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Calculation of Integer and Noninteger *n*-Dimensional Debye Functions Using Binomial Coefficients and Incomplete Gamma Functions

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Abstract Recursion and analytical relations for the evaluation of integer and noninteger n-dimensional Debye functions have been derived. Using the binomial expansion theorem, these functions are expressed through the binomial coefficients and familiar incomplete gamma functions. This simplification and the use of the memory of the computer for calculation of binomial coefficients may extend the limits to large arguments for users and result in speedier calculation, should such limits be required in practice. Comparison of numerical results shows that analytical solutions are accurate almost from the beginning of the calculation time. The series expansion relations obtained is sufficiently accurate over the entire range of parameters. The convergence rate of the series is estimated and discussed.

Keywords Binomial expansion theorem · Debye functions · Debye temperature · Free energy · Gamma functions · Heat capacity · Heat transfer · Mössbauer spectroscopy · Tarasov equation

1 Introduction

Debye functions are widely used in the study of many physical problems, especially in the evaluation of the heat capacity of solids [1–25]. The Mössbauer recoil-free fraction, which can be calculated from the area under the spectrum, gives the strength of the chemical binding through a parameter called the Debye temperature [26–32]. In the literature, various efficient numerical methods have been proposed for

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improving the evaluation of the n-dimensional Debye function, Debye temperature, and other type of Debye functions [12–19]. The accurate evaluation of the n-dimensional Debye function gives the Debye temperature of solids, which defines a boundary between the quantum-mechanical and classical behavior of phonons [33–35]. The Debye functions can also be used in the computation of heat capacities of solids using Tarasov equations [8].

The purpose of this paper is to present the series expansion formula for integer and noninteger n-dimensional Debye functions that contain a simple sum of binomial coefficients and incomplete gamma functions which can be easily evaluated for arbitrary values of parameters. The Debye functions with integer and noninteger positive values of n, β, and x have the following form [1–6,17–20]:

$$D_n(\beta, x) = \frac{n}{x^n} \int\limits_0^x \frac{t^n}{(e^t - 1)^\beta} \mathrm{d}t. \tag{1}$$

We see from [1–39] that the accurate and fast calculation of n-dimensional Debye functions is of considerable importance in various branches of physics and chemistry.

2 Series Expansion Relations for Integer and Noninteger *n*-Dimensional Debye Functions

In order to obtain the series expansion relation for n-dimensional Debye functions, Eq. 1, we use the following binomial expansion theorem for an arbitrary real n and $|x| > |y|$ (see [40–43]):

$$(x \pm y)^n = \sum_{m=0}^{\infty} (\pm 1)^m F_m(n) x^{n-m} y^m, \tag{2}$$

where $F_0(n) = 1$ and

$$F_m(n) = \begin{cases} n!/[m!(n-m)!] & \text{for integer } n \\ \frac{(-1)^m \Gamma(m-n)}{m!\Gamma(-n)} & \text{for noninteger } n \end{cases} \tag{3}$$

We notice that for $m < 0$ the binomial coefficient $F_m(n)$ in Eq. 3 is zero and the positive integer n terms with negative factorials do not contribute to the summation. The quantity $\Gamma(\sigma)$ in Eq. 3 is the well-known Gamma function defined by [40]

$$\Gamma(\sigma) = \int\limits_0^\infty t^{\sigma-1} e^{-t} \mathrm{d}t. \tag{4}$$

Now we can derive the series expansion relation for the n-dimensional Debye functions. Using Eq. 2 in Eq. 1, we obtain for n-dimensional Debye functions the following relation:

$$D_n(\beta, x) = \frac{n}{x^n} \lim_{N\to\infty} \sum_{i=0}^{N} (-1)^i F_i(-\beta) \frac{\gamma(n+1, (i+\beta)x)}{(i+\beta)^{n+1}}, \tag{5}$$

where n and β have integer and noninteger values. Here $\gamma(\alpha, x)$ is the well-known incomplete gamma function defined by [40]

$$\gamma(\alpha, x) = \int_0^x t^{\alpha-1} \mathrm{e}^{-t} \mathrm{d}t. \tag{6}$$

We note that the choice of reliable formulas for evaluation of an incomplete gamma function is of prime importance in the accurate calculation of n-dimensional Debye functions. Several useful procedures for evaluating the incomplete gamma function can be found in our previous papers [42,43].

3 Recurrence Relations for Debye Functions of Integers *n* and *β*

The Debye functions with integer values of parameters n and β satisfy the following recursive relations:

Upward recurrence

$$D_n(\beta, x) = \frac{nx}{(n+1)(e^x-1)^\beta} + \frac{n\beta x}{(n+1)^2}(D_{n+1}(\beta, x) + D_{n+1}(\beta+1, x)), \tag{7}$$

Downward recurrence

$$\begin{aligned} D_n(\beta, x) = &-\frac{n}{(\beta-1)(e^x-1)^{\beta-1}} \\ &+ \frac{n^2}{(n-1)(\beta-1)x} D_{n-1}(\beta-1, x) - D_n(\beta-1, x). \end{aligned} \tag{8}$$

This formula can be easily established from Eq. 1 by partial integration using $u = (e^t - 1)^{-\beta}$ and $\mathrm{d}v = t^n \mathrm{d}t$.

The integer n-dimensional Debye functions can be evaluated from the recursion relation of Eq. 8 using the following generating function [40,41]:

$$\frac{x}{e^x-1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!}, \tag{9}$$

where $|x| < 2\pi$ and B_n's are the Bernoulli numbers. Taking into account the expansion formula of Eq. 9, for n-dimensional Debye functions with integer n and $\beta = 1$, it is easy to establish the new relation in terms of the Bernoulli number:

$$D_n(1,x) = \frac{n}{x^n} \lim_{N' \to \infty} \sum_{i=0}^{N'} B_i \frac{x^{n+i}}{i!(n+i)}. \tag{10}$$

The indices N and N' occurring in Eqs. 5 and 10 are the upper limits of sums.

Taking into account Eq. 10 as the starting point, all the integer n-dimensional Debye functions for integer β can be calculated by repeated application of the recurrence relation, Eq. 8.

4 Numerical Results and Discussion

In this paper, an efficient and reliably accurate scheme is presented for the direct evaluation of n-dimensional Debye functions for arbitrary integer and noninteger values of n, β and x. To the best of our knowledge, there are no studies on the evaluation of n-dimensional Debye functions with noninteger values of n and β. The use of a simple numerical computational tool for modeling and simulation can be beneficial in various applications. To demonstrate the accuracy and efficiency of the methods described above, we present several numerical results. On the basis of formulas obtained in this paper, we constructed a program for computation of the n-dimensional Debye functions using Maple 7.0 international mathematical software. The examples of computer calculation for the n-dimensional Debye functions are shown in Tables 1–3. To demonstrate the reliability of the method, we compare our results with other calculations [44] and provide estimates of their range of applicability. The n-dimensional Debye functions is computed using the formulas presented in [44] and our formulas (Eqs. 5 and 10). Comparative values also are given in Table 1. These tests clearly indicate that the formulas obtained yield significant accuracy for arbitrary values of integral parameters. As shown in Table 1, Eq. 5 is significantly more accurate in the range for $n > 8$. The numerical experiment shows that the proposed algorithm slowly converges to the exact values for $n < 8$. Greater accuracy is attainable by the use of more terms of the expansion of Eq. 5. As can be seen from Table 1, Eq. 10 converges more rapidly for $n < 8$, but the situation is reversed in Table 3 for $n \geq 8$. The numbers of terms taken into account in series expansion formulas N and correct decimal figures m_u for upward recurrences determined from $\Delta f_{\mathrm{u}} = 10^{-m_{\mathrm{u}}}$ are given in these tables, where $\Delta f = \left| f^{\mathrm{L}} - f^{\mathrm{R}} \right|$. Here, the values f^{L} and f^{R} are obtained from the left-hand side (LHS) and the right-hand side (RHS) of Eqs. 7 and 8 for the recurrence relations.

5 Conclusions

By the use of the binomial expansion theorem, the series expansion relation for Debye functions with integer and noninteger values of parameters n and β are established. The recurrence relations are also derived for Debye functions of integers n and β. The series expansion and recurrence relations obtained in this work can be used in the study of many physical problems, especially in the calculation of the heat capacity

Table 1 Comparative values of n-dimensional Debye functions

n	β	x	Equation 5	N	Equation 10	N'	Ref. [44]	m_u
2	1	5	0.172329034857624782145	800	0.172329159390141389749	500	0.172329034857624782145	9
5	1	4.5	0.10164118339698890967	800	0.10164118339698910627	200	0.10164118339698890968	17
7	1	0.8	0.69112406526865230673	800	0.69112406526865241983	50	0.69112406526865230673	16
9	1	3.4	0.15413773867789254146	800	0.15413773867789254146	120	0.15413773867789254146	26
12	1	5.4	$0.36188492338281326047\times10^{-1}$	800	$0.36188492338281326047\times10^{-1}$	500	$0.36188492338281326047\times10^{-1}$	28
15	1	2.4	0.2661409156647294951955	300	0.2661409156647294951954	100	0.2661409156647294951955	20
20	1	1.24	0.523361585088859680745	300	0.523361585090032843766	50	0.523361585088859680745	10
25	1	4.2	$0.729649670621858713684\times10^{-1}$	100	$0.72964967062185871090\times10^{-1}$	150	$0.729649670621858713684\times10^{-1}$	17
30	1	3.42	0.1258426106590655660781	100	0.1258426106590368839497	150	0.1258426106590655660781	11
9.5	3	7	$0.116377879007503348241\times10^{-5}$	800				26
12.7	5.6	8.5	$0.684510482557800342\times10^{-11}$	800				30
16.3	8.5	13.8	$0.96664095558047506\times10^{-19}$	800				37
21	10	18	$0.23506677124764645229\times10^{-26}$	800				49
25	4.5	8.4	$0.317148833858837814525\times10^{-13}$	200				42
31.4	7.5	18.4	$0.101099399375459235780\times10^{-13}$	200				61
35.4	17.5	28.4	$0.672395938192198240331\times10^{-53}$	800				82
40.6	27.1	38.8	$0.35159426729202823\times10^{-69}$	800				87
15.3	0.7	8.6	$0.2968157089479756859\times10^{-1}$	100				20
25.3	0.3	18.6	$0.84653149137360178131\times10^{-1}$	50				20
23.3	3.5	0.6	1.4081313391923920653730	400				12

Table 2 Convergence of derived expression for D_{10} (1, 2.6) as a function of summation limits $N = N'$

N	Equation 5	Equation 10
40	0.24784443192313890161720143	0.24784443192315579483148500
50	0.24784443192315386610942504	0.24784443192315582138568381
60	0.24784443192315548967709313	0.24784443192315582138240808
70	0.24784443192315574783287120	0.24784443192315582138240849
80	0.24784443192315580151442033	0.24784443192315582138240849
85	0.24784443192315581042765708	0.24784443192315582138240849
90	0.24784443192315581513671130	
95	0.24784443192315581771345067	
100	0.24784443192315581916841693	

Table 3 Convergence of derived expression for $D_{24.3}$ (6.5, 4.3) as a function of summation limits N

N	Equation 5
70	$0.39278247788638890536026 08\times10^{-10}$
80	$0.3927824778863889054321194\times10^{-10}$
90	$0.3927824778863889054393176\times10^{-10}$
100	$0.3927824778863889054402370\times10^{-10}$
110	$0.3927824778863889054403799\times10^{-10}$
120	$0.3927824778863889054404060\times10^{-10}$
130	$0.3927824778863889054404115\times10^{-10}$
140	$0.3927824778863889054404128\times10^{-10}$
150	$0.3927824778863889054404131\times10^{-10}$
160	$0.3927824778863889054404132\times10^{-10}$
170	$0.3927824778863889054404132\times10^{-10}$

and Debye temperature of solids. The use of the computer programs presented for evaluation of n-dimensional Debye functions can be also applied in the investigation of the quantum-mechanical behavior of phonons.

We note that the derived expressions for the n-dimensional Debye functions can be evaluated most efficiently, fast, and accurately. We see from Table 3 that Eq. 5 displays the most rapid convergence to the numerical result with 26-digit precision when the 120 terms in the infinite summation are taken into account.

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