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THE BLOCH–GRUNEISEN FUNCTION OF ARBITRARY ORDER AND ITS SERIES REPRESENTATIONS

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We derive several series representations for the Bloch–Gruneisen function of an arbitrary (integer or noninteger) order and show that it is related to other, more familiar special functions more commonly used in mathematical physics. In particular, the Bloch–Gruneisen function of integer order is expressible in terms of the Bose–Einstein function of different orders.

Keywords: Bloch–Gruneisen formula, Bloch–Gruneisen function, Bose–Einstein function, Debye function, polylogarithm, incomplete gamma function, electrical resistivity

1. Introduction

The temperature-dependent electrical resistivity $\rho(T)$ in a nonmagnetic metallic crystalline solid is given by the Bloch–Gruneisen formula [1], [2]

$$\rho(T) = A\left(\frac{T}{\Theta_{\mathrm{R}}}\right)^n \int_0^{\Theta_{\mathrm{R}}/T} \frac{t^n}{(e^t-1)(1-e^{-t})}\,dt, \tag{1}$$

where T is the absolute temperature, A is a constant taking different values for different metals, and Θ_{R} is a characteristic temperature that very closely matches the values of the Debye temperature Θ_{D} obtained from specific heat measurements. The constant n is an integer that takes the values 2, 3, and 5 depending on which scattering mechanism is dominant.

Bloch–Gruneisen-like behavior has been observed in studying the effect of electron–phonon interaction on the resistivity of metallic nanowires [3], [4] and nanocrystalline metallic films and in studying the normal-state resistivity of superconductors [5], [6]. Fitting measured data over a wide temperature range using (1) yields not only integer but also noninteger values of n such as $n = 1.5$ and $n = 4.5$ [7], [8].

It is therefore quite relevant to study the analytic properties of functions of form (1) for some (not necessarily integer) n and to find computational procedures for determining A and Θ_{R} from the resistivity data. Here, we investigate the integral

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

hereafter called the Bloch–Gruneisen function of order s and argument x, derive several of its series expansions applicable for an arbitrary order, and discuss its relation to other special functions that are more familiar and more commonly used.

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2. Expansions for $\mathcal{F}_s(x)$

We first note that using integration by parts, we can recast the integrals in (2) in the form

$$\mathcal{F}_s(x) = \frac{x^s}{1-e^x} + s\int_0^x \frac{t^{s-1}}{e^t-1}dt = \frac{x^s}{1-e^x} + s\Gamma(s)z_s(x), \tag{3}$$

where $\Gamma(s)$ denotes the well-known gamma function and $z_s(x)$ denotes the incomplete Riemann zeta function. Such a name is explained by the fact that (Eq. 23.2.7 in [9])

$$z_s(\infty) = \zeta(s) := \frac{1}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}}{e^t-1}dt, \quad \operatorname{Re} s > 1,$$

where $\zeta(s)$ denotes the Riemann zeta function, which is usually defined by the series (Eq. 23.2.1 in [9])

$$\zeta(s) = \sum_{k=1}^\infty \frac{1}{k^s}, \quad \operatorname{Re} s > 1, \tag{4}$$

in its convergence region and by analytic continuation in the entire complex plane and also using the decomposition of the function $\zeta(s)$

$$\zeta(s) = \frac{1}{\Gamma(s)}\left(\int_0^x \frac{t^{s-1}}{e^t-1}dt + \int_x^\infty \frac{t^{s-1}}{e^t-1}dt\right) = z_s(x) + Z_s(x), \quad \operatorname{Re} s > 1, \quad 0 < x < \infty,$$

where $Z_s(x)$ is the complementary incomplete Riemann zeta function. But we also note that a classical special function called the Debye function is usually defined as $\Gamma(s+1)z_{s+1}(x)$ for *integers* $s = 1, 2, 3, \ldots$ (Eq. 27.1.1 in [9]; also see [10]–[14] for more details on exceptionally deep connections between properties of the Riemann zeta function and various outstanding problems in modern physics).

We first derive the expansions of $\mathcal{F}_s(x)$ for any real $s > 1$,

$$\mathcal{F}_s(x) = \sum_{k=0}^\infty \frac{B_k}{k!}\frac{(1-k)x^{k+s-1}}{k+s-1}, \quad 0 < x < 2\pi, \tag{5}$$

and

$$\mathcal{F}_s(x) = \sum_{k=0}^\infty \frac{B_k}{k!}\frac{(1-k)\xi^{k+s-1}}{k+s-1} + s\int_\xi^x \frac{t^{s-1}}{e^t-1}dt, \quad x \geq 2\pi, \quad 0 < \xi < 2\pi, \tag{6}$$

which involve the Bernoulli numbers B_k, $k = 0, 1, 2, \ldots$, defined (as usual) by the exponential generating function (Eq. 23.1.1 in [9])

$$\frac{t}{e^t-1} = \sum_{k=0}^\infty B_k \frac{t^k}{k!}, \quad |t| < 2\pi. \tag{7}$$

The series expansions in (5) and (6) can be somewhat simplified because in view of (see Eq. 23.1.19 in [9])

$$B_0 = 1, \qquad B_1 = -\frac{1}{2}, \qquad B_{2k+1} = 0, \quad k \in \mathbb{N},$$

they can be rewritten as

$$\sum_{k=0}^\infty \frac{B_k}{k!}\frac{x^{k+s-1}}{k+s-1} = \frac{x^{s-1}}{s-1} - \frac{x^s}{2s} + \sum_{k=1}^\infty \frac{B_{2k}}{(2k)!}\frac{x^{2k+s-1}}{2k+s-1}$$

and

$$\sum_{k=0}^{\infty} \frac{B_k}{k!} \frac{(1-k)x^{k+s-1}}{k+s-1} = \frac{x^{s-1}}{s-1} + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} \frac{(1-2k)x^{2k+s-1}}{2k+s-1}.$$

To derive these expansions, we evaluate the defining integral for $z_s(x)$ by splitting its integration interval into the intervals $[0, \xi]$ and $[\xi, x]$, $0 < \xi < 2\pi$. Substituting series (7) in the integral over $[0, \xi]$, we obtain

$$z_s(x) = \frac{1}{\Gamma(s)} \left(\sum_{k=0}^{\infty} \frac{B_k}{k!} \frac{\xi^{k+s-1}}{k+s-1} + \int_{\xi}^{x} \frac{t^{s-1}}{e^t - 1} dt \right) \tag{8}$$

and

$$z_s(x) = \frac{1}{\Gamma(s)} \sum_{k=0}^{\infty} \frac{B_k}{k!} \frac{x^{k+s-1}}{k+s-1} \tag{9}$$

in the case where $x = \xi$. Combining (3) with (8) and (9) now yields

$$\mathcal{F}_s(x) = \frac{x^s}{1-e^x} + s \sum_{k=0}^{\infty} \frac{B_k}{k!} \frac{x^{k+s-1}}{k+s-1}, \quad 0 < x < 2\pi, \tag{10}$$

and

$$\mathcal{F}_s(x) = \frac{x^s}{1-e^x} + s \sum_{k=0}^{\infty} \frac{B_k}{k!} \frac{\xi^{k+s-1}}{k+s-1} + s \int_{\xi}^{x} \frac{t^{s-1}}{e^t - 1} \, dt, \quad x \geq 2\pi, \quad 0 < \xi < 2\pi. \tag{11}$$

Finally, the expansions proposed in (5) and (6) easily follow from (10) and (11) by expanding the function $x^s/(1-e^x)$ as a series using (7).

The second set of expansions of $\mathcal{F}_s(x)$, applicable for any $s > 1$, is

$$\mathcal{F}_s(x) = \sum_{k=1}^{\infty} \frac{\gamma(s+1, kx)}{k^s}, \quad x > 0, \tag{12}$$

$$\mathcal{F}_s(x) = \Gamma(s)\zeta(s) - \sum_{k=1}^{\infty} \frac{\Gamma(s+1, kx)}{k^s}, \quad x > 0, \tag{13}$$

and it involves two related functions, the incomplete gamma function (Eq. 6.5.2 in [9])

$$\gamma(a, x) = \int_0^x t^{a-1} e^{-t} \, dt, \quad \operatorname{Re} a > 0, \quad x \geq \delta > 0, \tag{14}$$

and the complementary incomplete gamma function $\Gamma(s, x)$, which are the components in the decomposition of the gamma function (Eq. 6.5.3 in [9])

$$\Gamma(s) = \gamma(s, x) + \Gamma(s, x). \tag{15}$$

To prove (12) and (13), we again evaluate the defining integral of $z_s(x)$ and using the expansion

$$\frac{1}{e^t - 1} = \frac{e^{-t}}{1 - e^{-t}} = \sum_{k=1}^{\infty} e^{-kt}, \quad t > 0, \tag{16}$$

obtain

$$z_s(x) = \frac{1}{\Gamma(s)} \sum_{k=1}^{\infty} \int_0^x t^{s-1} e^{-kt} \, dt = \frac{1}{\Gamma(s)} \sum_{k=1}^{\infty} \frac{\gamma(s, kx)}{k^s}, \tag{17}$$

where interchanging the integration and summation is justified by absolute convergence, which in turn gives

$$\mathcal{F}_s(x) = \frac{x^s}{1-e^x} + s\sum_{k=1}^{\infty}\frac{\gamma(s,kx)}{k^s}, \quad x>0. \tag{18}$$

Recalling the definition of $\gamma(\alpha, x)$ in (14), we now easily use integration by parts to verify the recurrence relation

$$\gamma(\alpha,x) = \frac{1}{\alpha}\big(\gamma(\alpha+1,x) - x^{\alpha}e^{-x}\big).$$

Finally, this relation and series expansion (16) allow deriving the sought expansion in (12) from (18). It remains to show that by (15) and series (4), we obtain the required expansion in (13).

In the important case where the parameter s is an integer, we can deduce one more expansion for $\mathcal{F}_s(x)$,

$$\frac{\mathcal{F}_n(x)}{n!} = \zeta(n) - \sum_{j=0}^{n}\frac{x^j}{j!}\operatorname{Li}_{n-j}(e^{-x}), \quad n=2,3,\ldots, \tag{19}$$

where $\operatorname{Li}_s(x)$ denotes the polylogarithm function given by the series

$$\operatorname{Li}_s(z) = \sum_{k=1}^{\infty}\frac{z^k}{k^s} \tag{20}$$

in its convergence region and by analytic continuation in the rest of the complex plane (see, e.g., [15], [16]).

Indeed, starting from the definition of $\gamma(s,x)$ in (14) and using the easily derived formula

$$\int t^n e^{\alpha t}\,dt = e^{\alpha t}\sum_{j=0}^{n}(-1)^j\frac{n!}{\alpha^{k+1}(n-k)!}t^{n-k},$$

we obtain

$$\gamma(n+1,x) = n!\left(1 - e^{-x}\sum_{j=0}^{n}\frac{x^j}{j!}\right). \tag{21}$$

The sought result (19) now follows from (12) and (21). We note that (19) can be given in the form

$$\frac{\mathcal{F}_2(x)}{2!} = \zeta(2) + \frac{1}{1-e^x} + \log(1-e^{-x}). \tag{22}$$

For $n = 3, 4, \ldots,$ we then obtain

$$\frac{\mathcal{F}_n(x)}{n!} = \zeta(n) - \frac{e^{-x}}{1-e^{-x}} + \log(1-e^{-x}) - \sum_{j=0}^{n-2}\frac{x^j}{j!}\operatorname{Li}_{n-j}(e^{-x}) \tag{23}$$

because

$$\operatorname{Li}_0(x) = \frac{x}{1-x}, \qquad \operatorname{Li}_1(x) = -\log(1-x).$$

3. Concluding remarks

We note that the defining integral of $\mathcal{F}_s(x)$ cannot be evaluated in a closed form in terms of other functions. But at low and high temperatures, i.e., for $T \ll \Theta_{\mathrm{R}}$ and for $T \gg \Theta_{\mathrm{R}}$, it can be respectively approximated by

$$\mathcal{F}_s(x) \approx \Gamma(s+1) \qquad \text{and} \qquad \mathcal{F}_s(x) \sim \frac{x^{s-1}}{s-1}.$$

Computing the function $\mathcal{F}_s(x)$ in the intermediate temperature range can be based on one of several basic approaches: numerical quadrature, series expansions, polynomial or rational approximation schemes, and generation and interpolation of tabular values. An appropriate approximation to the integral would greatly facilitate determining A and Θ_{R} (see Eq. (1)) because a nonlinear least-squares fit requires a rather accurate numerical integration at each temperature. It is possible that certain kinds of Gauss quadrature or the use of continued fractions can give an optimal algorithm for calculating $\mathcal{F}_s(x)$ numerically, and this should be investigated further. In [17], an approximation was proposed for $n = 5$ in the form of a ninth-order polynomial in $\log(\Theta/T)$. In [18], an approximation was proposed for integer n in the form of a truncated series. In [19], expansions and approximations applicable for integer n were found, and this method was extended in [20].

We have derived series expansions for $\mathcal{F}_s(x)$. Formulas (5), (6), (12), and (13) are applicable for any real order $s > 1$, while series (23) is applicable only for an integer order $n \geq 2$. A detailed computational comparison of the different approximation methods based on these series is in progress, and we limit ourself to a few remarks here. Series (12) converges very quickly if x is small, while if x is large, it is extremely important to choose an appropriate way to compute $\gamma(a, x)$ in (12) because there are numerous computational schemes for it. Also, the computation of the Bernoulli numbers can be unstable, and care must be taken in using series (5) and (6).

Finally, we showed that $\mathcal{F}_s(x)$ is related to other special functions that are more familiar and more commonly used. In addition to the incomplete gamma function and the incomplete Riemann zeta function (or Debye function), we encountered the polylogarithm function. But we note that Eq. (23) for $n = 3, 4, \dots$ can be rewritten as

$$\frac{\mathcal{F}_n(x)}{n!} = \zeta(n) + \frac{1}{1-e^x} + \log(1-e^{-x}) - \sum_{j=0}^{n-2} \frac{x^j}{j!} B_{n-j-1}(-x), \tag{24}$$

where $B_s(x)$ is the Bose–Einstein function (see, e.g., [21]); in other words, the Bloch–Gruneisen function of integer order is expressible in terms of the Bose–Einstein function of different orders. It remains to be seen what impact these relations can have on computing the Bloch–Gruneisen function.

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