Ideal gas model of Bose-Einstein condensates confined in the parabolic trap

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Abstract. By using the one-dimensional canonical partition function, we modelled an ideal gas-like form of a set of Bose-Einstein condensates confined by a three-dimensional anisotropic parabolic trap. The model itself was constructed by taking the eigenenergies of the one-dimensional Gross-Pitaevskii equation in the longitudinal direction and enabling the harmonic volume as the inverse cube of average geometric trapping frequency to substitute the real volume. In this paper, we showed that the condensates form an ideal gas represented by its equation of state and have similar mature to Einstein’s solid-like model with the corrections in both the low and high temperatures in the internal energy formulations.

1. Introduction
Since it has been found the manifestation of Bose-Einstein Condensation (BEC) by cooling down the alkali atoms at the very low temperature in several experiments [1-3], see also Refs. [4-6], physicists are interested in finding a suitable formulation to explain the dynamics of Bose-Einstein condensates (BECs). Most of authors related to the papers of BEC and its related area have stated that the Gross-Pitaevskii equation (GPE) is the best model to study the mature of BECs even though it is considered as a successful theory only at $T \cong 0 \text{ K}$ (7-9). In fact, the GPE, which governs the dynamics of a condensate, is also well known as a kind of the nonlinear Schrödinger equation which is obtained by employing the Hartree-Fock and the mean field theories. In addition, it is also shown that the GPE has no analytical solutions [10] if the Thomas-Fermi approximation is not employed. Note that the modified GPE was also paid attention in the discussions, e.g., the nonlinear optic [11,12] and atom laser [13-15].

On the other side, a harmonic oscillator model has been well-known to formulate some physical quantities, such as the heat capacity of solid proposed by Einstein and Debye. Interestingly, the one-dimensional GPE can be treated as a quantum oscillator if the nonlinear term becomes very small and the solution can be provided by using the time-independent perturbation theory [10]. This fact motivates us to pursue a suspicion that by deriving the eigenenergies, a set of $N$ indistinguishable noninteracting condensates has a similar form to Einstein’s model of solid with a correction appearing from a very small nonlinear term. To follow this suspicion, we initially represent the integral factor as a linear equation since it cannot provide the recursion relation. In addition, to accept this model, we have to replace the real volume with the harmonic volume proposed by Romero-Rochín and his related papers [16-18]. If the above replacement is applied, we also show that the equation of state of a set of condensates will represent an ideal gas form.
To complete the paper, we present our model in section 2 by exploring the previous results based on the former available papers. Our focus in that section is to formulate the total partition function of \( N \) noninteracting indistinguishable condensates that includes the harmonic volume. Then, in the next section we apply our model to formulate the heat capacity of that set and show the figure in order to confirm our suspicion. At the end, we give some comments as a conclusion based on our results.

2. Method

In this section, we will be briefly reviewing the previous results that have been obtained. First, we write the three-dimensional GPE governing a single condensate as

\[
\frac{i\hbar}{\partial t} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) + U |\psi(\vec{r}, t)|^2 \psi(\vec{r}, t)
\]  

(1)

where \( \psi \) is the condensate wavefunction, \( U \) is the length scattering-dependent parameter, and the external potential is given by

\[
V(\vec{r}) = \frac{1}{2} m \omega_z^2 (x^2 + y^2 + \lambda z^2)
\]  

(2)

In this case, \( \lambda \equiv \omega_z^2 / \omega_L^2 < 1 \) represents the small parameter in the cigar-shaped trap, while the relationship between the longitudinal frequency \( \omega_z \) and transverse frequency \( \omega_L \) is denoted by \( \omega = (\omega_z^2 \omega_L^2)^{1/3} \), where \( \omega \) is taken into account as the trapping frequency [4]. By transforming the Cartesian coordinates and wavefunction into the dimensionless ones, Eq. (1) is cast into the one-dimensional GPE in the dimensionless form, see Refs. (10,19)

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

(3)

with the small dimensionless parameter \( \sigma \) can be positive or negative. Writing the solution \( \psi = \sum B_n \varphi_n(z) \exp(-iEt) \) and employing the time-independent perturbation theory where the quantum oscillator approach is held fixed in Eq. (3), we obtain the level of energy states

\[
E_n = \left( n + \frac{1}{2} \right) \hbar \omega_z - \sigma |B_n|^2 V_{\text{cub}} \sqrt{m \omega_L^2 / \hbar},
\]  

(4)

where \( \varphi_n \) represents a set of normalized quantum oscillator eigenfunctions

\[
\varphi_n(z) = (m \omega_z \sqrt{\pi})^{1/4} \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \exp \left( - \frac{m \omega_z \sqrt{\pi}}{2\hbar} z^2 \right) H_n \left( \frac{m \omega_z \sqrt{\pi}}{\hbar} z \right).
\]  

(5)

In the equation above, \( H_n \) denotes a set of Hermite polynomials and the integral factor

\[
V_{\text{cub}} = \int_{-\infty}^{\infty} \varphi_0(z) \varphi_0(z) \varphi_n(z) \varphi_n(z) \, dz,
\]  

(6)

comes from the nonlinear term. Equation (4), which is gained from reducing the three-dimensionless GPE, describes the propagation of a single condensate in the \( z \) direction where the parameter \( \sigma \) includes the length scattering of \( s \)-wave in the case of BEC. Therefore, by using a set of energy levels in Eq. (4), the canonical partition function for a single condensate is given by [19]

\[
Z = \sum_{n=0}^{\infty} e^{\frac{\beta (n+1/2) \hbar \omega_z - \sigma |B_n|^2 V_{\text{cub}} \sqrt{m \omega_L^2 / \hbar}}{kT}},
\]  

(7)

where the Boltzmann constant is given by the relation \( \beta = -1 / kT \).

To see the ideal gas form, we initially generalize our single condensate canonical partition function in Eq. (7) to \( N \)- noninteracting indistinguishable condensates partition function, which can be written as

\[
Z_T = \frac{1}{N!} \sum_{n=0}^{\infty} e^{\frac{\beta (n+1/2) \hbar \omega_z - \sigma |B_n|^2 V_{\text{cub}} \sqrt{m \omega_L^2 / \hbar}}{kT/N}}.
\]  

(8)

In Eq. (8) the purpose to include the noninteracting and indistinguishable aspects in order to avoid the Gibbs paradox possessed by some thermodynamic potentials, such as Helmholtz free energy, Gibbs free energy, etc. In addition, we see clearly that there is no real volume attached in Eq. (8), so we cannot directly formulate the thermodynamic properties. This can be solved if we define a new volume to replace the real volume. According to Romero-Rochín [16-18], since at a given temperature the gas will occupy the real volume at the order \( 1 / \omega_z^3 \), the new volume, namely the harmonic volume, is represented
by $\Omega = 1/\omega^3$. Using the latter definition to include the harmonic volume and applying the dimensionless transformation to the single canonical partition function, $Z \rightarrow Z(\omega^2_1/\omega^3)$ yield [20].

$$Z_T = \frac{1}{N!} \left( \omega^2_1 \omega_z \Omega \sum_{n=0}^{\infty} e^{\frac{-\left( n + \frac{1}{2} \right) \hbar \omega_z + \sigma |B_n|}{\sqrt{V_{nnm}} \sqrt{\lambda/h}}} \right)^N \tag{9}$$

3. Results and discussions

By observing the former results in the previous section, we explore our discussion on the gas ideal form by applying the available assumptions. Following our previous work, we assume that the number of condensates is so large that the Stirling’s approximation holds

$$\frac{1}{N} \ln N ! \approx \ln N - 1. \tag{10}$$

Using the expression of the Helmhotz free energy $F = -kT \ln Z_T$ the explicit form can be written as

$$F = -NkT \left( 1 + \ln \left[ \frac{\Omega}{\omega^2_1} \omega_z \sum_{n=0}^{\infty} \exp \left( -\left( n + \frac{1}{2} \right) \hbar \omega_z + \sigma |B_n| \sqrt{V_{nnm}} \sqrt{\lambda/h} / kT \right) \right] \right). \tag{11}$$

At last, by using the relation of pressure $P = -(\partial F / \partial \Omega)$, we exactly obtain the equation of state of an ideal gas $P \Omega = NkT$.

Next, we consider the discussion on the heat capacity of this model. It is clear that the integral results written in Eq. (7) do not achieve the recursion relation. Thus, it is better to replace $V_{nnm}$ with the linear equation, which is generally stated as $Mn + H$, by using the linear list-square fit. Here, $M$ and $H$ are constants that can be obtained by inputting several data from $V_{nnm}$. For the simplicity, we redefine

$$M' = M |B_n|^2 \sqrt{\lambda/h}, H' = H |B_n|^2 \sqrt{\lambda/h}. \tag{12}$$

Using the thermodynamic relation of the internal energy $E = kT \partial (\ln Z_T) / \partial T$, and substituting the total partition function in Eq. (9) into which, we attain the internal energy

$$E = N \left[ \frac{1}{2} \hbar \omega_z - \sigma H' + e^{-\left( \hbar \omega_z - \sigma M' \right) / kT} \right]. \tag{13}$$

Finally, by employing the relation of heat capacity $C_\Omega = \left( \partial E / \partial T \right)_{\Omega,N}$, we directly find

$$C_\Omega = N \left[ \frac{1}{2} \hbar \omega_z - \sigma M' \right] \frac{k^2}{\hbar^2 \omega_z - \sigma M'} \left( e^{-\left( \hbar \omega_z - \sigma M' \right) / kT} \right)^2. \tag{14}$$

where we reintroduce $\Theta = (\hbar \omega_z - \sigma M')^2 / k^2$ as the Einstein temperature. Figure 1 shows the similar behavior of the heat capacity in our model to the Einstein’s solid-like model.

![Figure 1. Heat capacity vs. temperature in Einstein’s solid-like model.](image-url)
By analyzing Eq. (12), we conclude
\[ C_\Omega \approx N k \] (15)
at the high temperature and
\[ C_\Omega \approx N \frac{(\hbar \omega_x - aM)^2}{kT^2} e^{-\frac{(\hbar \omega_x - aM)}{kT}} \] (16)
at the low temperature.

Note that the above model is only valid if we assume that the condensates do not interact each other. For the extension, we also can include the interaction between two condensates to deal with the real gas model. Unlike ours, who used a set of noninteracting condensates to study the ideal gas, Refs. [16-18,21-24] used the condensed atoms to study the ideal gas as well as the interacting gas in BEC via the Bose statistics. They also applied the similar condition, such as the Stirling’s approximation, to obtain the solution. The strong difference between us lies in the heat capacity although the same formulation was implemented. As previously written in Eqs. (15) and (16), we found the similar results to the Einstein’s solid-like model while they did not.

4. Conclusions
A model of a set of \( N \) noninteracting indistinguishable condensates has been proposed by using the canonical partition function and introducing a new thermodynamic volume, namely the harmonic volume, to replace the real volume. For deriving the thermodynamic properties, we also impose the large number of condensates in order to enable the Stirling’s approximation. The providing results seem to have the similar form to the ideal gas, as shown in the equation of state, but the internal energy and heat capacity take the similar forms to the Einstein’s solid-like model, which is only different in the parameter \( \sigma \). As we can see in Fig. 1, at the very high temperature the heat capacity tends to constant value as stated in Eq. (15) where we have redefined the Einstein temperature. In addition, the very small nonlinear term takes an effect on heat capacity at the low temperature in Eq. (16). We would like to remind that this model is valid only by accepting \( V_{nnn} \) as a linear equation.

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