

The Partition Function of the Bose-Einstein Condensation in Parabolic Trap

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Abstract

We have discussed the partition function of the Bose-Einstein condensation in parabolic trap associated to the one-dimensional Gross-Pitaevskii equation. The partition function itself is constructed by considering all the energy levels of the macroscopic quantum oscillator which is similar to statistical mechanics. The solutions of the energy levels for this case can be derived by pursuing the method that applies the time-independent perturbation theory. In this case, the one-dimensional Gross Pitaevskii equation can be treated as the one-dimensional macroscopic quantum oscillator on condition that the nonlinearity is very small. Moreover, the analytical expression for the ground state energy can be obtained by applying the method. However, the higher level states were not explicitly provided. In this research we followed up on the former work to derive explicitly the other states in order to formulate the partition function. However, we did not find the closed form of the partition function since the results of nonlinear term integral could not form the recursion relation. As a consequence, not only should the partition function but also the Helmholtz free energy and entropy should be reevaluated to check their convergences.

Abstrak

Fungsi Partisi dari Kondensasi Bose-Einstein di dalam Perangkap Parabola. Kami telah membahas fungsi partisi dari kondensasi Bose-Einstein di dalam perangkap parabola yang dinyatakan oleh persamaan Gross-Pitaevskii satu dimensi. Fungsi partisi itu sendiri dirumuskan hanya dengan meninjau semua tingkat-tingkat energi dari osilator kuantum makroskopik yang mirip seperti di dalam mekanika statistika. Solusi-solusi dari tingkat-tingkat energi untuk kasus ini dapat diturunkan dengan mengikuti metode yang menggunakan teori perturbasi bebas waktu. Pada kasus ini, persamaan Gross-Pitaevskii satu dimensi dapat diperlakukan sebagai osilator kuantum makroskopik dengan menerapkan kondisi bahwa faktor nonlinearnya sangat kecil. Selain itu, perumusan analitik untuk energi tingkat dasar dapat diperoleh dengan menggunakan metode tersebut. Namun demikian, tingkat-tingkat eksitasinya tidak diberikan secara eksplisit. Saat ini, kami melanjutkan pekerjaan sebelumnya untuk menurunkan tingkat-tingkat keadaan lainnya supaya dapat merumuskan fungsi partisi. Akan tetapi, kami tidak mendapatkan bentuk analitik dari fungsi partisi karena integral dari suku-suku nonlinear tidak dapat membentuk hubungan rekursif. Akibatnya, tidak hanya fungsi partisi tetapi juga energi bebas Helmholtz dan entropi harus dikaji ulang untuk memeriksa sifat konvergenya.

Keywords: Gross-Pitaevskii equation, partition function, quantum oscillator, thermodynamic properties

1. Introduction

It has been studied that the Gross-Pitaevskii equation (GPE) is used as a mathematical model to consider the realization of Bose-Einstein condensation (BEC) by the experiment series in recent years. The evidence of the existence of BEC was initially confirmed by Anderson *et al.* and Davis *et al.* through two separate experimental results [1]. Around 1995 to 2000 the three-dimensional GPE was introduced as a kind of nonlinear Schrödinger equation (NLSE) with the anisotropic trapping potential

while the parameter in the nonlinear term depends on the scattering length s -wave, which is then reduced to one-dimensional GPE. The trapping potential was chosen as an anisotropic three-dimensional harmonic potential which can be used to discuss the case of the cigar-shaped trap model. By applying the model some papers were published that presented numerical or approximation results and compared them to the other experimental results. For detailed discussions one can see Ref. [2-5]. Meanwhile, authors have also considered that GPE has two properties since this is due to the

characteristics of GPE itself. Some of them have treated GPE as a macroscopic quantum oscillator on the basis that the nonlinear term is so small [6-7]. And others have treated GPE as a NLSE coupled by parabolic potential [4,8]. However, they both concluded that the characteristics of solitary wave solutions do exist. Fortunately, one can also see some reviews on BEC which explain the basics of BEC in Ref. [9-10].

The published papers have triggered more and better theoretical explorations of GPE since the followed up experimental results need verification or are applied for application developments. During the years 2000, GPE has been used in discussions, not only in applied physics [11-16] but also in cosmology [17-20]. In GPE, the wave function describes the macroscopic wave function of the condensate having a different definition than in ordinary quantum mechanics when the integration over all space between the wave function and its conjugate is executed. First of all, we are interested in the question: "how can we get information about the physical quantities in thermodynamics?" The key to answer this question lies in the partition function which although the function itself has no physical meaning, yet it brings together all the information about the physical quantities in thermodynamics, for example one can derive Helmholtz free energy, entropy, etc. However, the problem is that the calculation of the partition function is so difficult to execute since the expression is usually formulated in the functional integral that needs some assumptions and boundary conditions, interested readers are welcome to see [21-26]. In this paper we introduce a simple way to formulate the appropriate partition function. To construct it, we initially explore an interesting case of GPE. By considering that the nonlinear term is ignored, the one-dimensional of GPE will be reduced to the ordinary Schrödinger equation in the presence of the harmonic oscillator potential. By pursuing this fact, we prove that it is possible to construct the appropriate partition function by using the approach of the one-dimensional macroscopic quantum oscillator.

The paper of Kivshar *et al.* [7] presents that by assuming that the nonlinear term is very small, the ground state energy can be analytically obtained by applying the time-independent perturbation theory. By observing this fact, in order to explicitly formulate the other energy levels we pursue the procedures of the recent work in [7]. After deriving some formulations on the energy level of the one-dimensional GPE, we attempt to construct the appropriate partition function as in statistical mechanics. In fact, although we followed their procedure, we obtained different results in the formulation of ground state energy. This difference will be considered in Sec. 3 with comments and comparisons of the obtained result in [7]. Furthermore, we also provide the calculations of the Helmholtz free energy

and entropy, and compare the results with the ordinary quantum oscillator. We structure the rest of the paper as follows: in sec 2 we review the important procedure based on the concepts of Kivshar *et al.* [7]. In this section we also comment on Rodriguez's formula used in their procedure since the formula can result in a different meaning when it is used in quantum mechanics. We initially formulated some energy level states and attached the figure of their modes so that the reader can compare our results with theirs. Then we wrote the partition function based on the previous results and also explored some values of the integration in the nonlinear potential term.

2. Methods

In order to seek the higher modes of the macroscopic quantum oscillator in the case of the one-dimensional GPE, our concern in this section is to review and rewrite the method proposed by Kivshar *et al.* [7]. Moreover we used some different notations without influencing the essential results. The standard formulation of the three-dimensional GPE equation is given as [4,7]

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) + U_0 |\psi(\vec{r}, t)|^2 \right) \psi(\vec{r}, t), \quad (1)$$

where $\psi(\vec{r}, t)$ denotes the wave function of the condensate, $V(\vec{r})$ is the anisotropic parabolic potential

$$V(\vec{r}) = \frac{1}{2} m \omega_{\perp}^2 (x^2 + y^2 + \lambda_z z^2), \quad (2)$$

where $\lambda_z \equiv \omega_z^2 / \omega_{\perp}^2$ is the very small parameter obtained by dividing between the angular frequency in the z direction and the transverse one, and $U_0 = 4\pi\hbar^2(a/m)$ is the parameter depending on the length scattering of s -wave, a . The length scattering can be positive or negative depending on whether the interaction of the particles is repulsive or attractive. In order to reduce the above three-dimensional GPE in Eq. (1), by following [7] we firstly used the following transformations for the coordinates and the wave function to become dimensionless equation as follows:

$$(x', y', z') = (x, y, z) / a_0, \quad (3)$$

$$t' = \frac{t}{2 / (\omega_z \sqrt{\lambda_z})}, \quad (4)$$

$$\psi' = \psi \sqrt{\frac{2U_0 \sqrt{\lambda_z}}{\hbar \omega_{\perp}}}, \quad (5)$$

where $a_0 = \sqrt{\hbar / m \omega_{\perp} \sqrt{\lambda_z}}$ defines the length of harmonic oscillator. After substituting Eq. (3-5) into Eq. (1), the dimensionless of the GPE equation becomes [7]

$$i \frac{\partial \psi'}{\partial t'} = -\nabla'^2 \psi' + (\lambda_z^{-1} (x'^2 + y'^2) + z'^2) \psi' - \sigma |\psi'|^2 \psi' \quad (6)$$

where σ only depends on the sign of the scattering length a .

Secondly, to get the final result of the reduced GPE in one dimension, it is convenient that the wave function in Eq. (6) should be transformed once again by the following transformation [7]

$$\psi'(r', z', t') = \Phi(\rho)\Psi(z', t')e^{-2i\gamma t'} \quad (7)$$

Note that the transformation in Eq. (7) is written in cylindrical coordinates. Thus, by writing the “del” operator written in Eq. (6) in cylindrical coordinates and substituting Eq. (7) into Eq. (6), we obtain the final one-dimensional GPE equation given by [7]

$$i \frac{\partial \Psi}{\partial t'} + \frac{\partial^2 \Psi}{\partial z'^2} - z'^2 \Psi + \sigma |\Psi|^2 \Psi = 0 \quad (8)$$

The above equation can directly be observed as the nonlinear Schrödinger equation with another potential that is described as a parabolic trapping potential or the ordinary Schrödinger equation for the harmonic oscillator potential if σ is ignored. Therefore the provided solution can numerically be achieved by two approaches considering whether we treat the equation as NLSE or the Schrödinger equation for harmonic oscillator as in quantum mechanics. In light of this, we choose the second solution by assuming that σ is very small [7].

Thirdly, to follow their choice that the one-dimensional GPE can be treated as a macroscopic quantum oscillator, [7] we went on to record some useful expressions that can be used to solve Eq. (8) as follows: The eigenfunctions of the harmonic oscillator satisfying the eigenvalue equation

$$-\frac{d^2 \phi_n}{dz'^2} + z'^2 \phi_n = E_n \phi_n \quad (9)$$

can be written as

$$\phi_n(z') = \sqrt{\frac{1}{2^n n! \sqrt{\pi}}} e^{-z'^2/2} H_n(z') \quad (10)$$

Note that all the variables are dimensionless. In Eq. (9) and (10) E_n denotes the discrete values of quantum harmonic oscillator

$$E_n = 2n + 1 \quad (11)$$

n are the sets of non negative integer while $H_n(z')$ associate as the set of Hermite Polynomials [27]

$$H_n(z') = (-1)^n e^{z'^2} \frac{d^n}{dz'^n} \left(e^{-z'^2} \right) \quad (12)$$

Here we would like to give our first comment. In their paper, Kivshar *et al.* [7] included the factor $\frac{1}{2}$ in the Rodriguez formula in Eq. (12). If it is executed, the eigenfunctions for harmonic oscillator in Eq. (10) should not normalize although they are still orthogonal.

Note that the eigenfunctions in quantum mechanics have always been chosen as the normalized functions. By following these expressions, we suggest that the solutions for Eq. (9) can be written as the superposition of the normalized eigenfunctions, as one uses in the case of time-independent perturbation theory [7].

$$\Psi(z', t') = e^{-iEt'} \sum_{n=0} B_n \phi_n(z') \quad (13)$$

3. Results and Discussion

Now, by following the same procedure suggested by Kivshar *et al.* [7], we will present our final result in the expression of the ground state energy that differs as in the result in [7]. Then we continue to explicitly derive the excitation states and attach the figures of some modes both for the case positive σ and negative one. After obtaining some energy levels we construct the partition function based on the previous results. First of all, we substitute Eq. (13) into Eq. (8) by also considering the relation in Eq. (9). By multiplying the achieved equation on both sides by the conjugate ϕ_m^* , then after integrating both sides over all space, we obtain the relation

$$B_m(E - E_m) + \sigma \sum_{nlk=0} B_n^* B_l B_k V_{mnlk} = 0 \quad (14)$$

where

$$V_{mnlk} = \int_{-\infty}^{\infty} \phi_m(z') \phi_n(z') \phi_l(z') \phi_k(z') dz' \quad (15)$$

Here we have written $\phi_m = \phi_m^*$ since the function itself is real. The result we obtain in Eq. (14) has the positive sign while Kivshar *et al.* obtained the negative sign [7]. Our second comment is that although the obtained result differs only in the sign, it influences both the formulations and probability density for all modes. Moreover, it also effects the formulation of the partition function since the function should be written in terms of energy levels.

Following Eq. (14-15), we construct the first three modes by pursuing the following assumptions

(a) Ground state level. To get energy in the ground state level, we take $m=0$ in Eq. (14) and assume that $B_0 \gg B_m$ should be maintained for all $m>0$ [7]. By imposing this condition, we directly obtain ground state energy from Eq. (14)

$$E = E_0 - \sigma |B_0|^2 V_{0000} \quad (16)$$

and the corresponding probability amplitude

$$|\Psi|^2 = |B_0|^2 |\phi_0|^2 \quad (17)$$

Note that Kivshar *et al.* have obtained the opposite sign result [7].

For achieving excitation levels, we assume that the calculation should be started in the appropriate excitation state by ignoring the ground state and the

lower excitation states and also following up on the previous assumption that the next expansion coefficients are smaller than its state.

(b) First excitation state level. Following the above procedure, by ignoring the ground state level, taking $m=1$ and assuming that $B_1 \gg B_m$ should be maintained for all $m > 1$, we obtain the first excitation energy

$$E = E_1 - \sigma |B_1|^2 V_{1111}, \tag{18}$$

and the appropriate probability amplitude

$$|\Psi|^2 = |B_1|^2 |\phi_1|^2. \tag{19}$$

(c) Second excitation state level. By ignoring the ground state and first excitation level, taking $m = 2$ and also assuming that $B_2 \gg B_m$ should be maintained for all $m > 2$, we obtain the second excitation energy and the corresponding probability amplitudes

$$E = E_2 - \sigma |B_2|^2 V_{2222}, \tag{20}$$

$$|\Psi|^2 = |B_2|^2 |\phi_2|^2. \tag{21}$$

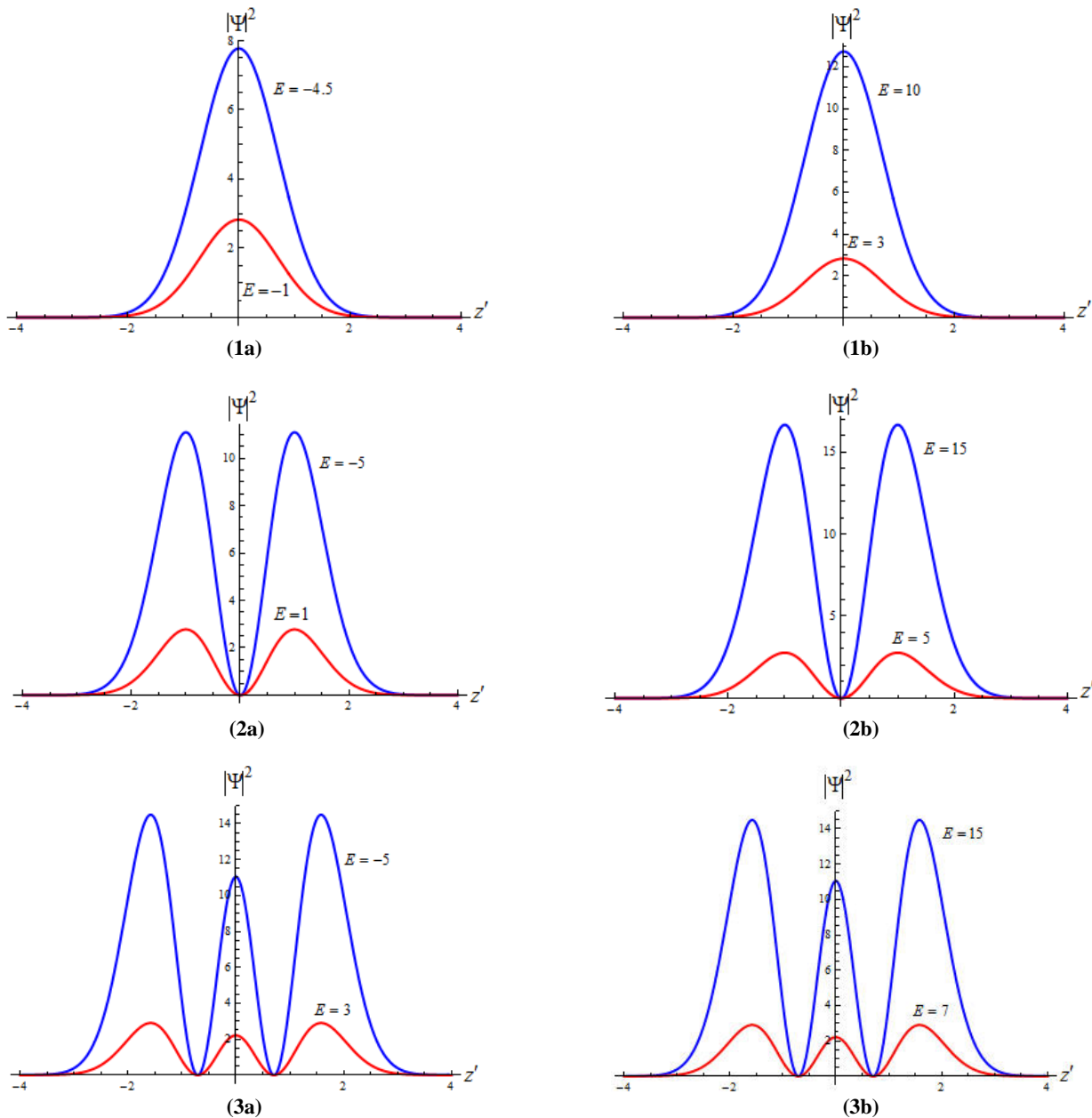


Figure 1. (1a) and (1b) State the Probability Amplitudes of the Ground State for $\sigma = 1$ and $\sigma = -1$, Respectively; (2a) and (2b) Describe the Probability Amplitudes of the First Excitation State for $\sigma = 1$ and $\sigma = -1$, Respectively; and (3a) and (3b) Address the Probability Amplitudes of the Second Excitation State for $\sigma = 1$ and $\sigma = -1$, Respectively

Here we have used *Mathematica* to produce our figures for the appropriate values.

Since we have used the approach of macroscopic quantum oscillator for the GPE with energy levels given by Eq. (16), (18), and (20), we directly conclude that the partition function can be formulated as the classical partition function in statistical mechanics. However, this statement leads to another question: “*is it possible to get the partition function in the closed form?*” In fact, to answer this we initially need to know whether all the values of Eq. (15) have the recursion relation or not. The values of Eq. (15) for the first three modes are given in the following Table 1.

In statistical mechanics the partition function for quantum oscillator can be defined as

$$Z = \sum_{n=0}^{\infty} e^{-E_n/kT} \tag{22}$$

Since the E_n/kT in the exponent should be dimensionless, we have to transform back some appropriate physical quantities used here

$$E_n \rightarrow \left(n + \frac{1}{2}\right) \hbar \omega_z \tag{23}$$

$$z' \rightarrow z' \sqrt{\frac{m\omega_{\perp} \sqrt{\lambda}}{\hbar}} \tag{24}$$

Therefore we formulate the explicit partition function as

$$Z = \sum_{n=0}^{\infty} e^{-\left\{ \left(n + \frac{1}{2}\right) \hbar \omega_z - \sigma |B_n|^2 V_{nnnn} \sqrt{\frac{m\omega_{\perp} \sqrt{\lambda}}{\hbar}} \right\} / kT} \tag{25}$$

By observing that there is no recursion relation in the values of the nonlinear term integral provided in Table 1, we state that the closed form of the partition function cannot be formulated.

Table 1. The Nonlinear Term Integral Values of the First Three Modes in Dimensionless Unit

nonlinear term integral	Values
V_{0000}	0.398942
V_{1111}	0.299207
V_{2222}	0.255572

This fact is sufficient since the nonlinear term integral contributes to determine the closed form of the partition function as stated in Eq. (25). Consequently, we have to examine the convergence of the partition function formulation. To prove it, one can refer to some previously noted testing series.

For closing this section, we wish to derive two thermodynamic properties, namely the Helmholtz free energy and entropy. In statistical mechanics the Helmholtz free energy and entropy are given respectively by

$$F = -kT \ln Z \tag{26}$$

$$S = -\frac{\partial F}{\partial T} \tag{27}$$

Meanwhile, the closed forms of Helmholtz free energy and entropy in the quantum oscillator are given respectively by

$$F = \frac{1}{2} \hbar \omega_z + kT \ln \left(1 - e^{-\frac{\hbar \omega_z}{kT}} \right), \tag{28}$$

$$S = k \left\{ \frac{\hbar \omega_z}{kT \left(1 - e^{-\frac{\hbar \omega_z}{kT}} \right)} - \ln \left(1 - e^{-\frac{\hbar \omega_z}{kT}} \right) \right\}. \tag{29}$$

After substituting Eq. (25) into Eq. (26), we obtain

$$F = -kT \ln \left(\sum_{n=0}^{\infty} e^{-\left[\left(n + \frac{1}{2}\right) \frac{\hbar \omega_z}{kT} + \sigma |B_n|^2 V_{nnnn} \frac{\sqrt{m\omega_{\perp} \sqrt{\lambda}}}{\hbar} \right] / kT} \right) \tag{30}$$

Finally, the entropy can be achieved by substituting Eq. (30) into Eq. (27)

Once more, we are dealing with the convergence problem stated by Eq. (30) and (31). It is clear that the Helmholtz free energy in Eq. (30) and entropy in Eq. (31) need evaluation to decide their convergences.

$$S = k \ln \left(\sum_{n=0}^{\infty} e^{-\left[\left(n + \frac{1}{2}\right) \frac{\hbar \omega_z}{kT} + \sigma |B_n|^2 V_{nnnn} \frac{\sqrt{m\omega_{\perp} \sqrt{\lambda}}}{\hbar} \right] / kT} \right) + kT \frac{\sum_{n=0}^{\infty} e^{-\left[\left(n + \frac{1}{2}\right) \frac{\hbar \omega_z}{kT} + \sigma |B_n|^2 V_{nnnn} \frac{\sqrt{m\omega_{\perp} \sqrt{\lambda}}}{\hbar} \right] / kT} \left[\left(n + \frac{1}{2}\right) \frac{\hbar \omega_z}{kT^2} - \sigma |B_n|^2 V_{nnnn} \frac{\sqrt{m\omega_{\perp} \sqrt{\lambda}}}{\hbar kT^2} \right]}{\sum_{n=0}^{\infty} e^{-\left[\left(n + \frac{1}{2}\right) \frac{\hbar \omega_z}{kT} + \sigma |B_n|^2 V_{nnnn} \frac{\sqrt{m\omega_{\perp} \sqrt{\lambda}}}{\hbar} \right] / kT}} \tag{31}$$

4. Conclusions

We have followed up the former work of Kivshar *et al.* and found that our final results differ in not only the opposite sign in Eq. (14) but also in the peak of the figures, a detailed discussion can be found in Kivshar *et al.* [7]. The localized probability amplitudes as stated in all figures are not surprising since the wave function is expanded by the Hermite-Gauss functions. Furthermore, all the above figures are similar to the probability amplitudes in the quantum oscillator, but the differences lie in the peak and width. This is caused by the nonlinear term which contributes to the amplitudes. By assuming that the nonlinear term is small, the use of the time-independent perturbation theory for finding the solutions of the level states by imposing the appropriate conditions is literally accepted. In addition, we can calculate some physical quantities in each mode, such as the probability, the energy expectation, etc. because of the localized probability amplitudes.

We have also proven that the method can be used to derive the partition function only from considering the relation of energy levels. By adding another assumption, one can see that the excitation levels also need a correction which is similar to the ground state. However, we can not obtain the closed form of the partition function since the values of the integral in the nonlinearity have no recursion relations as one can see in Table 1. If one continues the calculation, one can see that the values are monotonically decreasing. This result leads us to serious problems. As we mentioned before, we have found that the convergences of partition function, Helmholtz free energy, and entropy should be checked.

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