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Analytic Expressions for Debye Functions and the Heat Capacity of a Solid

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Abstract: Analytic expressions for the N-dimensional Debye function are obtained by the method of brackets. The new expressions are suitable for the study of heat capacity of solids and the analysis of the asymptotic behavior of this function, both in the high and low temperature limits.

Keywords: method of brackets; Debye functions; heat capacity

MSC: 33E20; 33F10

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1. Introduction

The N dimensional Debye function, defined by the integral representation

$$D_N(X) = \frac{N}{X^N}\int_0^X \frac{t^N}{e^t-1}dt, \quad |X| < 2\pi,\ \mathrm{Re}\, N \geq 1 \tag{1}$$

play an important role in study of a variety of problems in statistical physics and solid state physics, especially in calculations of heat capacity of solids. This function appeared first in a model proposed by Debye [1] describing the heat capacity of a crystalline solid, which, with some variations, is still used today [2,3]. This has created enough interest in their evaluation for arbitrary values of N and the parameter X. (Section 8 contains an example where $X = \Theta_D/T$, with Θ_D as the Debye temperature, and T is the absolute temperature.) The alternative expression for (1) (appearing in [4], ch. 27) :

$$D_N(X) = N\left(\frac{1}{N} - \frac{X}{2(N+1)} + \sum_{k=1}^{\infty}\frac{B_{2k}}{(2k+N)\Gamma(2k+1)}X^{2k}\right), \tag{2}$$

valid for $|X| < 2\pi$ and $N \geq 1$, comes from the expansion

$$\frac{t}{e^t-1} = \sum_{k=0}^{\infty}\frac{B_k}{k!}t^k, \quad |t| < 2\pi \tag{3}$$

where B_k are the Bernoulli numbers. The values $B_0 = 1$, $B_1 = -\frac{1}{2}$ and the vanishing of B_k for odd $k \geq 3$, gives the representation

$$D_N(X) = N\left(\frac{1}{N} - \frac{X}{2(N+1)} + \sum_{k=1}^{\infty}\frac{B_{2k}}{(2k+N)\Gamma(2k+1)}X^{2k}\right), \tag{4}$$

with the restrictions given in (1). The goal of this paper is to present some expressions for $D_N(X)$ in terms of polylogarithm functions. These results are established by evaluating the integral defining $D_N(X)$ by the method of brackets [5]. This is a relatively new method of integration. Its basic rules are reviewed in Section 4. An alternative proof using the Mellin–Barnes transformation is also given. The analytic expressions for $D_N(X)$, given in [6], are may be reproduced by the formulas presented here. Numerical computation of the Debye function appears in [7,8]. The direct calculation presented here involves polylogarithms and it is simpler to compute for $N \in \mathbb{N}$.

The method of brackets was developed in the context of calculations of multidimensional definite integrals appearing in evaluation of Feynman diagrams. It consists of a small number of heuristic rules that yield the evaluation of a wide range of integrals. These rules admit an easy implementation in a computer algebra system. The reader will find more details in [5,9–12].

The Debye function $D_N(X)$ is generalized by the introduction of a parameter α as follows:

$$D_N(\alpha, X) = \frac{N}{X^N} \int_0^X \frac{t^N}{e^t - \alpha} dt, \quad \text{for } |\alpha| \leq 1, \tag{5}$$

where X is restricted by $|X| < \sqrt{\log^2 |\alpha| + (\operatorname{Arg} \alpha)^2}$, so as to have a continuous integrand. This is referred to as the generalized Debye function.

The manipulation below shows how to express the case $N = 1$, with a notation $\beta \equiv \ln \alpha$

$$\begin{aligned}
\frac{t}{e^t - \alpha} &= \frac{t - \beta + \beta}{\alpha(e^{t-\beta} - 1)} \\
&= \frac{1}{\alpha} \frac{1}{t - \beta} \left[\frac{(t-\beta)^2}{e^{t-\beta} - 1} + \frac{\beta(t-\beta)}{e^{t-\beta} - 1} \right] \\
&= \frac{1}{\alpha} \frac{1}{t - \beta} \left[(t-\beta) \sum_{k=0}^{\infty} \frac{B_k}{k!} (t-\beta)^k + \beta \sum_{k=0}^{\infty} \frac{B_k}{k!} (t-\beta)^k \right] \\
&= \frac{1}{\alpha} \frac{1}{t - \beta} \left[\sum_{k=0}^{\infty} \frac{B_k}{k!} (t-\beta)^{k+1} + \beta + \beta \sum_{k=1}^{\infty} \frac{B_k}{k!} (t-\beta)^k \right] \\
&= \frac{1}{\alpha} \frac{1}{t - \beta} \left[\beta + \sum_{k=0}^{\infty} \left(\frac{B_k}{k!} + \frac{\beta B_{k+1}}{(k+1)!} \right) (t-\beta)^{k+1} \right].
\end{aligned} \tag{6}$$

Therefore,

$$\begin{aligned}
D_1(\alpha, X) &= \frac{1}{X} \int_0^X \frac{t}{e^t - \alpha} dt \\
&= \frac{1}{X\alpha} \int_0^X \left[\frac{\beta}{t - \beta} + \sum_{k=0}^{\infty} \left(\frac{B_k}{k!} + \frac{\beta B_{k+1}}{(k+1)!} \right) (t-\beta)^k \right] dt,
\end{aligned}$$

where the only (possible) singular term is the first one

$$\frac{1}{X\alpha} \int_0^X \frac{\beta}{t - \beta} dt. \tag{7}$$

Observe that when $X < \ln \alpha$, there are no singularities, but for $X > \ln \alpha$ the integrand is singular, but it can be integrated in a sense of the principal value. The method of bracket gives the same analytic result in both the cases.

The content of the paper is described next. Sections 2 and 3 describe analytic relations between the Debye function and the polylogarithms appearing in the literature. Section 4 introduces the method of brackets. Section 5 uses this method to evaluate Debye functions and their analytic expressions. In particular, expressions that are free of integral representations are presented here, recovering those presented by [6]. These results are then used to study the asymptotic behavior of these functions in limiting values of the temperature (the relation of temperature T and the variable X is given in the previous section). Section 6 evaluates the generalized Debye function $D_N(\alpha, X)$ using the Mellin–Barnes transformations and Section 7 extends these calculations to $N \in \mathbb{C}$. Section 8 uses these representations to evaluate the internal energy and heat capacity in solids. The emphasis here is on the new expression for Debye functions to show that the manipulation of them simplifies the computation of the limits $T \to 0$ and $T \to \infty$ for temperature presented in [6].

Remark 1. *The results given here complement a variety of analytic expressions for the Debye function appearing in the literature. Kölbig considered in [13] the incomplete Riemann zeta function*

$$A(s, \lambda) = \frac{1}{\Gamma(s)} \int_0^\lambda \frac{x^{s-1}\,dx}{e^x - 1}, \tag{8}$$

a function included in the NIST Handbook [14]. The relation to the Debye function is

$$D_N(X) = \frac{N}{X^N}\Gamma(N+1)A(N+1, X). \tag{9}$$

In [15] (p. 553, Equation (14)) Kölbig pointed out that

$$A)s, \lambda) = S_{1,s-1}(1 - e^{-\lambda}), \tag{10}$$

where

$$S_{n,p}(s) := \frac{(-1)^{n+p-1}}{(n-1)!p!} \int_0^1 \log^{n-1} u \, \log^p(1 - xu) \frac{du}{u} \tag{11}$$

is the Nielsen's generalized polylogarithm. Therefore,

$$D_N(X) = \frac{N}{X^N}\Gamma(N+1)S_{1,N}(1 - e^{-X}). \tag{12}$$

On the other hand, it has been shown that [16] (p. 127, Equation (22)) and [17]

$$S_{1,p}(z) = \zeta(p+1) + \sum_{k=0}^{p} \frac{(-1)^{k-1}}{k!} Li_{p+1-k}(1-z) \log^k(1-z). \tag{13}$$

Thus

$$\begin{aligned} D_N(X) &= \frac{N}{X^N}\Gamma(N+1)\left[\zeta(N+1) + \sum_{k=0}^{N} \frac{(-1)^{k-1}}{k!} Li_{N+1-k}(e^{-X}) \log^k(e^{-X})\right] \\ &= \frac{N}{X^N}\Gamma(N+1)\left[Li_{N+1}(1) - \sum_{k=0}^{N} \frac{X^k}{k!} Li_{N+1-k}(e^{-X})\right]. \end{aligned} \tag{14}$$

The expressions above show that the main result stated in this paper may also be derived from Kölbig's work.

Remark 2. *Alternative expressions for the Debye function are given by Kölbig in [15] in terms of the incomplete Bose-Einstein function defined by*

$$B_p(\eta, u) = \frac{1}{\Gamma(p+1)} \int_0^u \frac{x^p\,dx}{e^{x-\eta} - 1} \tag{15}$$

in the form

$$D_N(\alpha, X) = \frac{N}{\alpha X^N}\Gamma(N+1)B_N(\beta, X). \tag{16}$$

Cvijovic [18] considered (14) *in terms of the function*

$$\mathcal{F}_s(x) = \int_0^x \frac{t^s e^t \, dt}{(e^t-1)^2}, \quad x \geq \delta > 0, \; s > 1, \tag{17}$$

and proved that

$$\mathcal{F}_s(x) = \frac{x^s}{1-e^x} + s\Gamma(s)A(s,x) \tag{18}$$

with A defined in (10). *The result [18] (p. 40, Equation (19))*

$$\frac{\mathcal{F}_1(x)}{n!} = \zeta(n) - \sum_{j=0}^{n} \frac{x^j}{j!} Li_{n-j}(e^{-x}), \tag{19}$$

shows the relation between $D_N(X)$ and these special functions.

2. Debye Functions in Quantum Field Theory

Debye functions are closely related to polylogarithms. As mentioned in the Introduction, they have applications in quantum optics and are related to the Planck formula of the black body radiation. The Debye functions frequently appears in Feynman diagrams with quantized energy, so called sum-integral, in the finite temperature field theory. A typical example is given by Tornheim sums, $T(a,b,c)$, defined by

$$T(a,b,c) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{m^a n^b (m+n)^c}. \tag{20}$$

References for these sums include [19,20], where they appear in the context of evaluating classes of definite integrals, and [21] is a book with a good introduction to them, mostly with a combinatorial and number-theoretical emphasis. These sums also provide a good introduction to the theory of polylogarithms, which is the main function involved in the result of this paper.

A direct manipulation provides

$$\begin{aligned} T(a,b,c) &= \frac{1}{2\pi i} \frac{1}{\Gamma(c)} \int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(c+z) \sum_{m>0} \sum_{n>0} \frac{1}{m^a n^{b+c}} \left(\frac{m}{n}\right)^z dz \\ &= \frac{1}{2\pi i} \frac{1}{\Gamma(c)} \int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(c+z)\zeta(a-z)\zeta(b+c+z) dz. \end{aligned} \tag{21}$$

As an example, we reproduce the well-known result $T(1,1,1) = 2\zeta(3)$. This is obtained in terms of the integral

$$\begin{aligned} T(1,1,1) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{mn(m+n)} \\ &= \frac{1}{2\pi i} \int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)\zeta(1-z)\zeta(2+z) dz. \end{aligned}$$

On the line of integration the real part of the argument of ζ function is greater than 1 and, using the integral representation,

$$\zeta(z)\Gamma(z) = \int_0^{\infty} \frac{t^{z-1}}{e^t-1} dt, \quad \mathrm{Re}\, z > 1, \tag{22}$$

gives the representation of the Debye function in the limit $X \to \infty$. A simple transformation gives

$$
\begin{aligned}
T(1,1,1) &= \frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)\zeta(1-z)\zeta(2+z)dz \\
&= \frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(1-z)\Gamma(2+z)\zeta(1-z)\zeta(2+z)}{(-z)(1+z)}dz \\
&= \frac{1}{2\pi i}\int_0^\infty \frac{udu}{e^u-1}\int_0^\infty \frac{d\tau}{e^\tau-1}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{1}{(-z)(1+z)}\left(\frac{u}{\tau}\right)^z dz \\
&= \frac{1}{2\pi i}\int_0^\infty \frac{udu}{e^u-1}\left(\int_0^u+\int_u^\infty\right)\frac{d\tau}{e^\tau-1}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{1}{(-z)(1+z)}\left(\frac{u}{\tau}\right)^z dz \\
&= \int_0^\infty \frac{udu}{e^u-1}\int_0^u \frac{d\tau}{e^\tau-1}\left(\frac{u}{\tau}\right)^{-1}+\int_0^\infty \frac{udu}{e^u-1}\int_u^\infty \frac{d\tau}{e^\tau-1} \\
&= \int_0^\infty \frac{du}{e^u-1}\int_0^u \frac{\tau d\tau}{e^\tau-1}+\int_0^\infty \frac{udu}{e^u-1}\int_u^\infty \frac{d\tau}{e^\tau-1} \\
&= \int_0^\infty \frac{\tau d\tau}{e^\tau-1}\int_\tau^\infty \frac{du}{e^u-1}+\int_0^\infty \frac{udu}{e^u-1}\int_u^\infty \frac{d\tau}{e^\tau-1} \\
&= 2\int_0^\infty \frac{udu}{e^u-1}\int_u^\infty \frac{d\tau}{e^\tau-1} = -2\int_0^\infty \frac{udu}{e^u-1}\ln\left(1-e^{-u}\right) \\
&= -2\int_0^\infty \frac{ue^{-u}}{1-e^{-u}}\ln\left(1-e^{-u}\right)du = \int_0^\infty \ln^2\left(1-e^{-u}\right)du \\
&= \int_0^1 \frac{\ln^2(1-t)}{t}dt = 2\zeta(3).
\end{aligned}
\tag{23}
$$

The equality in the penultimate line follows by integration by parts.

The Debye function appears in calculation of Tornheim sums at the intermediate steps which are closely related to polylogarithms and ζ function. The reader is encouraged to use this procedure for other evaluations.

3. Polylogarithms

In this section, we describe the basic definitions of polylogarithms. They will be used in the calculations of the generalized Debye functions, as in [6]. The polylogarithm function [22] is defined by

$$
\mathrm{Li}_s(x) = \sum_{k\geq 1}\frac{x^k}{k^s}, \quad \text{for } |x| \leq 1. \tag{24}
$$

The first few examples are given by

$$
\begin{aligned}
\mathrm{Li}_1(x) &= \sum_{k\geq 1}\frac{x^k}{k} = -\ln(1-x), \\
\mathrm{Li}_2(x) &= \sum_{k\geq 1}\frac{x^k}{k^2} = \int_0^x \frac{\mathrm{Li}_1(t)}{t}dt = -\int_0^x \frac{\ln(1-t)}{t}dt, \\
\mathrm{Li}_3(x) &= \sum_{k\geq 1}\frac{x^k}{k^3} = \int_0^x \frac{\mathrm{Li}_2(t)}{t}dt = -\int_0^x \frac{dt}{t}\int_0^t \frac{\ln(1-u)}{u}du.
\end{aligned}
\tag{25}
$$

These expressions may be transformed to produce other useful relations,

$$\begin{aligned}
\mathrm{Li}_3(x) &= -\int_0^x \frac{dt}{t}\int_0^t \frac{\ln(1-u)}{u}du = -\int_0^x \frac{\ln(1-u)}{u}du\int_u^x \frac{dt}{t} \\
&= \ln x\,\mathrm{Li}_2(x) + \int_0^x \frac{\ln(1-u)\ln u}{u}du \\
&= \ln x\,\mathrm{Li}_2(x) + \frac{1}{2}\ln(1-x)\ln^2 x + \frac{1}{2}\int_0^x \frac{\ln^2 u}{1-u}du \\
&= \ln x\,\mathrm{Li}_2(x) + \frac{1}{2}\ln(1-x)\ln^2 x + \frac{1}{2}\int_{1-x}^1 \frac{\ln^2(1-u)}{u}du.
\end{aligned}$$

From here and (23), it follows that

$$\zeta(3) = \mathrm{Li}_3(1) = \frac{1}{2}\int_0^1 \frac{\ln^2(1-u)}{u}du.$$

A long list of evaluations of this type may be found in [23].

4. Basic of Method of Brackets

The method of brackets is a generalized version of the Negative Dimensional Integration Method (NDIM) [24–28], a technique developed to evaluate Feynman diagrams. In quantum field theories, Feynman diagrams correspond to multi-variable integrals that represent physical processes.

This method evaluates definite integrals in one or several dimensions over the interval $[0,\infty]$. The procedure introduces the notion of a bracket and converts the integrand in a series of brackets. The method contains a small number of heuristic rules which transform the evaluation of an integral into the solution of a small linear system of equations. A summary of these rules is presented below. More details may be found in [5,9,10,12].

Rule 0. For $a \in \mathbb{C}$, the bracket associated to a is the divergent integral

$$\langle a\rangle = \int_0^\infty x^{a-1}\,dx. \tag{26}$$

Rule 1. The expansion of an arbitrary function. The use of the method of brackets requires to replace components of the integrand by their corresponding power series, that is, it is required to represent an arbitrary function $f(x)$ as:

$$f(x) = \sum_n \phi_n C(n) x^{\beta n+\alpha}, \tag{27}$$

where $C(n)$ are the coefficients in the expansion, α and β are arbitrary (complex) exponents and ϕ_n is defined by:

$$\phi_n = \frac{(-1)^n}{\Gamma(n+1)}. \tag{28}$$

For multidimensional integrals one needs an expansion in several variables, such as

$$f(x_1,x_2) = \sum_{n_1}\sum_{n_2}\phi_{n_1}\phi_{n_2}\ C(n_1,n_2)\ x_1^{\beta_1 n_1+\alpha_1}x_2^{\beta_2 n_2+\alpha_2}. \tag{29}$$

The notation ϕ_{12} is frequently used for $\phi_{n_1}\phi_{n_2}$, with similar notation for a higher number of indices.

Rule 2. Multinomial expansion. An expression of the form $(A_1+\cdots+A_r)^\mu$ often appears in the evaluation of integrals. The bracket expansion

$$(A_1+\cdots+A_r)^\mu = \sum_{n_1}\cdots\sum_{n_r}\phi_{n_1}\cdots\phi_{n_r}\ A_1^{n_1}\cdots A_r^{n_r}\frac{\langle -\mu+n_1+\cdots+n_r\rangle}{\Gamma(-\mu)},$$

has been established in [5].

Rule 3: Eliminating integration symbols. Once the first two rules are applied, the integral is converted into a bracket series. The evaluation of these series is described next.

Rule 4: Finding solutions. The result of applying the previous rules to an integral is that its value is represented by a bracket series J. The rule to evaluate this series is given first in the special case when number of sums and brackets is the same (this is the so-called index zero case): the bracket series is now written as

$$J = \sum_{n_1} \cdots \sum_{n_r} \phi_{n_1} \cdots \phi_{n_r} \, C(n_1, \cdots, n_r) \langle a_{11}n_1 + \cdots + a_{1r}n_r + c_1 \rangle \cdots \langle a_{r1}n_1 + \cdots + a_{rr}n_r + c_r \rangle.$$

The coefficient $C(n_1, \cdots, n_r)$ depends on the parameters of the integral and the index of the sum $\{n_i\}$, $i = 1, \cdots, r$. The value of this multiple sum is declared to be

$$\mathbf{J} = \frac{1}{|\det(\mathbf{A})|} \, \Gamma(-n_1^*) \cdots \Gamma(-n_r^*) \, C(n_1^*, \cdots, n_r^*), \tag{30}$$

where $\mathbf{A} = \{a_{ij}\}$ and the values $\{n_i^*\}$ $(i = 1, \cdots, r)$ are the solutions of the linear system obtained by the vanishing of the brackets:

$$\begin{cases} a_{11}n_1 + \cdots + a_{1r}n_r & = & -c_1 \\ \vdots & & \vdots \\ a_{r1}n_1 + \cdots + a_r n_r & = & -c_r. \end{cases} \tag{31}$$

If the matrix $\mathbf{A}$ is not invertible and the number of sums is larger than the number of brackets, there is an extension of the procedure described here to evaluate the integral. Details may be found in [5,12].

5. The Debye Function $D_N(\alpha, X)$ by the Method of Brackets

The Debye function has been defined by:

$$D_N(X) = \frac{N}{X^N} \int_0^X \frac{t^N \, dt}{e^t - 1}, \tag{32}$$

and the generalization considered here is defined by

$$D_N(\alpha, X) = \frac{N}{X^N} \int_0^X \frac{t^N \, dt}{e^t - \alpha}. \tag{33}$$

Here N is zero or a positive integer, X and α are positive parameters. The parameter α is introduced here to find alternative expressions for these new functions.

5.1. A Bracket Series for $D_N(\alpha, X)$

The computation of a bracket series for $D_N(\alpha, X)$ is described next. The first step is the expansion of the denominator in the integrand according to Rule 2, to obtain:

$$D_N(\alpha, X) = \frac{N}{X^N} \sum_{n_1} \sum_{n_2} \phi_{n_1} \phi_{n_2} \, (-1)^{n_2} \alpha^{n_2} \langle 1 + n_1 + n_2 \rangle \int_0^X t^N e^{t n_1} dt. \tag{34}$$

The expansion of the exponential function is

$$e^{t n_1} = \sum_{n_3} \frac{1}{n_3!} t^{n_3} n_1^{n_3} = \sum_{n_3} \phi_{n_3} (-1)^{-n_3} t^{n_3} n_1^{n_3}, \tag{35}$$

and replacing in (34) produces

$$D_N(\alpha, X) = \frac{N}{X^N} \sum_{n_1} \sum_{n_2} \sum_{n_3} \phi_{n_1} \phi_{n_2} \phi_{n_3} \, (-1)^{n_2 - n_3} \alpha^{n_2} n_1^{n_3} \langle 1 + n_1 + n_2 \rangle \int_0^X t^{N+n_3} \, dt.$$

The change of variables $y = t/(X - t)$ converts the last integral to

$$\int_0^X t^{N+n_3} \, dt = X^{N+n_3+1} \int_0^\infty \frac{y^{N+n_3}}{(y+1)^{N+n_3+2}} dy, \tag{36}$$

and the desired bracket series is

$$\int_0^X t^{N+n_3} \, dt = \frac{X^{N+n_3+1}}{\Gamma(N+n_3+2)} \sum_{n_4} \sum_{n_5} \phi_{n_4} \phi_{n_5} \langle N + n_3 + 2 + n_4 + n_5 \rangle \langle N + n_3 + n_4 + 1 \rangle.$$

This produces the final bracket series for $D_N(\alpha, X)$ as

$$\begin{aligned} D_N(\alpha, X) = \;& NX \sum_{n_1} \cdots \sum_{n_5} \phi_{n_1} \cdots \phi_{n_5} \, (-1)^{n_2 - n_3} \tfrac{n_1^{n_3}}{\Gamma(N+n_3+2)} \alpha^{n_2} X^{n_3} \\ & \times \langle 1 + n_1 + n_2 \rangle \langle N + n_3 + 2 + n_4 + n_5 \rangle \langle N + n_3 + n_4 + 1 \rangle. \end{aligned} \tag{37}$$

An expression for the integral (33) is now obtained from (37). The method of brackets yields four different series:

$$S_1 = -\frac{NX}{\alpha} \sum_{n_1 \geq 0} \sum_{n_2 \geq 0} \frac{\Gamma(N+1+n_2)}{\Gamma(N+2+n_2)} \frac{n_1^{n_2}}{n_2!} \left(\frac{1}{\alpha} \right)^{n_1} X^{n_2}, \tag{38}$$

$$S_2 = NX \sum_{n_1 \geq 0} \sum_{n_2 \geq 0} (-1)^{n_2} \frac{\Gamma(N+1+n_2)}{\Gamma(N+2+n_2)} \frac{(1+n_1)^{n_2}}{n_2!} \alpha^{n_1} X^{n_2}, \tag{39}$$

$$S_3 = \frac{N}{X^N} \sum_{n_1 \geq 0} \sum_{n_2 \geq 0} (-1)^{n_2} \frac{\Gamma(N+1+n_2)}{\Gamma(1-n_2)} \frac{(1+n_1)^{-1-N-n_2}}{n_2!} \frac{\alpha^{n_1}}{X^{n_2}}, \tag{40}$$

$$S_4 = (-1)^N \frac{N}{X^N \alpha} \sum_{n_1 \geq 0} \sum_{n_2 \geq 0} \frac{\Gamma(N+1+n_2)}{\Gamma(1-n_2)} \frac{n_1^{-N-1-n_2}}{n_2!} \left(\frac{1}{\alpha} \right)^{n_1} X^{n_2}. \tag{41}$$

The influence of the parameter α is discussed first. The four solutions S_j are power series in α or $1/\alpha$. This gives S_1 and S_4 as expansions in α in a neighborhood of infinity and S_2 and S_3 as expansions in α in a neighborhood of zero. A similar situation occurs with the parameter X. Each series represents the integral (33). Their analysis is described next.

1. The series S_4 must be neglected because the term with $n_1 = 0$ diverges.
2. The series S_3 is naturally truncated at $n_2 = 0$. Since this index is associated to the powers of X^{-1}, it represents an asymptotic approximation for case $X >> 1$. A detailed study including condition $\alpha \to 1$ yields:

$$S_4 \approx \frac{N\Gamma(N+1)}{X^N} \sum_{n_1 \geq 0} \frac{1}{(1+n_1)^{N+1}} = \frac{N\Gamma(N+1)}{X^N} \zeta(N+1), \tag{42}$$

where $\zeta(s)$ is the Riemann zeta function.
3. The series S_1 and S_2 are both convergent as power series in X. Both are expressions for $D_N(\alpha, X)$. It turns out that these are equivalent.

5.2. Analysis of the Expressions Obtained Above

5.2.1. S_1 as Solution

Rearranging the defining series produces a hypergeometric representation:

$$\begin{aligned} S_1 &= -\frac{NX}{\alpha}\sum_{n_1\geq 0}\left(\alpha^{-1}\right)^{n_1}\sum_{n_2\geq 0}\frac{\Gamma(N+1+n_2)}{\Gamma(N+2+n_2)}\frac{(Xn_1)^{n_2}}{n_2!} \\ &= -\frac{NX}{\alpha(N+1)}\sum_{n_1\geq 0}\left(\alpha^{-1}\right)^{n_1}{}_1F_1\left(\begin{matrix}N+1\\N+2\end{matrix}\middle| Xn_1\right). \end{aligned} \tag{43}$$

The previous expression may be written as

$$S_1 = -\left(\frac{N}{N+1}\right)\frac{X}{\alpha} - \left(\frac{N}{N+1}\right)\frac{X}{\alpha}\sum_{n_1\geq 1}\left(\alpha^{-1}\right)^{n_1}{}_1F_1\left(\begin{matrix}N+1\\N+2\end{matrix}\middle| Xn_1\right), \tag{44}$$

where the hypergeometric function ${}_1F_1$ is known as the Kummer function. The relation

$${}_1F_1\left(\begin{matrix}n\\n+1\end{matrix}\middle| -Z\right) = \frac{n}{Z^n}\gamma(n,Z), \tag{45}$$

where $\gamma(n,Z)$ is the incomplete Gamma function defined by the integral representation

$$\gamma(n,Z) = \int_0^Z t^{n-1}e^{-t}\,dt, \tag{46}$$

finally produces an expression for S_1 in terms of the incomplete gamma function.

In the important special case of $n \in \mathbb{N}$, the function $\gamma(n,Z)$ can be written as a finite sum

$$\gamma(n,Z) = \Gamma(n)\left[1 - e^{-Z}\sum_{k=0}^{n-1}\frac{Z^k}{k!}\right], \tag{47}$$

and then

$${}_1F_1\left(\begin{matrix}n\\n+1\end{matrix}\middle| -Z\right) = \frac{\Gamma(n+1)}{Z^n}\left[1 - e^{-Z}\sum_{k=0}^{n-1}\frac{Z^k}{k!}\right]. \tag{48}$$

The Formula (45) is now transformed to

$$\begin{aligned} {}_1F_1\left(\begin{matrix}N+1\\N+2\end{matrix}\middle| Xn_1\right) &= \frac{\Gamma(N+2)}{(-Xn_1)^{N+1}}\left[1 - e^{Xn_1}\sum_{k=0}^{N}\frac{(-Xn_1)^k}{k!}\right] \\ &= (-1)^{N+1}\frac{(N+1)\Gamma(N+1)}{X^{N+1}n_1^{N+1}}\left[1 - e^{Xn_1}\sum_{k=0}^{N}\frac{(-Xn_1)^k}{k!}\right], \end{aligned}$$

and the series S_1 can be written as

$$S_1 = -\left(\frac{N}{N+1}\right)\frac{X}{\alpha} + (-1)^N\frac{N\Gamma(N+1)}{X^N\alpha}\sum_{n_1\geq 1}\frac{\left(\alpha^{-1}\right)^{n_1}}{n_1^{N+1}}\left[1 - e^{Xn_1}\sum_{k=0}^{N}\frac{(-Xn_1)^k}{k!}\right].$$

After some algebraic manipulations, the previous expression is written as

$$\begin{aligned} S_1 &= -\left(\frac{N}{N+1}\right)\frac{X}{\alpha} + (-1)^N\frac{N\Gamma(N+1)}{X^N\alpha}\times\left[\sum_{n_1\geq 1}\frac{\left(\alpha^{-1}\right)^{n_1}}{n_1^{N+1}} - \sum_{n_1\geq 1}\frac{\left[\frac{e^X}{\alpha}\right]^{n_1}}{n_1^{N+1}}\sum_{k=0}^{N}\frac{(-Xn_1)^k}{k!}\right] \\ &= -\left(\frac{N}{N+1}\right)\frac{X}{\alpha} + (-1)^N\frac{N\Gamma(N+1)}{X^N\alpha}\times\left[\sum_{n_1\geq 1}\frac{\left(\alpha^{-1}\right)^{n_1}}{n_1^{N+1}} - \sum_{k=0}^{N}\frac{(-X)^k}{k!}\sum_{n_1\geq 1}\frac{\left[\frac{e^X}{\alpha}\right]^{n_1}}{n_1^{N+1-k}}\right]. \end{aligned}$$

The polylogarithm function [22], defined in (24), is now used to obtain an expression for the Debye function $D_N(\alpha, X)$ in the form

$$\begin{aligned} D_N(\alpha, X) &= -\left(\frac{N}{N+1}\right)\frac{X}{\alpha} \\ &+ (-1)^N \frac{N\Gamma(N+1)}{X^N \alpha} \times \left[\mathrm{Li}_{N+1}\left(\alpha^{-1}\right) - \sum_{k=0}^{N} \mathrm{Li}_{N+1-k}\left(\frac{e^X}{\alpha}\right)\frac{(-X)^k}{k!} \right]. \end{aligned} \tag{49}$$

This formula was first presented in [6].

In addition to this representation, the method of brackets produces a new expression for the Debye function using the series S_2. This is described next.

5.2.2. The Series S_2: A New Solution

As in the computation of S_1, the series defining S_2 can be written as a sum of values of the incomplete Gamma function:

$$\begin{aligned} S_2 &= NX \sum_{n_1 \geq 0} \sum_{n_2 \geq 0} \alpha^{n_1} \frac{\Gamma(N+1+n_2)}{\Gamma(N+2+n_2)} \frac{(-X)^{n_2}(1+n_1)^{n_2}}{n_2!} \\ &= \frac{N}{N+1} X \sum_{n_1 \geq 0} \alpha^{n_1} \, {}_1F_1\left(\begin{matrix} N+1 \\ N+2 \end{matrix} \,\middle|\, -(1+n_1)X \right) \\ &= \frac{N}{X^N} \sum_{n_1 \geq 0} \frac{\alpha^{n_1}}{(1+n_1)^{N+1}} \gamma(N+1, (1+n_1)X), \end{aligned} \tag{50}$$

and using (48), this becomes

$$S_2 = \frac{N\Gamma(N+1)}{X^N \alpha} \times \left[\sum_{n_1 \geq 0} \frac{\alpha^{n_1+1}}{(1+n_1)^{N+1}} - \sum_{k=0}^{N} \frac{X^k}{k!} \sum_{n_1 \geq 0} \frac{\left[\alpha e^{-X}\right]^{n_1}}{(1+n_1)^{N+1-k}} \right]. \tag{51}$$

Proceeding as in the previous case, the Debye function $D_N(\alpha, X)$ is now

$$D_N(\alpha, X) = \frac{N\Gamma(N+1)}{X^N \alpha} \left[\mathrm{Li}_{N+1}(\alpha) - \sum_{k=0}^{N} \mathrm{Li}_{N+1-k}\left(\alpha e^{-X}\right) \frac{X^k}{k!} \right]. \tag{52}$$

In summary, the method of brackets has produced two equivalent formulations of the representation of the Debye function. The first one in (49), reproducing the solution presented in [6] and the second expression, given in (52), is a new representation for $D_N(\alpha, X)$.

6. Debye Function $D_N(\alpha, X)$ by Other Methods: Comparative Analysis

The representations of the generalized Debye function given in (49) and (52), are now obtained by a direct calculation of the integral (25). This is exactly how (49) was obtained in [6].

6.1. Formula via Definition of Polylogarithms

The formula is (52). It appears that it is easier to reproduce (52) than (49). Indeed, write (in case of $N = 0$ formally)

$$\int \frac{1}{e^t - 1} dt = -\int \frac{1}{1 - e^{-t}} de^{-t} = \ln(1 - e^{-t}) = -\mathrm{Li}_1\left(e^{-t}\right). \tag{53}$$

From (1) write the formal expression $D_0(X) = 0\left[\mathrm{Li}_1(1) - \mathrm{Li}_1\left(e^{-X}\right)\right]$. This expression matches (52) for the case $N = 0$ and $\alpha = 1$. Similarly we may reproduce the results in (49) for all the higher numbers of the index N. For example, for the case $N = 1$, the indefinite integral involved is

$$\begin{aligned}
\int \frac{t}{e^t - 1} dt &= \int t\, d\ln(1 - e^{-t}) = t\ln(1 - e^{-t}) - \int \ln(1 - e^{-t}) dt \\
&= t\ \ln(1 - e^{-t}) + \int \frac{\ln(1 - e^{-t})}{e^{-t}} de^{-t} = -t\mathrm{Li}_1(e^{-t}) - \mathrm{Li}_2(e^{-t}).
\end{aligned}$$

Then (1) gives

$$\begin{aligned}
D_1(X) &= \frac{1}{X}\int_0^X \frac{t}{e^t - 1} dt = \frac{1}{X}\left[-t\mathrm{Li}_1(e^{-t}) - \mathrm{Li}_2(e^{-t})\right]\Big|_0^X \\
&= \frac{1}{X}\left[\mathrm{Li}_2(1) - X\mathrm{Li}_1\left(e^{-X}\right) - \mathrm{Li}_2\left(e^{-X}\right)\right].
\end{aligned} \tag{54}$$

This expression coincides with (52) for the case $N = 1$ and $\alpha = 1$. Similar arguments proves (52) by induction on N, using (25).

Indeed, for the case $N = 2$,

$$\begin{aligned}
\int \frac{t^2}{e^t - 1} dt &= \int t\, d\left[-t\mathrm{Li}_1(e^{-t}) - \mathrm{Li}_2(e^{-t})\right] \\
&= -t\left[t\mathrm{Li}_1(e^{-t}) + \mathrm{Li}_2(e^{-t})\right] + \int \left[t\mathrm{Li}_1(e^{-t}) + \mathrm{Li}_2(e^{-t})\right] dt \\
&= -t\left[t\mathrm{Li}_1(e^{-t}) + \mathrm{Li}_2(e^{-t})\right] - \int \frac{t\mathrm{Li}_1(e^{-t}) + \mathrm{Li}_2(e^{-t})}{e^{-t}} de^{-t} \\
&= -t\left[t\mathrm{Li}_1(e^{-t}) + \mathrm{Li}_2(e^{-t})\right] - \int t d\mathrm{Li}_2(e^{-t}) - \mathrm{Li}_3(e^{-t}) \\
&= -t\left[t\mathrm{Li}_1(e^{-t}) + \mathrm{Li}_2(e^{-t})\right] - t\mathrm{Li}_2(e^{-t}) + \int \mathrm{Li}_2(e^{-t}) dt - \mathrm{Li}_3(e^{-t}) \\
&= -t^2\mathrm{Li}_1(e^{-t}) - 2t\mathrm{Li}_2(e^{-t}) + \int \frac{\mathrm{Li}_2(e^{-t})}{e^{-t}} e^{-t} dt - \mathrm{Li}_3(e^{-t}) \\
&= -t^2\mathrm{Li}_1(e^{-t}) - 2t\mathrm{Li}_2(e^{-t}) - 2\mathrm{Li}_3(e^{-t}).
\end{aligned}$$

In this case, (1) gives

$$\begin{aligned}
D_2(X) &= \frac{2}{X^2}\left[-t^2\mathrm{Li}_1(e^{-t}) - 2t\mathrm{Li}_2(e^{-t}) - 2\mathrm{Li}_3(e^{-t})\right]\Big|_0^X \\
&= \frac{4}{X^2}\left[\mathrm{Li}_3(1) - \tfrac{1}{2}X^2\mathrm{Li}_1\left(e^{-X}\right) - X\mathrm{Li}_2\left(e^{-X}\right) - \mathrm{Li}_3\left(e^{-X}\right)\right].
\end{aligned}$$

This expression coincides with (52) when $N = 2$ and $\alpha = 1$. The case of general N is handled in a similar manner.

6.2. Formula via the Mellin–Barnes Transformation

The formula is (52). The calculation via Mellin–Barnes transformation is simpler. Apply this transformation to represent the Debye function D_1 as

$$\begin{aligned} D_1(X) &= \frac{1}{X}\int_0^X \frac{t}{e^t-1}dt = \frac{1}{X}\int_0^X \frac{te^{-t}}{1-e^{-t}}dt \\ &= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)\int_0^X te^{-t}\left(-e^{-t}\right)^z dtdz \\ &= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z\int_0^X t\left(e^{-t}\right)^{z+1} dtdz \\ &= -\frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z\left[\frac{t\left(e^{-t}\right)^{z+1}}{z+1}+\frac{\left(e^{-t}\right)^{(z+1)}}{(z+1)^2}\right]\Bigg|_0^X dz \\ &= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z\left[\frac{1}{(z+1)^2}-\frac{X\left(e^{-X}\right)^{z+1}}{z+1}-\frac{\left(e^{-X}\right)^{(z+1)}}{(z+1)^2}\right]dz. \end{aligned}$$

The method of residues is now used to produce

$$\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \frac{\Gamma(-z)\Gamma(1+z)}{z+1}x^{z+1}dz = \ln(1+x) = -\mathrm{Li}_1(-x) \tag{55}$$

$$\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^2}x^{z+1}dz = -\mathrm{Li}_2(-x) \tag{56}$$

and this yields

$$\begin{aligned} D_1(X) &= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)\left[-\frac{(-1)^{z+1}}{(z+1)^2}+\frac{X\left(-e^{-X}\right)^{z+1}}{z+1}\frac{\left(-e^{-X}\right)^{(z+1)}}{(z+1)^2}\right]dz \\ &= \frac{1}{X}\left[\mathrm{Li}_2(1) - X\mathrm{Li}_1\left(e^{-X}\right) - \mathrm{Li}_2\left(e^{-X}\right)\right]. \end{aligned}$$

This result coincides with (54).

For the arbitrary $N \in \mathbb{N}$ the calculation is a simple generalization of $N = 1$. This is presented next:

$$\begin{aligned} D_N(X) &= \frac{N}{X^N}\int_0^X \frac{t}{e^t-1}dt = \frac{1}{X}\int_0^X \frac{t^Ne^{-t}}{1-e^{-t}}dt \\ &= \frac{N}{X^N}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)\int_0^X t^Ne^{-t}\left(-e^{-t}\right)^z dtdz \\ &= \frac{N}{X^N}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z\int_0^X t^N\left(e^{-t}\right)^{z+1} dtdz \\ &= \frac{N}{X^N}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} \frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^{N+1}}(-1)^z\int_0^{X(z+1)} \tau^Ne^{-\tau}d\tau dz. \end{aligned}$$

Observe that in the last line above, the path of integration is arbitrary subject to the condition connecting the upper and lower limits of the integral. In the case $N \in \mathbb{N}$, the integrand has no branch points. Using the incomplete gamma function (46), it follows that

$$
\begin{aligned}
&\frac{N}{X^N}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^{N+1}}(-1)^z\gamma(N+1,X(z+1)) \\
&= \frac{N}{X^N}\frac{\Gamma(N+1)}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^{N+1}}(-1)^z \times \\
&\qquad \left[1-e^{-X(z+1)}\sum_{k=0}^{N}\frac{(X(z+1))^k}{k!}\right]dz \\
&= \frac{N}{X^N}\frac{\Gamma(N+1)}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^z \times \\
&\qquad \left[\frac{1}{(z+1)^{N+1}}-e^{-X(z+1)}\sum_{k=0}^{N}\frac{X^k}{k!(z+1)^{N+1-k}}\right]dz \\
&= \frac{N\Gamma(N+1)}{X^N}\left[\mathrm{Li}_{N+1}(1)-\sum_{k=0}^{N}\mathrm{Li}_{N+1-k}\left(e^{-X}\right)\frac{X^k}{k!}\right].
\end{aligned}
\tag{57}
$$

The result is now obtained from the formula

$$
\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^n}x^{z+1}dz \quad = \quad -\mathrm{Li}_n(-x) \tag{58}
$$

Thus, the combination of polylogarithms in this the last line of (57) just reproduces the formula for the incomplete gamma function (46).

6.3. Formula via Definition of Polylogarithms

A direct calculation of polylogarithms and Mellin–Barnes transformations is now used to reproduce (49). The version in (49) is more difficult to obtain and it is the only one found in [6]. The equivalence of the two formulations (49) and (52) is presented in two different ways.

Consider first the direct calculation. Using the Mellin–Barnes transformation in the case $N=0$ it follows that $D_0(X)$ is given by

$$
\begin{aligned}
\int\frac{1}{e^t-1}dt &= -\int\left[\frac{1}{e^t}+\frac{1}{1-e^t}\right]de^t \\
&= -t+\ln(1-e^t) \\
&= -t-\mathrm{Li}_1(e^t).
\end{aligned}
\tag{59}
$$

From (1) we have a formal expression $D_0(X) = 0\left[\mathrm{Li}_1(1)-X-\mathrm{Li}_1\left(e^X\right)\right]$. This agrees with (49) for the case $N=0$ and $\alpha=1$, via (25). The results in (49) also extend to higher numbers N. For example, for $N=1$, the corresponding indefinite integral is

$$
\begin{aligned}
\int\frac{t}{e^t-1}dt &= -\int\frac{te^t}{(1-e^t)e^t}dt = -\int\left[\frac{1}{e^t}+\frac{1}{1-e^t}\right]te^t dt \\
&= -\frac{t^2}{2}+\int t\,d\ln(1-e^t) = -\frac{t^2}{2}+t\ln(1-e^t)-\int\ln(1-e^t)dt \\
&= -\frac{t^2}{2}+t\ln(1-e^t)-\int\frac{\ln(1-e^t)}{e^t}de^t \\
&= -\frac{t^2}{2}-t\mathrm{Li}_1\left(e^t\right)+\mathrm{Li}_2\left(e^t\right).
\end{aligned}
$$

Then (1) implies

$$\begin{aligned}
D_1(X) &= \frac{1}{X}\int_0^X \frac{t}{e^t-1}dt = \frac{1}{X}\left[-\frac{t^2}{2} - t\mathrm{Li}_1\left(e^t\right) + \mathrm{Li}_2\left(e^t\right)\right]\Bigg|_0^X \\
&= \frac{1}{X}\left[-\frac{X^2}{2} - \mathrm{Li}_2(1) - X\mathrm{Li}_1\left(e^X\right) + \mathrm{Li}_2\left(e^X\right)\right],
\end{aligned}$$

confirming (49) for $N = 1$ and $\alpha = 1$. An induction procedure extends the result to arbitrary $N \in \mathbb{N}$.

6.4. Formula via the Mellin–Barnes Transformation

The formula is (49). The calculation via Mellin–Barnes transformation is simpler than in the previous case. The $D_1(X)$ Debye function is represented as

$$\begin{aligned}
D_1(X) &= \frac{1}{X}\int_0^X \frac{t}{e^t-1}dt = -\frac{1}{X}\int_0^X \frac{t}{1-e^t}dt \\
&= -\frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)\int_0^X t\left(-e^t\right)^z dtdz \\
&= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^{z+1}\int_0^X t\left(e^t\right)^z dtdz \\
&= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^{z+1}\left[\frac{te^{tz}}{z} - \frac{e^{tz}}{z^2}\right]\Bigg|_0^X dz \\
&= \frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^{z+1}\left[\frac{Xe^{Xz}}{z} - \frac{e^{Xz}}{z^2} + \frac{1}{z^2}\right]dz.
\end{aligned}$$

The formulae below can be obtained using residue calculations:

$$\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{z}x^z dz = \ln x - \ln(1+x) \tag{60}$$

$$\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{z^2}x^z dz = \frac{1}{2}\ln^2 x + \zeta(2) + \mathrm{Li}_2(-x) \tag{61}$$

and this yields

$$\begin{aligned}
D_1(X) &= -\frac{1}{X}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)\left[\frac{X\left(-e^X\right)^z}{z} - \frac{\left(-e^X\right)^z}{z^2} + \frac{(-1)^z}{z^2}\right]dz \\
&= \frac{1}{X}\left[-X\left[\ln(-e^X) - \ln(1-e^X)\right] + \frac{1}{2}\ln^2(-e^X) + \zeta(2) + \mathrm{Li}_2\left(e^X\right)\right. \\
&\qquad \left. -\frac{1}{2}\ln^2(-1) - 2\zeta(2)\right] = \frac{1}{X}\left[-X\left[\ln(-1) + X - \ln(1-e^X)\right]\right. \\
&\qquad \left. + X\ln(-1) + \frac{X^2}{2} - \zeta(2) + \mathrm{Li}_2\left(e^X\right)\right] \\
&= \frac{1}{X}\left[-\frac{X^2}{2} + X\ln(1-e^X) - \zeta(2) + \mathrm{Li}_2\left(e^X\right)\right] \\
&= \frac{1}{X}\left[-\frac{X^2}{2} - X\mathrm{Li}_1\left(e^X\right) - \mathrm{Li}_2(1) + \mathrm{Li}_2\left(e^X\right)\right].
\end{aligned}$$

This proves the equivalence of (49) and (52). In (49) there are no divergent series appearing making this a more convenient form.

7. Debye Function $D_N(X)$ for Complex N via Mellin–Barnes Transform

Section 6.2 shows that the simplest analysis when $N \in \mathbb{N}$ is via the Mellin–Barnes transformation of the integrand in (1). From the beginning of the proof (as in the expression (57)) it becomes clear that (52) is controlled by the incomplete gamma function. The goal of this section is to extend these arguments to $N \in \mathbb{C}$, beginning by establishing representations for $D_N(X)$ via Mellin–Barnes integrals. The Debye function has been defined for $\mathrm{Re}N \geq 1$. An extension to $N \in \mathbb{C}$ is presented next.

The analysis of $D_N(X)$ for $N \in \mathbb{C}$ proceeds via Mellin–Barnes transformations, as in the case $N \in \mathbb{N}$. Section 6.1 shows that the definitions of polylogarithm is enough to reproduce (52) by the method of brackets. On the other hand, the Mellin–Barnes transformation succeeds for $N \in \mathbb{N}$, since it reduces to the integration of elementary functions of the incomplete gamma function. Therefore, instead of obtaining an infinite series in X, as appearing in the original representation with coefficients involving Bernoulli numbers, the results is now expressed as a finite combination of polylogarithmic functions. This section verifies that a similar phenomenon occurs for $N \in \mathbb{C}$.

The analysis of the Debye function requires some representations of the incomplete gamma function. These are presented next.

7.1. ζ Function as Mellin–Barnes Transform of the Debye Function

Consider first the Mellin–Barnes representation for the incomplete gamma function. Starting with the first line in (57) as before, rewrite the incomplete gamma function in terms of the Kummer function using (45). This justifies the first line of (57), now with $N \in \mathbb{C}$. It follows that

$$\begin{aligned}
& \frac{N}{X^N}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^{N+1}}(-1)^z\gamma(N+1,X(z+1)) \\
=\;& \frac{N}{X^N}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\frac{\Gamma(-z)\Gamma(1+z)}{(z+1)^{N+1}}(-1)^z\frac{(X(z+1))^{N+1}}{N+1}\times {}_1F_1\left(\left.\begin{matrix}N+1\\N+2\end{matrix}\right|-X(z+1)\right) \\
=\;& \frac{NX}{N+1}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^z{}_1F_1\left(\left.\begin{matrix}N+1\\N+2\end{matrix}\right|-X(z+1)\right) \\
=\;& NX\left(\frac{1}{2\pi i}\right)^2\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^z\int_{-\varepsilon-i\infty}^{-\varepsilon+i\infty}\frac{\Gamma(-u)(X(z+1))^u}{N+1+u}du,
\end{aligned} \tag{62}$$

using the standard Mellin–Barnes representation of the Kummer function [29],

$$\begin{aligned}
{}_1F_1\left(\left.\begin{matrix}a\\c\end{matrix}\right|x\right) &= \frac{\Gamma(c)}{\Gamma(a)}\int_{-\varepsilon-i\infty}^{-\varepsilon+i\infty}dz\frac{\Gamma(a+z)\Gamma(-z)}{\Gamma(c+z)}(-x)^z \\
&= \frac{\Gamma(c)}{\Gamma(a)}\oint_C dz\frac{\Gamma(a+z)\Gamma(-z)}{\Gamma(c+z)}(-x)^z \\
&= \sum_{k=0}^{\infty}\frac{(a)_k}{(c)_k}\frac{x^k}{k!}.
\end{aligned} \tag{63}$$

The contour contains the vertical line, infinitesimally close to the imaginary axis (ε, δ are small positive real numbers) and it is closed at complex infinity in order to satisfy the standard convergence conditions. See [30] (Section 2.4) for details. Now, taking into account that Re $N \geq 1$ in $D_N(X)$, the last line of (62) is transformed as

$$
\begin{aligned}
& NX\left(\frac{1}{2\pi i}\right)^2 \int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z dz \\
\times & \int_{-\varepsilon-i\infty}^{-\varepsilon+i\infty} \frac{\Gamma(-u)(X(z+1))^u}{N+1+u} du \\
= & NX\left(\frac{1}{2\pi i}\right)^2 \int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z dz \\
\times & \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{\Gamma(-u)(X(z+1))^u}{N+1+u} du \\
= & NX\left(\frac{1}{2\pi i}\right)^2 \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{\Gamma(-u)X^u du}{N+1+u} \\
\times & \int_{-\delta-i\infty}^{-\delta+i\infty} \Gamma(-z)\Gamma(1+z)(-1)^z (z+1)^u dz \\
= & \frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{\Gamma(-u)X^u}{N+1+u} \left(\sum_{k=1}^{\infty} k^u\right) du \\
= & \frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{\zeta(-u)\Gamma(-u)X^u}{N+1+u} du \\
= & \frac{NX}{2\pi i} \oint \frac{\zeta(-u)\Gamma(-u)X^u}{N+1+u} du
\end{aligned}
\tag{64}
$$

This contour should be closed to the right complex infinity and the residue calculus due to gamma function in the numerator results in the initial series (1) because the Bernoulli numbers are related to the values of ζ function at the negative integers. The only residue due to ζ function is responsible for the first term in the classical series (1).

Thus, for (64) we may write

$$
\begin{aligned}
\frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{\zeta(-u)\Gamma(-u)X^u}{N+1+u} du &= 1 + NX \sum_{k=0}^{\infty} \frac{\zeta(-k)(-X)^k}{(N+1+k)k!} \\
&= 1 + NX \sum_{k=0}^{\infty} \frac{B_{k+1}X^k}{(N+1+k)(k+1)!} \\
&= 1 - \frac{NX}{2(N+1)} + N \sum_{k=1}^{\infty} \frac{B_{2k}X^{2k}}{(2k+N)(2k)!}.
\end{aligned}
$$

This produces an integral representation of the Debye function as a Mellin–Barnes transformation

$$
\frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \zeta(-u) \frac{\Gamma(-u)X^u}{N+1+u} du = D_N(X). \tag{65}
$$

It is now shown that (65) may be transformed to the initial definition of the Debye function:

$$
\begin{aligned}
\frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{\zeta(-u)\Gamma(-u)X^u}{N+1+u} du &= \frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{X^u du}{N+1+u} \int_0^{\infty} \frac{\tau^{-u-1}}{e^\tau - 1} d\tau \\
&= \frac{NX}{2\pi i} \int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty} \frac{du}{N+1+u} \left(\int_0^X + \int_X^\infty\right) \frac{\tau^{-1} d\tau}{e^\tau - 1} \left(\frac{X}{\tau}\right)^u \\
&= NX \int_0^X \frac{\tau^{-1} d\tau}{e^\tau - 1} \left(\frac{X}{\tau}\right)^{-N-1} \\
&= \frac{N}{X^N} \int_0^X \frac{\tau^N d\tau}{e^\tau - 1}.
\end{aligned}
$$

7.2. Mellin–Barnes Transform of the Kummer Function Series

Finally, the Kummer function ${}_1F_1\left(\begin{smallmatrix} N+1 \\ N+2 \end{smallmatrix}\middle| -X(z+1)\right)$ in (62) is replaced by the series (63)

$$\begin{aligned} &\frac{NX}{N+1}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^z{}_1F_1\left(\begin{matrix} N+1 \\ N+2 \end{matrix}\middle| -X(z+1)\right)dz \\ &= NX\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty}\Gamma(-z)\Gamma(1+z)(-1)^z\sum_{k=0}^{\infty}\frac{(-X(z+1))^k}{(N+1+k)k!}dz \end{aligned}$$

to obtain a final representation for $D_N(X)$ valid for $N \in \mathbb{C}$.

However, this process involves divergent sums coming from the z-integration. In this intermediate step, the divergent sums may be combined into a finite sum and the initial result (2) in terms of Bernoulli numbers is recovered. In the integral (64) this divergent sum was regularized by shifting the contour to the left in the complex plain of the Mellin–Barnes integral representation of the Kummer function (63). Further shifting the vertical line part of the contour in (64) produces analytic continuation of the result, giving an expression for $D_N(X)$ on the whole complex plane.

7.3. ζ Function in Terms of Integral over Hankel Contour

The polylogarithms and the ζ function may be represented in terms of Hankel contour integrals for arbitrary values of their arguments. Deformations of the vertical lines of the Mellin–Barnes contours to Hankel contours are useful in the transforming the contour integrals appearing in the solution of the integro-differential equations in QCD [29]. In other words, the Hankel contours may be deformed to vertical lines in order to obtain the Barnes integrals from integrals over contours of different shapes [29].

The classical representation

$$\begin{aligned} \zeta(z)\Gamma(z) &= \frac{i}{2\sin\pi z}\oint_H \frac{(-w)^{z-1}}{e^w-1}dw \\ &= -\frac{\Gamma(z)\Gamma(1-z)}{2\pi i}\oint_H \frac{(-w)^{z-1}}{e^w-1}dw, \end{aligned} \tag{66}$$

valid for arbitrary $z \in \mathbb{C}$ should be compared with (22). This last representation has restrictions on the arguments. The well-known identity for the gamma function,

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin\pi z} \quad z \notin \mathbb{Z} \tag{67}$$

was used in (66). The identity for the polylogarithm with an arbitrary index in which the integration over Hankel contour is invoked, is

$$\mathrm{Li}_N\left(e^{-\beta}\right) = -\frac{\Gamma(1-N)}{2\pi i}\oint_H \frac{(-w)^{N-1}}{e^{w+\beta}-1}dw,$$

here $N \in \mathbb{C}/\mathbb{N}$, and β is arbitrary real positive. This type of integral representations produces an alternative proof of (65):

$$
\begin{aligned}
&\frac{NX}{2\pi i}\int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty}\frac{\zeta(-u)\Gamma(-u)X^u}{N+1+u}du \\
&= -\frac{NX}{(2\pi i)^2}\int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty}\frac{\Gamma(-u)\Gamma(1+u)X^u}{N+1+u}du\oint_H\frac{(-w)^{-u-1}}{e^w-1}dw \\
&= -\frac{NX}{(2\pi i)^2}\oint_H\frac{(-w)^{-1}}{e^w-1}dw\int_{-2+\varepsilon-i\infty}^{-2+\varepsilon+i\infty}\frac{\Gamma(-u)\Gamma(1+u)}{N+1+u}\left(-\frac{X}{w}\right)^u du \\
&= -\frac{NX}{2\pi i}\oint_H\frac{(-w)^{-1}}{e^w-1}dw\left[\frac{1}{N}\left(-\frac{X}{w}\right)^{-1}+\sum_{k=0}^{\infty}\frac{1}{N+1+k}\left(\frac{X}{w}\right)^k\right] \\
&= -\frac{1}{2\pi i}\oint_H\frac{1}{e^w-1}dw-\frac{NX}{2\pi i}\sum_{k=0}^{\infty}\frac{(-X)^k}{N+1+k}\oint_H\frac{(-w)^{-1-k}}{e^w-1}dw \\
&= -\frac{1}{2\pi i}\oint_H\frac{1}{e^w-1}dw+NX\sum_{k=0}^{\infty}\frac{\zeta(-k)(-X)^k}{(N+1+k)\Gamma(k+1)} \\
&= 1+NX\sum_{k=0}^{\infty}\frac{B_{k+1}X^k}{(N+1+k)(k+1)!} \\
&= 1-\frac{NX}{2(N+1)}+N\sum_{k=1}^{\infty}\frac{B_{2k}X^{2k}}{(2k+N)(2k)!}=D_N(X).
\end{aligned}
\tag{68}
$$

8. Application: Debye Model and the Heat Capacity in Solids

An important problem in solid state physics is the determination of heat capacity using quantum treatments [1,31]. The integral expression (32) is associated to this question through a model proposed by Debye [1]. According to this model, the internal energy in solids is given as a function of the absolute temperature T, by

$$
U = 3Nk_BTD_3\left(\frac{\Theta_D}{T}\right), \tag{69}
$$

with the usual notation for Debye functions, i.e., $D_3\left(\frac{\Theta_D}{T}\right) = D_3\left(1, \frac{\Theta_D}{T}\right)$; that is, the parameter α is set to be 1. Here, k_B is the Boltzmann constant, Θ_D is called the *Debye temperature* and N the number of particles in the system.

Using (49), and with the notation $X = \Theta_D/T$, one obtains

$$
\begin{aligned}
D_3(X) = -\frac{3X}{4} - \frac{18}{X^3}\zeta(4) \\
+\frac{18}{X^3}\left[\mathrm{Li}_4\left(e^X\right) - X\,\mathrm{Li}_3\left(e^X\right) + \tfrac{1}{2}X^2\,\mathrm{Li}_2\left(e^X\right) - \tfrac{1}{6}X^3\mathrm{Li}_1\left(e^X\right)\right].
\end{aligned}
\tag{70}
$$

The expressions (70) and (71) below, are analytical expressions for the Debye function $D_3\left(\frac{\Theta_D}{T}\right) \equiv D_2(X)$, complementing the original Formula (1).

The analysis of (70) as $T \to 0\,(X \to \infty)$ is not easy to obtain directly from here. An analysis of this limiting behavior, based on the new expression (52), is presented next. Keeping the the same notation as before, start with

$$
D_3(X) = \frac{18}{X^3}\zeta(4) - \frac{18}{X^3}\mathrm{Li}_4\left(e^{-X}\right) - \frac{18}{X^2}\mathrm{Li}_3\left(e^{-X}\right) - \frac{9}{X}\mathrm{Li}_2\left(e^{-X}\right) - 3\mathrm{Li}_1\left(e^{-X}\right). \tag{71}
$$

The limiting behavior of this representation is described next. Observe that in the limiting case $T \to 0\,(X \to \infty)$, the asymptotic behavior is much simpler to obtain from (71) than from the classical (70).

8.1. Asymptotic Limits

The classical approach to study limiting behavior of these functions is usually based on their integral representations. These procedures are valid in some specific limits (high and low temperatures). An alternative procedure, based on the analytical expressions presented in this work, is described next. The new formulae permit the analysis of limiting high and low temperatures, reproducing in a unified manner the results of [7,8]. A general form of the asymptotic expansion appearing in (73) may be found in [7] (p. 285, formula 12.36). This can be verified directly: start with the integral representation for $D_N(X)$ in (1) and expand the integrand to produce

$$\begin{aligned} D_N(X) &= \frac{N}{X^N}\int_0^X \frac{t^N}{e^t-1}\,dt \\ &= \frac{N}{X^N}\sum_{k=0}^{\infty}\frac{B_k}{k!}\int_0^X t^{N-1+k}\,dt \\ &= \frac{N}{X^N}\sum_{k=0}^{\infty}\frac{B_k}{k!}\frac{X^{N+k}}{N+k}. \end{aligned} \tag{72}$$

Now $N=3$ gives (73).

The asymptotic behavior is stated next.

- As $T\to\infty$,

$$D_3\left(\frac{\Theta_D}{T}\right) \approx 1-\frac{3}{8}\frac{\Theta_D}{T}+\frac{1}{20}\left(\frac{\Theta_D}{T}\right)^2-\frac{1}{1680}\left(\frac{\Theta_D}{T}\right)^4+O\left(T^{-6}\right). \tag{73}$$

- As $T\to 0$

$$D_3\left(\frac{\Theta_D}{T}\right) \approx \frac{18}{\left(\frac{\Theta_D}{T}\right)^3}\zeta(4). \tag{74}$$

In the analysis of this last formula, the behavior of the polylogaritmic function $\mathrm{Li}_n\left(e^{-\Theta_D/T}\right) \ll 1$ as $T\to 0$ obtained from the power series expansion

$$\mathrm{Li}_n\left(e^{-\frac{\Theta_D}{T}}\right) = e^{-\Theta_D/T}+\frac{1}{2^n}e^{-2\Theta_D/T}+\frac{1}{3^n}e^{-3\Theta_D/T}+\cdots \tag{75}$$

shows that this contribution is negligible in relation to $18\zeta(4)\left(\frac{\Theta_D}{T}\right)^{-3}$. This expansion comes directly from the series definition of the polylogarithm function. From these approximations, it follows that the internal energy satisfies

- As $T\to\infty$

$$U \approx 3Nk_BT-\frac{9}{8}Nk_B\Theta_D+\frac{3}{20}Nk_B\left(\frac{\Theta_D^2}{T}\right)-\frac{1}{560}Nk_B\left(\frac{\Theta_D^4}{T^3}\right). \tag{76}$$

- As $T\to 0$

$$U \approx \frac{3}{5}\frac{\pi^4}{\Theta_D^3}Nk_BT^4. \tag{77}$$

These results are in agreement with the results appearing in the literature [7,8].

8.2. Heat Capacity

This time one employs the relation $c_V = \left(\frac{\partial U}{\partial T}\right)_V$. The limiting behaviors are now

- For $T\to\infty$

$$c_V \approx 3Nk_B - \frac{3}{20}Nk_B\left(\frac{\Theta_D}{T}\right)^2 + \frac{3}{560}Nk_B\left(\frac{\Theta_D}{T}\right)^4 + O\left(T^{-6}\right). \tag{78}$$

- For $T \to 0$

$$c_V \approx \frac{12\pi^4}{5}\left(\frac{T}{\Theta_D}\right)^3 Nk_B. \tag{79}$$

The analytical expressions for the Debye functions presented in this work now produce results valid for arbitrary temperature. From (69), and with the notation $X = \Theta_D/T$, the value c_V is given by

$$\begin{aligned} c_V \quad = \quad & -\frac{12}{5}\pi^4 Nk_B X^{-3} + 216Nk_B X^{-3}\mathrm{Li}_4\left(e^X\right) - 216Nk_B X^{-2}\mathrm{Li}_3\left(e^X\right) \\ & +108Nk_B X^{-1}\mathrm{Li}_2\left(e^X\right) - 36Nk_B\mathrm{Li}_1\left(e^X\right) + 9Nk_B X\left(\frac{e^X}{1-e^X}\right), \end{aligned}$$

and using the result in (71), it follows that

$$\begin{aligned} c_V \quad = \quad & \frac{12}{5}\pi^4 Nk_B X^{-3} - 216Nk_B X^{-3}\mathrm{Li}_4\left(e^{-X}\right) - 216Nk_B X^{-2}\mathrm{Li}_3\left(e^{-X}\right) \\ & -108Nk_B X^{-1}\mathrm{Li}_2\left(e^{-X}\right) - 36Nk_B\mathrm{Li}_1\left(e^{-X}\right) - 9Nk_B X\left(\frac{e^{-X}}{1-e^{-X}}\right). \end{aligned}$$

9. Conclusions

Analytic expressions for the Debye functions are produced using the method of brackets. These expressions differ from the classical integral representations and are given as sums of the polylogarithm functions. The results presented here reproduce formulas developed in [6]. The new expressions produced in this work, provide an efficient manner to evaluate limiting behaviors at both high and low temperatures.

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