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Analytical computation of Bose-Einstein integral functions

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Abstract

The study of Bose-Einstein integral functions is important in the fact that such functions arise in various numerical calculations of different domains of physics. The significance of gamma function and Riemann zeta function in solving such integrals has been studied and functional equations are evaluated thereby enabling the integrals of all orders to be calculated.

Keywords

Bose-Einstein integral function, Gamma function, Riemann zeta function, Lanczos approximation, Gauss-Laguerre Quadrature.

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1. Introduction

Over the years, several authors [1-8] have worked on the analysis and evaluation of Bose-Einstein integrals using different approaches. The Bose-Einstein distribution function describes the statistical behaviour of integer spin particles called bosons. The probability $f_{BE}(\epsilon)$ that a boson occupies a state of energy ϵ is given by

$$f_{BE}(\epsilon) = \frac{1}{e^{\alpha + \frac{\epsilon}{kT}} - 1} \tag{1}$$

where k is Boltzmann constant, T is absolute temperature and α depends on the properties of the system and is a function of T. The sum over all energy states of $n(\epsilon) = g(\epsilon) f(\epsilon)$ is equal to the total number of particles N in the system, i.e. $N = \sum n_i$.

The distribution of the average number of molecules n_i in an energy level ϵ_i of statistical weight g_i is then given as

$$n_i = \frac{g_i}{e^{\alpha + \frac{\epsilon}{kT}} - 1} \tag{2}$$

The energy spectrum of an ideal monatomic gas of mass m enclosed in a cubic volume V can be represented by the smoothed weight function given as

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$$g(\epsilon) = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} \epsilon^{\frac{1}{2}} \tag{3}$$

where $g(\epsilon)\, d(\epsilon)$ gives the number of energy levels in the interval $(\epsilon, \epsilon + d\epsilon)$.

Replacing the summation $\sum n_i$ by an integral for a macroscopic volume and using Eq.(3) in Eq.(2), we obtain [9, 10]

$$N = \frac{2\pi V}{h^3} (2m)^{3/2} \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\alpha + \frac{\epsilon}{kT}} - 1} \tag{4}$$

This expression of N can be written as

$$N = V \left(\frac{2\pi mkT}{h^2} \right)^{3/2} F_{3/2}(\alpha) \tag{5}$$

where $F_{3/2}(\alpha)$ is the case of $\sigma = 3/2$ of the Bose-Einstein integral functions of the form

$$F_\sigma(\alpha) = \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}}{e^{x+\alpha} - 1} dx \tag{6}$$

Here $\Gamma(\sigma)$ is the gamma function. For $\alpha = 0$ and $\sigma > 1$, the function $F_\sigma(0)$ is identical with the Riemann zeta function.

The aim of the present work is the numerical computation of the special functions, viz. Gamma function and Riemann zeta function, and the Bose-Einstein integral function. A comparative study and analysis are done among the different expressions of σ and α of the Bose-Einstein integral functions. Both gamma function and Riemann zeta function are often encountered while evaluating such integrals. These two functions are discussed in the next section.

2 Gamma function and Riemann zeta function

Most special functions come as solutions of first or second order differential equations. However, two most important special functions, Gamma function and Riemann zeta function, do not arise from differential equations.

The Gamma function is a component in various probability distribution function. For a given complex number z, it is defined by the definite integral [11, 12]

$$\Gamma(z) = \int_0^\infty e^{-x} x^{z-1} dx \tag{7}$$

For any complex number σ, the Riemann zeta function is defined by the Dirichlet series: [13]

$$\zeta(\sigma) = \sum_{n=1}^{\infty} \frac{1}{n^\sigma} \tag{8}$$

On the real line with any variable $\sigma > 1$, it can be defined by the integral

$$\zeta(\sigma) = \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}}{e^x - 1} dx \tag{9}$$

which relates it to the Gamma function.

2.1 Lanczos approximation

The complex values of Gamma function can be computed numerically with arbitrary precision using the Lanczos approximation [14]. Gamma function is undefined for negative integers but using Lanczos approximation, the function can be calculated not only for positive arguments but also for negative fractions to a very high order of accuracy. The Lanczos approximation is given as

$$\Gamma(z) = \left[\frac{\sqrt{2\pi}}{z}\left(p_0 + \sum_{n=1}^{6}\frac{p_n}{z+n}\right)\right](z+5.5)^{(z+0.5)}\, e^{-(z+5.5)} \tag{10}$$

where

$$\begin{aligned}
p_0 &= 1.000000000190015 \\
p_1 &= 76.18009172947146 \\
p_2 &= -86.50532032941677 \\
p_3 &= 24.01409824083091 \\
p_4 &= -1.231739572450155 \\
p_5 &= 1.208650973866179 \times 10^{-3} \\
p_6 &= -5.395239384953 \times 10^{-6}
\end{aligned} \tag{11}$$

The Gamma function of a few rational numbers, computed using the Lanczos approximation, has been listed in Table 1. It should be noted that the approximation is not defined at $z = -5.5$ upto $z = -7.4$. It works well again at $z = -7.5$ and beyond. The calculated values are agreeable with the theoretical ones.

Table 1: Gamma function of some rational numbers.

z	Γ(z)	Remarks
-1.5	2.363271713	
-1.25	3.921333551	
-0.75	-4.834146500	
-0.50	-3.544907808	
-0.25	-4.901666641	
0.25	3.625609875	
0.50	1.772453904	$\sqrt{\pi} \approx 1.772453851$
0.75	1.225416660	
1	1.000000000	
1.25	0.906402469	
1.5	0.886226925	$\sqrt{\pi}/2 \approx 0.886226925$
1.75	0.919062555	
2	1.000000000	
2.5	1.329340388	$3\sqrt{\pi}/4 \approx 1.329340388$
2.75	1.608359456	

From Table 1, it can be inferred that the values of Gamma function obtained using the Lanczos approximation agrees well with those of the theoretical values, e.g. the most well-known value $\Gamma(1/2) = \sqrt{\pi} \approx 1.772453851$ and $\Gamma(1.5) = \sqrt{\pi}/2 \approx 0.886226925$ are almost equal to the calculated values. Thus, despite its limitations, this approximation proves to be of great importance in computing and evaluating the Gamma function of any argument to a high order of accuracy.

2.2 Plot of Gamma graph and the location of minima

It can be checked that using the values of Gamma function of any argument in the range $1 \le x \le 2$, one can compute the Gamma function of any other arguments, irrespective of the sign. Following is the tabulation used for plotting the Gamma graph and the location of minima.

Table 2: Gamma function of some arguments.

$\mathbf{x}$	$\mathbf{\Gamma(x)}$
1.435	0.885910
1.437	0.885865
1.439	0.885824
1.441	0.885787
1.443	0.885753
1.445	0.885722
1.447	0.885695
1.449	0.885672
1.451	0.885652
1.453	0.885635
1.455	0.885622
1.457	0.885612
1.459	0.885606
1.461	0.885603
1.462	0.885603
1.464	0.885606
1.466	0.885611
1.468	0.885621
1.470	0.885633
1.472	0.885649
1.474	0.885669

Using Table 2, the Gamma graph is plotted taking the values of the variable along x-axis and $\Gamma(x)$ along y-axis. With the increase in values of the variable, the values of Gamma function decrease gradually and then after attaining a *minima* it increases gradually. We know that $\Gamma(1) = 1$ and $\Gamma(2) = 1$. Hence one may expect the minima to be located at the midpoint, i.e. $(1+2)/2 = 1.5$. But the expectation **cannot** be a proof. $\Gamma(1.5) = \sqrt{\pi}/2 \approx 0.886226$. It is clearly observed from the graph that the minima lies between $x = 1.461$ and $x = 1.462$ and its Gamma function is approximately equal to 0.885603, which is less than $\sqrt{\pi}/2$. Figure 1 shows the Gamma graph and the location of minima.

2.3 Riemann's functional equation

Using Eq.(8), the computation of the Riemann zeta function is restricted only to non-negative arguments. The function for negative integers and fractions can be calculated using the *functional equation* [15]

$$\Gamma\left(\frac{\sigma}{2}\right)\pi^{-\sigma/2}\zeta(\sigma) = \Gamma\left(\frac{1-\sigma}{2}\right)\pi^{-(1-\sigma)/2}\zeta(1-\sigma) \tag{12}$$

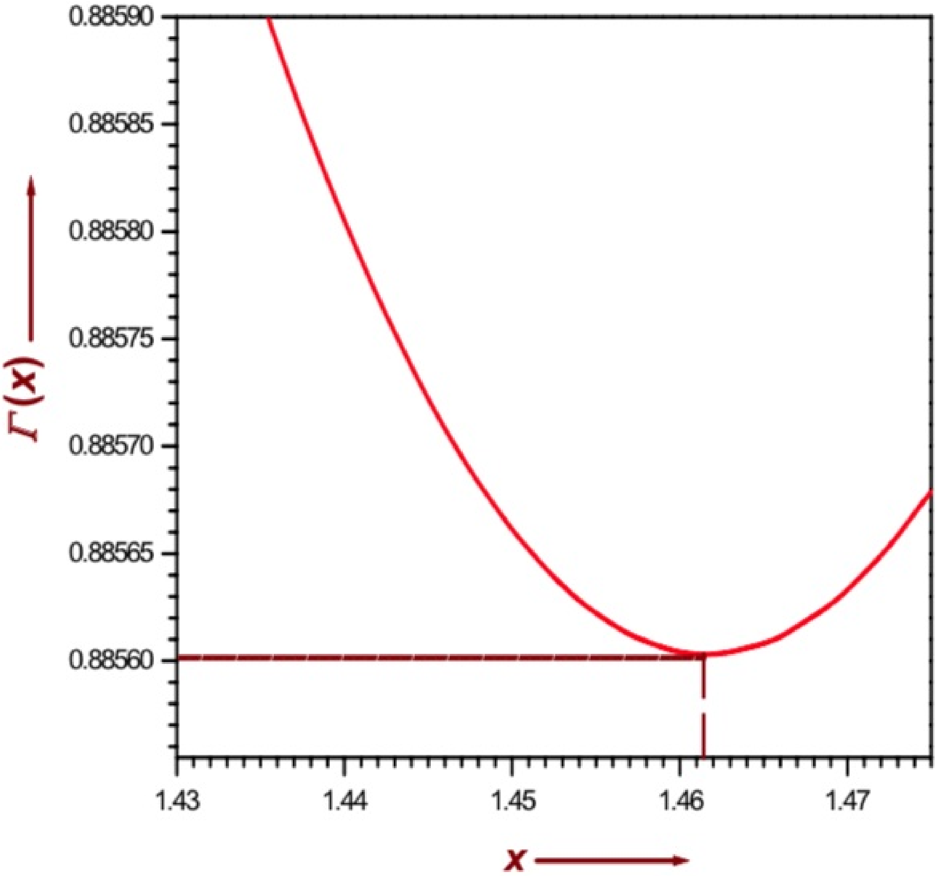

Figure 1: **Plot of Gamma graph and the location of minima.**

The values of positive arguments are used simultaneously while computing the Riemann zeta function of negative arguments.

The Riemann zeta function of some rational numbers computed using the functional equation (Eq.(12)) are listed in Table 3.

The values of Riemann zeta function computed using the functional equation formula (Eq.(12)) accords with the theoretical values. It can be observed that the Riemann zeta function has zeros at the negative even integers and it is an important property of this function.

3 Bose-Einstein integral functions

The expansions in Dirichlet series for the Bose-Einstein integral functions (Eq. (6)) in powers of α are desirable in the study of the behaviour of $F_\sigma(\alpha)$ for small α. Here, σ and α are the parameters of the Bose-Einstein gas where α is a function of total number of molecules at absolute temperature T. The power series expression for the Bose-Einstein integral function $F_\sigma(\alpha)$ as obtained in Ref. [16] is given as

Table 3: Riemann zeta function of some rational numbers.

σ	$\zeta(\sigma)$
-5	-0.003968253
-4	0
-3.5	0.004441010
-3	0.008333333
-2.5	0.008516913
-2	0
-1.5	-0.025484722
-1	-0.08333333
-0.5	-0.207000464
0	-0.5
0.5	-1.460354508
1	∞
1.5	2.601244688
2	1.644725323
2.5	1.341462016
3	1.202050686
3.5	1.126731873
4	1.082322121
5	1.036927462

$$F_\sigma(\alpha) = \alpha^{\sigma-1}\Gamma(1-\sigma) + \sum_{n=0}^{\infty} (-\alpha)^n \frac{\zeta(\sigma-n)}{n!} \tag{13}$$

By the principle of analytic continuation, Eq.(13) holds for all σ. A comparative study and analyses are done for the functions $F_{1/2}(\alpha)$, $F_{3/2}(\alpha)$, $F_{5/2}(\alpha)$ and $F_{7/2}(\alpha)$ for different values of σ and α. While evaluating the infinite series of these functions, both Gamma function and Riemann zeta function of positive and negative rational numbers are used. Following are the infinite series of these functions, which are obtained using Eq. (13):

$$\begin{aligned}
F_{1/2}(\alpha) &= 1.77245\,\alpha^{-1/2} - 1.46035 + 0.20789\,\alpha - 0.01274\,\alpha^2 - 0.00142\,\alpha^3 + \\
&\quad 0.00018\,\alpha^4 - 0.000026\,\alpha^5 + ... \\
F_{3/2}(\alpha) &= -3.544908\,\alpha^{1/2} + 2.61237 + 1.46035\,\alpha - 0.10394\,\alpha^2 + 0.00425\,\alpha^3 + \\
&\quad 0.00035\,\alpha^4 - 0.000037\,\alpha^5 + ... \\
F_{5/2}(\alpha) &= 2.36327\,\alpha^{3/2} + 1.34148 - 2.61237\,\alpha - 0.73017\,\alpha^2 + 0.03465\,\alpha^3 - \\
&\quad 0.00106\,\alpha^4 - 0.000071\,\alpha^5 + ... \\
F_{7/2}(\alpha) &= -0.94531\,\alpha^{5/2} + 1.12670 - 1.34148\,\alpha + 1.30619\,\alpha^2 + 0.24339\,\alpha^3 - \\
&\quad 0.00866\,\alpha^4 + ...
\end{aligned} \tag{14}$$

Table 4 gives the list of some arguments of the Bose-Einstein integral functions given by Eq.(13). They are evaluated using *Gauss-Laguerre Quadrature* [11, 17] for different values of σ and α and are compared with the values of exponential function.

Table 4: Bose-Einstein integral functions for different values of σ and α.

α	$\mathbf{F_{1/2}}(\alpha)$	$\mathbf{F_{3/2}}(\alpha)$	$\mathbf{F_{5/2}}(\alpha)$	$\mathbf{F_{7/2}}(\alpha)$	$\mathbf{e}^{-\alpha}$
0	∞	2.612	1.341	1.127	1.000
0.1	4.165	1.636	1.477	1.003	0.905
0.2	2.544	1.315	1.001	0.896	0.819
0.3	1.837	1.099	0.881	0.802	0.741
0.4	1.423	0.938	0.779	0.719	0.670
0.5	1.147	0.811	0.692	0.645	0.606
0.6	0.948	0.706	0.617	0.579	0.549
0.7	0.797	0.619	0.551	0.522	0.497
0.8	0.679	0.546	0.493	0.469	0.449
0.9	0.584	0.483	0.441	0.423	0.407
1.0	0.506	0.428	0.396	0.381	0.368
2.0	0.149	0.142	0.139	0.137	0.135

It can be observed from Table 4 that the function $F_{1/2}(\alpha)$ has no finite maximum value. The functions $F_{3/2}(\alpha)$, $F_{5/2}(\alpha)$ and $F_{7/2}(\alpha)$, on the other hand, have respective finite maximum values 2.612, 1.341 and 1.127 at $\alpha = 0$, from which they decrease monotonically with increasing α and then merge with the exponential function $e^{-\alpha}$. Figure 2 shows the plot of Bose-Einstein integral functions against α.

4 Conclusions

This paper is mainly concerned with the study of two special functions, viz. Gamma function and Riemann zeta function, followed by the numerical evaluation of the Bose-Einstein integral functions. The present work follows the discussion of Bose-Einstein integrals in Ref. [16].

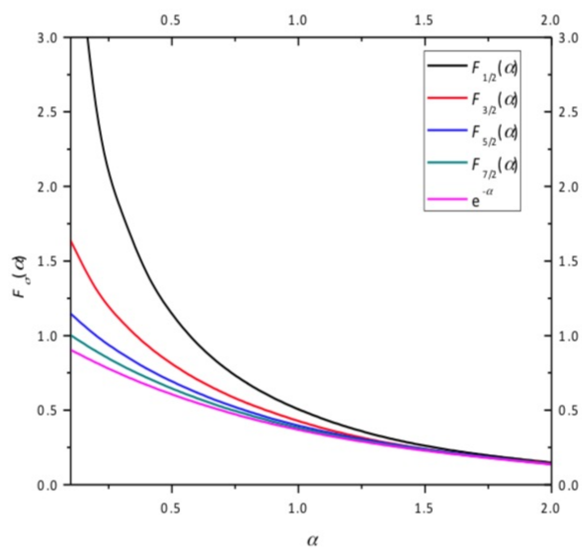

Figure 2: Plot of Bose-Einstein integral functions $F_{1/2}(\alpha)$, $F_{3/2}(\alpha)$, $F_{5/2}(\alpha)$ and $F_{7/2}(\alpha)$ with $e^{-\alpha}$ for the range $0 \leq \alpha \leq 2$.

It is found that the Gamma function of positive as well as negative rational numbers can be computed to a very high order of accuracy using Lanczos approximation. The significance and the limitation of this approximation have been discussed.

It is also observed that the Gamma function gradually decreases with the increase in the value of arguments and then after attaining a minima it increases gradually. A very significant analysis of the function is the location of the minima.

The Riemann zeta function is also discussed and then analysed the reduction of its integral form to the well-known functional equation, using which the Riemann zeta function has been computed not only for non-negative arguments but also for negative integers and fractions. The function is found to be zero for negative even integers.

From the plot of the Bose-Einstein integral functions against the Bose-Einstein gas parameter α, it is evident that the functions decrease gradually as α increases and then finally merge with the exponential function.

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