The equation of state of one-dimensional Gross-Pitaevskii equation

T. B. Prayitno

Physics Department, Faculty of Mathematics and Natural Science, Universitas Negeri Jakarta, Jl. Pemuda Rawamangun 13220, Indonesia

E-mail: trunk_.002@unj.ac.id

Abstract. We have constructed the equation of state of one-dimensional Gross-Pitaevskii equation by benefiting from the formulation of a single macroscopic particle partition function and then modeling \( N \) undistinguishable macroscopic particles in canonical ensemble. This macroscopic particle, in which two or more atoms include, is literally a condensate that can be observed as an assembly in the system. In this case, we suppose all condensates are confined in the anisotropic parabolic trap and interaction between two condensates can be ignored by applying semi infinite cigar-shaped trap. It is also shown that the equation of state is indeed an ideal gas with the new thermodynamic interpretation of volume and pressure. Moreover, even though our resulting partition function was portrayed as a sum of exponential functions, we prove that the series is indeed convergent.

1. Introduction

The phenomenon of Bose-Einstein condensation (BEC) has driven physicists to establish the new possibilities in order to utilize the condensed Bose gas. To produce the condensed Bose gas, one only has to cool down several atoms, such as alkali atoms [1, 2], below its specific critical temperature until the atomic waves overlap each other [3, 4]. It means that all atoms will occupy the lowest energy where some of them are condensed. Appropriate mathematical tools to characterize the nature of Bose gas in the very low temperature are of the most interest of this case. It has been noted that some authors have explored theoretically the properties of Bose gas, such as the soliton solution [5, 6, 7, 8, 9, 10], the propagation of atom laser wave [11, 12, 13, 14, 15, 16, 17], etc, by solving the Gross-Pitaevskii equation (GPE) which describes the dynamics of condensate or atom laser beam.

In thermodynamics, the property of gas can be understood by formulating the equation of state which provides the mathematical relation of two or more the thermodynamic quantities. The above equation is usually obtained by initially expressing the appropriate partition function which the assemblies can exchange both matter and energy. However, the problem to derive the partition function emerges in the nonlinear case since it is needed some assumptions and conditions. Nevertheless, in fact, in the case of BEC we have two options in order to deal with thermodynamic case by focusing on the particles or the condensates. In the previous papers, some authors proposed the grand canonical partition function to achieve some thermodynamic properties associated with \( N \) bosons confined by three-dimensional anisotropic harmonic trap [18, 19, 20, 21], for other similar discussions see also [22, 23]. They concerned with \( N \) weakly interacting particles by proposing a new variable thermodynamic quantity, namely harmonic
volume, which replaces the role of real volume. In contrast to them, in order to achieve the thermodynamic quantities we consider the $N$ noninteracting condensates, each of which is represented by the GPE, to formulate the canonical partition function by solving the GPE to obtain the energy levels. In our opinion, the most possible way to achieve the partition function simply is to consider the GPE as a macroscopic quantum oscillator since the trapping potential can be reduced to the harmonic potential. Here, we adopt the idea by allowing the definition of harmonic volume since we also cannot find the available real volume. By pursuing our previous work, we offer the simplest way to attain the partition function by applying the canonical ensemble for $N$ noninteracting condensates confined by the anisotropic harmonic trap. This model allows that a condensate may be treated as a macroscopic oscillator whose energy states are corrected on condition that the nonlinearity is considered as a small term. The derivation of the energy states, which were obtained by employing the time-independent perturbation theory, were proposed by Kivshar et al. [24], but we corrected the formulation in our previous paper where we only differ in the negative sign [25]. This textbook-like treatment generates a new perspective of the nonlinear modes presence like quantum mechanics version. In this paper, we present how to use the providing partition function to acquire the equation of state which relates to the pressure, volume and temperature. Besides, we also provide the other quantity, namely, the internal energy and heat capacity.

In the second section, we will be acquainting the canonical partition function of single condensate built by only considering the energy levels of macroscopic quantum oscillator, from which we extend for $N$ noninteracting condensates. The convergence of the partition function is also explored by means of representing suitable function in the nonlinear term. In addition, we also introduce a new definition related to volume since the real volume is not provided in the partition function. We present in practice in section three how to derive the equation of state in the simplest way like in the textbook of statistical mechanics, as well as the internal energy and heat capacity. To convince us the validity of relation, we also prove that the thermodynamic relations are still hold. We close our work in section four by giving the conclusions.

2. Model of $N$ noninteracting condensates partition function

We start by initially considering the one-dimensional GPE

$$i \frac{\psi}{\partial t} + \frac{\partial^2 \psi}{\partial z^2} - z^2 \psi + \sigma |\psi|^2 \psi = 0,$$

(1)

where the wave function $\psi$ propagates in $z$ direction and $\sigma$ denotes the very small parameter in which the $s$ wave scattering length has been absorbed, so $\sigma$ can be negative or positive. It has been derived in our previous work by following up the former work of Kivshar et al. [24] the canonical partition function of the above equation of a single condensate [25]

$$Z = \sum_{n=0}^{\infty} e^{\beta \left( \hbar \omega_z (n+1/2) - \sigma |B_n|^2 V_{nnn} \right) V_{nnn} / \hbar} \sqrt{m \omega_z \sqrt{\lambda / \hbar}}.$$

(2)

where we set $\lambda = \omega_z^2 / \omega_\perp^2 << 1$ in the cigar-shaped trap and define $\beta = -1 / kT$. Here, we refer $\omega_z$ and $\omega_\perp$ to the longitudinal frequency and transverse frequency, respectively. The sum can be convergent or divergent based on the chosen function representing $V_{nnn}$. The simplest method to choose the available function is linear least-square fit which provides linear combination of polynomials based on the list of values. If this method is applied, we note that the highest order of polynomials should be odd if considering the positive $\sigma$ and even if $\sigma$ is taken negative. For example, for listing ten data of $V_{nnn}$ versus $n$ for the positive $\sigma$, by setting all entities to unity we are able to obtain the stable value of the sum, namely $9.75451 \times 10^9$, starting $n = 42$. Later,
by observing the formulation (1), it is clear that the partition function is constructed from the energy states of quantum oscillator containing a correction that comes from the nonlinearity

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega_z - \sigma |B_n|^2 V_{mmm}, \quad (3)$$

where

$$V_{nmlk} = \int_{-\infty}^{\infty} \phi_n(z) \phi_m(z) \phi_l(z) \phi_k(z) \, dz, \quad (4)$$

and $\phi_n$ is a set of dimensionless normalized eigen functions of harmonic oscillator

$$\phi_n(z) = (-1)^n \sqrt{\frac{1}{2^n n! \sqrt{\pi}}} \frac{e^{-z^2/2}}{d^n (e^{-z^2})}. \quad (5)$$

This derivation was first presented by Kivshar et al. by treating the GPE in equation (1) as macroscopic quantum oscillator where the nonlinear term is considered as a very small term [24].

In order to obtain the equation of state in terms of pressure, temperature, and volume, we must fix the partition function in equation (2) to be an extensive entity. The problem is, there is no an extensive variable related to volume. Interestingly, this problem has been solved by Romero-Rochín by replacing the ordinary volume to harmonic volume which is the inverse cube of average geometric trapping frequency [18, 19, 20]

$$V = \frac{1}{\omega^3}. \quad (6)$$

This introduced volume is motivated from the fact that an available volume in which gas fills at a given temperature, is proportional to $1/\omega^3$ [18]. Meanwhile, in the cigar-shaped trap the relation among the appropriate frequencies is given by [3]

$$\omega = (\omega_1^2 \omega_2) \omega^3 \quad (7)$$

If we define the dimensionless parameter $\omega^2 \omega_z / \omega^3$, then by observing the relation, we transform the partition function with this parameter without loosing the meaning

$$Z \to \left(\frac{\omega^2 \omega_z}{\omega^3}\right) Z \quad (8)$$

or, in the complete form

$$Z = \omega^2 \omega_z V \sum_{n=0}^{\infty} e^{\beta \left(\hbar \omega_z (n+1/2) - \sigma |B_n|^2 V_{mmm} \sqrt{m \omega_1 \sqrt{\hbar}}\right)}. \quad (9)$$

Since the dimensionless parameter can be set to unity, we claim then the thermodynamic potentials derived from the partition function does not lose the physical meaning. It is clear that our partition function now has become the extensive quantity since by transforming $V \to \gamma V$ with $\gamma$ is an arbitrary positive constant, the partition function will also transform $Z \to \gamma Z$.

To build the noninteracting $N$ condensates partition function, we have to choose whether the condensates form a set of distinguishable oscillators or indistinguishable oscillators. Nevertheless, we have examined that the treatment should be the second one since the set
of $N$ distinguishable oscillators leads to Gibbs paradox experienced by some thermodynamic
quantities and it must be noted that the paradox is not available in the previous papers
[18, 19, 20, 21, 22, 23] At this point, the total partition function of the set of $N$ indistinguishable
condensates is given by

$$Z_t = \frac{1}{N!} \left( \omega_\perp \omega_\parallel \sum_{n=0}^{\infty} e^{\beta \left( \frac{h \omega_z (n+1/2) - \sigma |B_n|^2 V_{nmmn} \sqrt{m \omega_\perp \sqrt{\lambda / \hbar}}}{kT} \right)} \right)^N. \quad (10)$$

In this case we assume that the number of condensates is so large, then we can use the Stirling’s
formula by agreeing the approximation

$$\frac{1}{N} \ln N! \approx \ln N - 1. \quad (11)$$

3. Equation of state

It is worth initially applying the partition function to derived one of the thermodynamic
potentials, namely, the Helmholtz free energy

$$F = -kT \ln Z_t. \quad (12)$$

Then, by substituting equation (10) into equation (12) and imposing the condition (11), we
obtain

$$F = -NkT \ln \left( \frac{\nu}{N!} \omega_\perp \omega_\parallel \sum_{n=0}^{\infty} e^{\beta \left( \frac{h \omega_z (n+1/2) - \sigma |B_n|^2 V_{nmmn} \sqrt{m \omega_\perp \sqrt{\lambda / \hbar}}}{kT} \right)} \right) - NkT.$$ 

In statistical mechanics, the equation of state can be derived directly by using the equation
of pressure. Since the pressure is indeed a pair conjugate of the volume, we call it as the
harmonic pressure, $P$, which is one of the intensive variables. In this case, by using the relation
$\mathcal{P} = -\left( \frac{\partial F}{\partial V} \right)_{N,T}$, we find the equation state as an ideal gas form

$$\mathcal{P}V = NkT. \quad (13)$$

It must be noted that the above equation of state can also be achieved with other thermodynamic
relations, for example we are able to use the relation $\mathcal{P} = -\left( \frac{\partial F}{\partial V} \right)_{N,S}$, where $E$ and $S$ are
internal energy and entropy, respectively.

However, even though the equation state has ideal gas formula, the internal energy and heat
capacity are literally different. To show the differences, we use first the relation for the internal
energy

$$E = kT^2 \frac{\partial \ln Z_t}{\partial T}$$

$$= N \sum_{n=0}^{\infty} \left[ \left( n + \frac{1}{2} \right) \frac{h \omega_z}{kT} - \sigma |B_n|^2 V_{nmmn} \sqrt{m \omega_\perp \sqrt{\lambda / \hbar}} \right] \exp \left[ - \left( n + \frac{1}{2} \right) \frac{h \omega_z}{kT} + \sigma |B_n|^2 V_{nmmn} \sqrt{m \omega_\perp \sqrt{\lambda / \hbar}} \right]$$

$$\sum_{s=0}^{\infty} \exp \left[ - \left( s + \frac{1}{2} \right) \frac{h \omega_z}{kT} + \sigma |B_s|^2 V_{ssss} \sqrt{m \omega_\perp \sqrt{\lambda / \hbar}} \right]$$

$$\sum_{s=0}^{\infty} \exp \left[ - \left( s + \frac{1}{2} \right) \frac{h \omega_z}{kT} + \sigma |B_s|^2 V_{ssss} \sqrt{m \omega_\perp \sqrt{\lambda / \hbar}} \right]$$

(14)

In order to plot the graphic $E$, it is convenient to replace $V_{nmmn}$ in the numerator and
denominator by a representing function. Realizing that $V_{nmmn}$ cannot form recursion relation,
we take ten data and employing linear least-square fit to represent $V_{nmmn}$. To end our discussion,
we attach another thermodynamic quantity, namely heat capacity at volume constant, which is derived from \( C_V = (\frac{\partial E}{\partial T})_{V,N} \). To produces all graphics, we replace \( V_{nnnn} \) with third order polynomial for positive \( \sigma \) and second order polynomial for negative \( \sigma \), take \( n = 42 \), and set the other constants to unity. In figure 1, we show that raising temperature to the specific temperature in the interval of low temperature will not change the internal energy both positive and negative \( \sigma \), and from that specific temperature the internal energy will linearly increase with the raising temperature. These results are not completely different with the ref. [19] since in the former paper the authors found that the internal energy is linear dependence with the temperature. Meanwhile, from another paper with the similar discussion [21] our results are fully different in calculating the heat capacity given in figure 2. In the previous paper [21],
Sandoval-Figueroa and Romero-Rochín found that at the specific temperature the heat capacity remains constant, while ours did not. We can see that at the very low temperature our heat capacity has a specific peak and monotonically decline from it.

4. Conclusions
As a conclusion, we confirm that the equation of state of $N$ noninteracting undistinguishable condensates, which is confined by anisotropic parabolic trap, is derived by means of introducing $1/\omega^3$ as a harmonic volume to replace the ordinary volume in thermodynamics. This replacement is intended to discuss the thermodynamic entities through the partition function of a set of discrete energies of the one-dimensional GPE formulated by approaching time-independent perturbation theory. In addition, it also must be emphasized that we focus only on the dynamics of condensates, not the particles, by solving the GPE. As stated above, using canonical partition function to obtain the thermodynamic quantities will create the Gibbs paradox if we only consider the distinguishable condensate and the interaction of particles has been included explicitly in the GPE.

We also realize that this model causes the problem both in the internal energy and heat capacity, each of which is discontinuous at $T = 0$. Furthermore, in the case of heat capacity, we also cannot find the realistic entity since it must have a constant value in the higher temperature. This situation appears, in our opinion, since we neglect the interaction between condensates, minimally the attractive interaction.

4.1. Acknowledgments
It is a pleasure to acknowledge Dr. Anto Sulaksono for the encouragement and comments.

5. References
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