[
S^{(5)} = \int_0^\beta d\tau \int d\vec{r}\left[\Sigma_{11}\tilde{\psi}^* \psi + \frac{1}{2}\Sigma_{12}(\tilde{\psi}^* \tilde{\psi}^* + \psi \psi^*)\right]. \tag{17}
\]

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

\[
\tilde{\psi} = \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2), \quad \tilde{\psi}^* = \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2). \tag{18}
\]

After some algebraic manipulations 14, 15, one can split the action into “classical”, “free”, and “interaction” parts:

\[
S = S_{\text{cl}} + S_{\text{free}} + S_{\text{int}}.
\]

\[
S_{\text{cl}} = V\beta(-v^2\mu_0 + \frac{gv^4}{2}),
\]

\[
S_{\text{free}} = \frac{1}{2} \int_0^\beta d\tau \int d\vec{r} \left[ i\epsilon_{ab}\psi_a \partial_r \psi_b + \psi_1(-\nabla^2/2m + X_1)\psi_1
+ \psi_2(-\nabla^2/2m + X_2)\psi_2 \right]. \tag{19}
\]

\[
S_{\text{int}} = S^{(2)}_{\text{int}} + S^{(3)}_{\text{int}} + S^{(4)}_{\text{int}}.
\]

\[
S^{(2)}_{\text{int}} = \frac{1}{2} \int_0^\beta d\tau \int d\vec{r} \left[ \psi_1^2(3gv^2 - \Pi_{11}) + \psi_2^2(gv^2 - \Pi_{22}) \right],
\]

\[
S^{(3)}_{\text{int}} = g \int_0^\beta d\tau \int d\vec{r} \psi_1(\psi_1^2 + \psi_2^2),
\]

\[
S^{(4)}_{\text{int}} = \frac{g}{2} \int_0^\beta d\tau \int d\vec{r} \left[ \tilde{\psi}^* \psi_1^2 + \tilde{\psi} \psi_2^2 + \tilde{\psi} \psi_2 \psi_1^2 \right]. \tag{20}
\]

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

\[
\Pi_{11} = \Sigma_{11} + \Sigma_{12}, \quad \Pi_{22} = \Sigma_{11} - \Sigma_{12}, \quad X_1 = \Pi_{11} - \mu_1, \quad X_2 = \Pi_{22} - \mu_1. \tag{21}
\]

In accordance with Refs. 11, 16, \( \Pi_{ab} \) are the components of the 2 \times 2 self-energy matrix.

The free part of the action, \( S_{\text{free}} \) in Eq. (20), gives rise to a propagator, which can be used in perturbative framework. In a momentum space,

\[
\tilde{\psi}_a(\tau, r) = \frac{1}{\sqrt{2\beta v^2}} \sum_{n=-\infty}^{\infty} \sum_{k} \tilde{\psi}_n(\omega_n, \vec{k}) \exp(i\omega_n \tau + ik\vec{r}), \tag{22}
\]

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

\[
G(\omega_n, k) = \frac{1}{\omega_n^2 + E_k^2} \begin{pmatrix} \varepsilon_k + X_2 & \omega_n \\ -\omega_n & \varepsilon_k + X_1 \end{pmatrix}, \tag{23}
\]

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

With this Green’s function using Eqs. (24) and (25), and neglecting terms \( S^{(3)}_{\text{int}} \) and \( S^{(4)}_{\text{int}} \), one may get the thermodynamic potential in the one loop approximation:

\[
\Omega^{(1L)}(\mu_0, \mu_1, v) = V \left( -\mu_0 v^2 + \frac{gv^4}{2} \right)
+ \frac{1}{2} \sum_k E_k + \frac{g}{2} \sum_k \ln[1 - e^{-\beta E_k}]
+ \frac{1}{2} \left( B(3gv^2 - \Pi_{11}) + A(gv^2 - \Pi_{22}) \right), \tag{24}
\]

with \( \Pi_{11} = 3gv^2 \) and \( \Pi_{22} = gv^2 \) ( \( A \) and \( B \) will be given below), so that the last term in square bracket can be
dropped. Note that, hereafter we perform explicit summation by Matsubara frequencies (see e.g. [15]). As to the BPA, it can be obtained by introducing an auxiliary expansion parameter $\eta_{1L}$ as it was shown by Kleinert [17].

Loop expansion of $\Omega$ may be organized by using the propagator $G(\omega_n, \vec{k})$ with constraints $X_1 = 2g v^2$ and $X_2 = 0$ as illustrated in Ref. [18]. To take into account higher order quantum fluctuations, one has to calculate $\langle S_{\text{int}}^{(3)} \rangle$ and $\langle S_{\text{int}}^{(4)} \rangle$. Although these quantities can not be evaluated exactly, they may be estimated in the Gaussian approximation [23], where for the homogeneous system:

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

$$\langle \psi_{\alpha}^2 \rangle = G_{\alpha\alpha}(r-r'), \quad \langle \psi_{\alpha}^4 \rangle = 3G_{\alpha\alpha}^2(0),$$

$$G_{11}(0) = \frac{1}{V^2} \sum_{\omega_n \to \infty} \sum_k G_{11}(\omega_n, \vec{k}) = V^{-1}B,$$

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

Finally, combining Eqs. (24) and (25), we get the following expressions for the thermodynamic potential:

$$\Omega(X_1, X_2, v, \mu_0, \mu_1) = V(-\mu_0 v^2 + \frac{g v^4}{2})$$

$$+ \frac{1}{2} \sum_k E_k + T \sum_k \ln[1 - e^{-\beta E_k}]$$

$$+ \frac{1}{2} \left[ B(3g v^2 - \Pi_{11}) + A(g v^2 - \Pi_{22}) \right]$$

$$+ \frac{g}{8N} [3(A^2 + B^2) + 2AB],$$

where

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

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

The free energy in Eq. (26) is supposed to have all the information about the system. Particularly taking it’s derivative with respect to $\mu_1$, one gets the expression for the uncondensed fraction $N_1$:

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

$$= \frac{1}{2} \left[ A + B - (3g v^2 - \Pi_{11})B' - (g v^2 - \Pi_{22})A' \right]$$

$$- \frac{g}{2V} [(3A + B)A' + (3B + A)B'],$$

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

$$\rho_1 = \frac{N_1}{V} = \langle \hat{\psi}^{\dagger} \hat{\psi} \rangle = \frac{1}{Z} \int \mathcal{D}\hat{\psi} \mathcal{D}\hat{\psi}^{\dagger} \exp \{-S[\psi, \psi^{\dagger}]\} \hat{\psi}^{\dagger} \hat{\psi}$$

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

In this section, the variational parameters $\Pi_{11}$ and $\Pi_{22}$ will be determined using the principle of minimal sensitivity [8]. From Eqs. (20) and (24), the gap equations may be found:

$$\frac{\partial \Omega(X_1, X_2, v, \mu_0, \mu_1)}{\partial X_1} = 0$$

$$= \frac{1}{2} \left\{ A_1'[gv^2 - \mu_1 - X_2] + B_1'[3gv^2 - \mu_1 - X_1] \right\}$$

$$+ g[A_1'(3A + B) + B_1'(3B + A)]/2V = 0,$$

and

$$\frac{\partial \Omega(X_1, X_2, v, \mu_0, \mu_1)}{\partial X_2} = 0$$

$$= \frac{1}{2} \left\{ A_2'[gv^2 - \mu_1 - X_2] + B_2'[3gv^2 - \mu_1 - X_1] \right\}$$

$$+ g[A_2'(3A + B) + B_2'(3B + A)]/2V = 0,$$

where

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

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

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

Above, we have two equations (30) and (31) 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 H-P theorem. So, from Eqs. (13) and (21), one can immediately conclude $X_2 = 0$, and, hence, in the long wavelength limit ($k \rightarrow 0$), 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

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

$$I_{0,1}(X_1)[3gv^2 - \mu_1 - X_1] - I_{-2,-1}(X_1)[g v^2 - \mu_1]$$

$$+ \frac{g}{8V} [5I_{0,1}(X_1) + I_{-2,-1}(X_1)] = 0,$$

and Eq. (28) as

$$N_1 = \frac{1}{8} J_{1,1}(X_1)$$

$$+ \frac{J_{0,1}(X_1) - 2I_{-2,-1}(X_1)}{128V m} [8g v^2 - g I_{1,1}(X_1) - 8V \mu_1].$$

Here, the following dimensionless integral

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

is introduced. Their explicit expressions and the relations between them evaluated in dimensional regularization are
presented in the Appendix of Ref. [11]. In particular, \( I_{1,1}(X_1) = \frac{V(2mX_1)\rho^2}{\pi^2} = 2B|X_2=0 = -4A|X_2=0, \) \( \frac{dI_{1,1}(X_1)}{dX_1} = \frac{I_{0,1}(X_1)}{m}. \) (37) Note that Eqs. (34) and (35) 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. (33) as
\[
X_1 = \frac{-\mu_1}{2} + \frac{5g\rho^2}{2} + \frac{11gI_{1,1}(X_1)}{16V}, \] (38) and substituting it into Eq. (33), one observes that the latter is factorized:
\[
[I_{0,1}(X_1) - 2I_{-2,-1}(X_1)]gI_{1,1}(X_1) = 8Vg\rho^2 + 8V\mu_1 = 0. \] (39) Finally, from the last two equations, we find the formal solutions of the gap equations
\[
X_1 = 2g\rho^2 + \frac{3g}{4V}I_{1,1}(X_1), \] (40) \[
\mu_1 = g\rho^2 - \frac{g}{8V}I_{1,1}(X_1). \] (41) We denote these optimum values of \( X_1 \) and \( \mu_1 \) by \( \bar{X}_1 \) and \( \bar{\mu}_1, \) respectively, which are explicitly dependent on \( v^2. \) Now, comparing Eqs. (35) and (39), one can easily see that only the first term in Eq. (35) survives
\[
N_1 = \frac{1}{8}I_{1,1}(X_1). \] (42) Now, inserting these formal solutions into Eq. (29) and using the relations between the integrals, Eq. (37), gives the following form for \( \Omega \)
\[
\Omega(\bar{X}_1, v, \mu_0) = V(-\mu_0v^2 + \frac{g\rho^2}{2} + \frac{m}{2}I_{0,-1}(X_1)) - \frac{11gI_{1,1}^2(\bar{X}_1)}{128V}, \] (43)
where
\[
I_{0,-1}(X_1) = \frac{1}{m} \sum_k \sqrt{\varepsilon_k - \varepsilon_0 + X_1} = \frac{2\sqrt{V}(m\bar{X}_1)^{5/2}}{15m^2\pi^2}. \] (44) In particular, neglecting in Eq. (43) the last term gives the one-loop result:
\[
\Omega(\bar{X}_1, v, \mu_0)|_{\bar{X}_1 = 2g\rho^2} = \Omega^{(1L)}(\mu_0, \mu_1, v)|_{\mu_1 = g\rho^2}. \] (45) presented in the previous section. In the stable equilibrium, the grand canonical potential reaches the global minimum as a function of \( v : \)
\[
\frac{d\Omega}{d\mu_0} = V\rho(-\mu_0 + g\rho n_0) + \frac{X_1^2I_{1,1}(\bar{X}_1)}{4} + \frac{11gI_{0,1}(X_1)}{16V_{m}} = 0 \] (46) where \( n_0 = \rho^2/\rho = N_0/N \) and \( X_1' = (d\bar{X}_1/dn_0). \) Note that the same equation could be obtained from the original equation (26) as:
\[
\frac{d\Omega}{d\mu_0} = \frac{\partial \Omega}{\partial \mu_1} \frac{\partial \mu_1}{\partial \bar{X}_1} + \frac{\partial \Omega}{\partial X_1} \frac{\partial X_1}{\partial \bar{X}_1} + \frac{\partial \Omega}{\partial X_2} \frac{\partial X_2}{\partial \bar{X}_1} = 0, \] (47) where the last two terms may be omitted due to the gap Eqs. (30) and (31), and the factor in the second term is related to \( N_1 \) by (15). Clearly, the optimal value of \( \rho^2, \) i.e. \( \bar{\rho}^2 \) defined by Eq. (48), should correspond to the normalization condition in Eq. (11) (constraint):
\[
\bar{\rho}^2 + \rho_1(\bar{X}_1) = \bar{\rho}^2 + \frac{I_{1,1}(\bar{X}_1)}{8V} = \rho, \] (48) which may be considered as a nonlinear equation with respect to the c-number \( \bar{\rho}^2 \) with a fixed \( \rho \) and \( \bar{X}_1(\bar{\rho}^2). \) Strictly speaking, \( \bar{\rho}^2 \) must be determined from Eq. (46) as a function of \( \mu_0, \) and after substituting it into Eq. (48), the latter should be solved with respect to \( \mu_0. \) However, this would be a rather complicated way, since Eq. (46) is a highly nonlinear equation. On the other hand, one may assume that \( \bar{\rho}^2 \) is known as a solution of Eq. (48) and \( \mu_0 \) could be extracted from Eq. (46). Following this strategy, we obtain
\[
\bar{\mu}_0 = g\rho n_0 + \frac{X_1^2I_{1,1}(\bar{X}_1)}{4V\rho} \left[ 1 + \frac{11gI_{0,1}(\bar{X}_1)}{16V_{m}} \right], \] (49) in particular, neglecting the second term in square brackets and taking into account \( X_1^{1L} = 2g\rho n_0, \) we have \( \mu_0 \) for the one-loop approximation
\[
\mu_0^{1L} = g\rho \left[ n_0 + \frac{I_{1,1}(X_1^{1L})}{2V^{1/2}} \right]. \] (50) Further simplification, by introducing an auxiliary expansion parameter \( \eta_1, \) as in Ref. [17], gives \( \mu_0 \) for the BPA
\[
\mu_0^{BP} = g\rho \left[ 1 - \frac{gI_{0,1}(X_1) - 2g\rho}{2V_{m}} \right]. \] (51) As to the total system chemical potential \( \mu, \) it follows from Eqs. (11) and (12) as
\[
\mu = \bar{\mu}_1 + \bar{\mu}_0 n_0, \] (52) where \( \bar{\mu}_1 = 1 - \bar{n}_0, \) and \( \bar{\mu}_0 \) and \( \bar{\mu}_0 \) are given by Eqs. (11) and (49), respectively. Now, substituting (49) into (13), one may obtain the pressure as \( P = -\Omega/V \)
\[
P = \frac{1}{2}g\rho^2 n_0^2 + \frac{1}{4V}[n_0X_1^2I_{1,1}(\bar{X}_1) - 2mI_{0,-1}(\bar{X}_1)] + \frac{11gI_{0,1}(\bar{X}_1)}{128m^2V^2}[2n_0X_1^2I_{0,1}(X_1) + mI_{1,1}(X_1)]. \] (53) 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 \( \mu_0\bar{\rho}^2 V \) in
Eq. (43) as \( \mu_0 v^2 V = \mu N - \mu_1 n_1 N \) (which follows from Eq. (50) and using Eq. (41):

\[
\Omega(\tilde{X}_1, \tilde{\varphi}) = -\mu N + \frac{V^2 \tilde{g} n_0^2}{2} + \frac{m}{2} I_{0,-1}(\tilde{X}_1) + \frac{g}{8} I_{1,1}(\tilde{X}_1) - \frac{13g}{128V^2} I_{1,1}(\tilde{X}_1).
\]

Now, one may immediately obtain

\[
\mathcal{E} = \frac{g v^2}{2} + \frac{m}{2V} I_{0,-1}(\tilde{X}_1) + \frac{g}{8} I_{1,1}(\tilde{X}_1) - \frac{13g}{128V^2} I_{1,1}(\tilde{X}_1),
\]

and

\[
\mathcal{E}^{\text{BP}} = \frac{g v^2}{2} + \frac{m}{2V} I_{0,-1}(X_1)|_{X_1=2g\rho},
\]

for the Gaussian and Bogoliubov - Popov approximations respectively.

It is well known that in the BPA, the normal (\( \Sigma_{11} \)) and the anomalous self-energies (\( \Sigma_{12} \)) are rather simple [17]:

\[
\Sigma_{11}^{\text{BP}} = 2g\rho, \quad \Sigma_{12}^{\text{BP}} = g\rho.
\]

In the Gaussian approximation using Eqs. (21), (40), and (41), one obtains

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

\[
\Sigma_{12} = \frac{X_1}{2} = g v^2 + \frac{3g}{8V} I_{1,1}(X_1),
\]

which can be further simplified at the stationary point as

\[
\Sigma_{11} = 2g\rho, \quad \Sigma_{12} = g\rho(1 + 2\tilde{n}_1).
\]

Clearly, neglecting the uncondensed fraction \( \tilde{n}_1 \) in the last equation, we recover the Bogoliubov - Popov approximation. (57). The dimensionless sound velocity defined as \( c = \lim_{k \to 0} E_k / k = \sqrt{\tilde{X}_1 / 2m} \) is simply related to \( \Sigma_{12} \) as

\[
c^2 = \frac{\tilde{\Sigma}_{12}}{m}.
\]

V. SOLUTIONS TO THE GAP EQUATIONS

In this section, we analyse possible solutions to the gap equation (40) which can be written as

\[
X_1 = 2g v^2 + \frac{g(mX_1)^{(3/2)}}{\sqrt{2\pi}}.
\]

Before solving this equation, we emphasize that in accordance with the general principle of the variational Gaussian approximation, the constraint in Eq. (48) 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. (61) analytically. Note that when the second term on the RHS of Eq. (61) is neglected, one obtains a well known result of the one-loop approximation: \( X_1^{(1)} = 2g v^2 \), and further, assuming here \( v^2 = \rho \) gives the self-energy for BPA: \( V_{BP} = 2g\rho \).

In general, the Eq. (61) can be rewritten in a dimensionless form

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

where the following dimensionless quantities were introduced

\[
Z = \gamma X_1 / 2g\rho, \quad N_\gamma = \frac{432\gamma n_0}{\pi},
\]

with \( \gamma = a^3/\rho \) is the gas parameter. Analysis shows that Eq. (62) has no real positive solution when \( N_\gamma > 1 \). This is illustrated in Fig. 1 where the solid curve presents RHS, and the dashed straight lines present LHS of Eq. (62) for \( N_\gamma = 0.1; 0.3; 0.7; 1.0; 1.1 \) 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 \( \gamma \), or more exactly critical value of \( N_\gamma/\gamma \) which controls the stability of the uniform Bose condensate at \( T = 0 \). When \( N_\gamma = 432\gamma n_0/\pi \) exceeds unity, \( N_\gamma > 1 \), \( X_1 \) and hence the self-energy becomes complex, and the BEC will be unstable.

Differentiating Eq. (62) by \( N_\gamma \) and solving with respect to \( dZ/dN_\gamma \), one obtains:

\[
Z' = \frac{dZ}{dN_\gamma} = -\frac{\pi^{3/2}}{432(\pi - 12\sqrt{Z})},
\]

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

\[
\lim_{N_\gamma \to 1} \frac{\partial X_1}{\partial n_0} = \infty,
\]

and hence, at this point the chemical potential of the condensate \( \mu_0 \) in Eq. (49), which is responsible for the thermodynamical stability of the system, has a singularity.

For \( N_\gamma \leq 1 \), the solutions are given as [20]

\[
Z_1 = \frac{\pi}{576} [2c_1 \cos(c_2) + 3]
\]

\[
\approx \frac{\pi}{64} - \frac{\pi N_{\gamma}}{216} + O(N_{\gamma}^2),
\]

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

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

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

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,
for the solutions of Eq. (69) in power series of density expansion of physical quantities, one may search to deal with weakly interacting atoms, so that the majority of experiments with ultracold trapped gases 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. (69) in power series of\(\sqrt{\gamma}\) to get

\[
\bar{n}_1 = 1 - \bar{n}_0 = \frac{8}{3} \left(\frac{\gamma}{\pi}\right)^{1/2} + \frac{64}{3} \frac{\gamma}{\pi} + O(\gamma^{3/2}).
\]

(70)

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. (70) is exactly the same as the one obtained in the modified Hartree-Fock Bogoliubov (HFB) approximation. Now, using Eqs. (61), (69), (65), (59), (60) and (70) we obtain the following low density expansions for the energy density, chemical potentials, self energies, the sound velocity and the pressure:

\[
E \approx \gamma \rho \left\{1 + \frac{128 \sqrt{\gamma}}{9 \pi} + \frac{128 \gamma}{9 \pi}\right\}, \quad \mu_0 \approx g \rho \left\{1 + \frac{32 \sqrt{\gamma}}{3 \pi} + \frac{24 \gamma}{3 \pi}\right\}.
\]

(71)

VI. RESULTS AND DISCUSSIONS

Expansion for small \(\gamma\). The starting point of our numerical calculations is the Eq. (61), which can be rewritten as

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

(69)

Before analyzing this nonlinear equation we note that the majority of experiments with ultracold trapped gases deal with weakly interacting atoms, so that \(\gamma\) 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. (69) in power series of \(\sqrt{\gamma}\) to get

\[
\bar{n}_1 = 1 - \bar{n}_0 = \frac{8}{3} \left(\frac{\gamma}{\pi}\right)^{1/2} + \frac{64}{3} \frac{\gamma}{\pi} + O(\gamma^{3/2}).
\]

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. (70) is exactly the same as the one obtained in the modified Hartree-Fock Bogoliubov (HFB) approximation. Now, using Eqs. (61), (69), (65), (59), (60) and (70) we obtain the following low density expansions for the energy density, chemical potentials, self energies, the sound velocity and the pressure:

\[
E \approx \gamma \rho \left\{1 + \frac{128 \sqrt{\gamma}}{9 \pi} + \frac{128 \gamma}{9 \pi}\right\}, \quad \mu_0 \approx g \rho \left\{1 + \frac{32 \sqrt{\gamma}}{3 \pi} + \frac{24 \gamma}{3 \pi}\right\}.
\]

(71)

Critical density and exact solutions. In order to discuss exact solutions of the equation, (69), we first establish the boundary for \(\gamma\) which is related to the critical value of \(\gamma_c\) found in the previous section. This may be evaluated directly by substituting \(\gamma_c = 1, Z = \pi/144\) into Eq. (69), which immediately gives \(\gamma_c = 5\pi/1296 \approx 0.012120\). It is interesting to observe that when \(\gamma\) approaches this critical value, the condensed fraction remains still large, \(\lim_{\gamma \to \gamma_c} \bar{n}(\gamma) = \pi/432\gamma_c = 3/5 = 0.6\) but the condensate as a whole become unstable.

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

The chemical potential \(\mu \approx \mu_0 + \mu_1 n_1\) is presented in Fig. 3. One may observe that, in the Gaussian approximation it varies slowly with increasing \(\gamma\), almost coinciding with that for the BPA. However, when \(\gamma\) approaches the critical value \(\gamma_{crit} = 0.012\) it starts to increase very fast in this region, when \(\gamma \to \gamma_{crit}\) in Eq. (49) becomes very large and so does \(\mu_0\). 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 \(\gamma\) (or more exactly \(\gamma_{crit}\)) 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. (53) 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 sound velocity remain finite, since corresponding expressions Eqs. (55)-(60) do not include \( X'_1 \) explicitly.

Now we consider 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 3 body interaction in our starting Lagrangian, it was shown that [21], at \( T \to 0 \), the repulsive two body interaction leads to a three body recombination with the rate constant \( a_{\text{rec}} \propto a^4 \) and, hence, the three body recombination becomes very significant for a large scattering length i.e. large \( \gamma \). This seems to be one of the main reasons for the fact that a stable condensate with large gas parameter is inaccessible experimentally. When \( \gamma \) 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.

FIG. 3: The chemical potential in the Gaussian (solid line) and Bogoliubov-Popov approximations.

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 [22]. 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 \( N_\gamma \propto n_0 a^3 \) 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 \( N_\gamma \) exceeds the critical value the condensate becomes unstable, in similar fashion to the BEC with an attractive interaction. Note that this phenomena cannot be obtained in ordinary perturbative framework.

It would be quite interesting to study the dependence of critical \( N_\gamma \) on temperature. It was discovered long ago by Bethe [23] that the inelastic cross section, which tends to destroy the condensate, varies as \( 1/k \), (called as 1/velocity law), and hence the bad collisions can be surprisingly large near zero temperature. Thus, the temperature dependence of the critical \( N_\gamma \) seems not to be trivial. This work is on progress.

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