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PHONONS BLOCH-GRÜNEISEN FUNCTION AND ITS APPLICATIONS TO NOBLE METALS RESISTIVITY, PART I

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Abstract: Internal thermal energy in solids contributes to all kinds of bosons and fermions energy across very complicated mechanisms. Bloch-Grüneisen (BG) function is considered a main term which controls in phonons resistivity.

Mathematical treatment had been applied on BG resistivity equation, which gave a Semi-empirical relationship between integral constant and Debye temperature in noble metals as a function of temperature. Comparison between theoretical and experimental was examined.

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1. Introduction

Bosons mean phonons, magnons or photons, where phonons are a cornerstone

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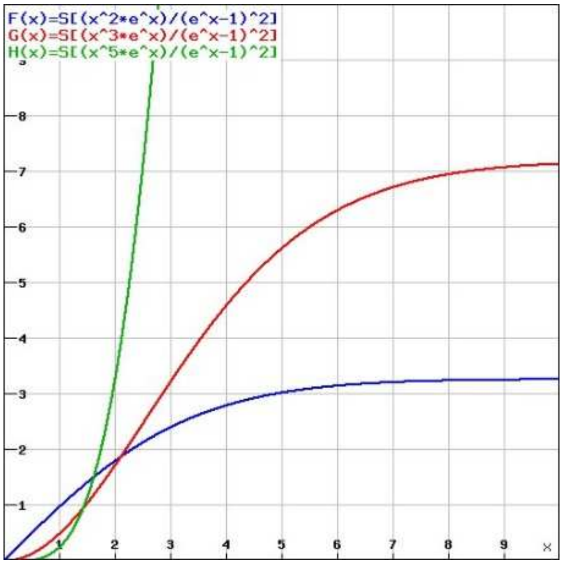

Figure 1: Mathematical integral graph of equation (1) for small $J(2, 3, 5, x)$ values (see http://rechneronline.de/function-graphs/)

in solid state physics. They are contributing to thermal and electrical conductivity, specific heat, melting, and superconductivity, if there are no phonons, transmission of sound in all materials would be acoustic insulators.

In solid-state physics, phonons BG function $J(n, x)$, see[1]-[4], is defined by:

$$J(n,x) = \int_0^x t^n \frac{e^t}{(e^t-1)^2} dt \qquad (1)$$

Figure 1 and Figure 2 show graphs of BG function $J(n, x)$ for n=2, 3, 5.

Nevertheless, in mathematics, equation (1) may be named as the transport function. Most components of expression (1) come from, Bose-Einstein statistics [5 - 10] and According to the type of particles or quasi-particles, whether they were phonons or magnons.

The temperature-dependent electrical resistivity or specific heat in most kinds of metals and their alloys must have in its relationship part of equation (1).

The aim of this paper is to find algebraic value of the mathematical integration in equation (1), and get a semi-empirical equation to the noble metal resistivity to calculate some of the physical constants.

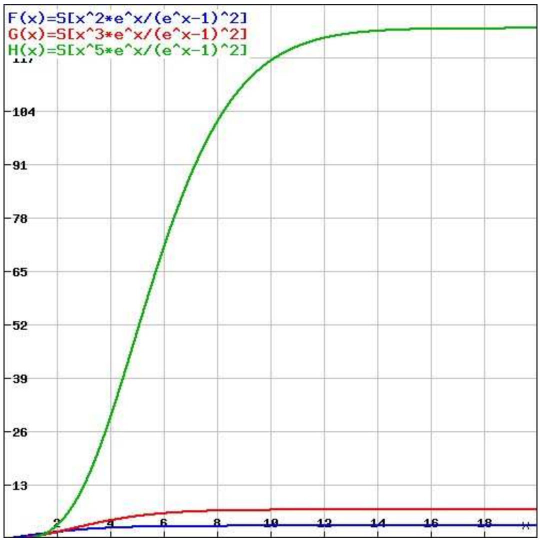

Figure 2: Mathematical integral graph of equation (1) for high $J(2,3,5,x)$ values

2. Quantum Statistical Mechanics

The expected number of particles with energy ε_i for all statistical distributions are n_i where [11]:

$$\begin{aligned} n_i =& \frac{1}{e^{(\varepsilon_i-\mu)/\mathrm{K_B T}+1}}, && \text{Fermi-Dirac distribution,} \\ n(\omega) =& \frac{1}{e^{(\hbar\omega/\mathrm{K_B T})-1}}, && \text{Bose-Einstein distribution,} \\ n_i =& \frac{g_i}{e^{\left(\varepsilon_i-\mu\right)/K_B T}}, && \text{Maxwell-Boltzmann distribution.} \end{aligned} \tag{2}$$

Here Bose-Einstein and Fermi-Dirac integrals given by (see [12], [13]):

$$\begin{aligned} B_s(\mu) =& (p!)^{-1} \int_0^\infty \frac{\varepsilon^s}{e^{(\varepsilon-\mu)}-1}\, d\varepsilon, && \text{Bose-Einstein integrals,} \\ F_s(\mu) =& (p!)^{-1} \int_0^\infty \frac{\varepsilon^s}{e^{(\varepsilon-\mu)}+1}\, d\varepsilon && \text{Ferml-Dirac integrals.} \end{aligned} \tag{3}$$

Estimation of Bloch-Grüneisen, Bose-Einstein and Fermi-Dirac integrals are not easy, but Pass through very complex mathematical treatments.

Bloch-Grüneisen resistivity ($n = 5$) or Bloch-Wilson (BW) formula ($n = 3$) (see [14]) was physically presented by this equation (see [15]-[17]):

$$\begin{aligned}\rho_{electron-\text{phonon}}(T) &= \frac{C}{M\theta_R}\left(\frac{T}{\theta_R}\right)^5 \int_0^{\frac{\theta}{T}} \frac{z^5}{(e^z-1)(1-e^{-z})}dz \\ &= \frac{C}{M\theta_R}\left(\frac{T}{\theta_R}\right)^5 J_5\left(\frac{T}{\theta_R}\right) \\ \rho^{N-process}_{electron-\text{phonon}}(T) &= 4A\left(\frac{T}{\theta_R}\right)^5 J_5\left(\frac{T}{\theta_R}\right) \\ \rho^{U-process}_{electron-\text{phonon}}(T) &= BT^3 J_3\left(\frac{T}{\theta_R}\right),\end{aligned} \tag{4}$$

where

$$J_n\left(\frac{T}{\theta_R}\right) = \int_0^{\frac{\theta}{T}} \frac{z^n}{(e^z-1)(1-e^{-z})}dz = \int_0^{\frac{\theta}{T}} \frac{z^n e^z}{(e^z-1)^2}dz.$$

Here A is a constant, proportional to the square of the electron-lattice interaction constant C (constant of the metal), θ_R is the Debye temperature obtained from resistivity measurements, $J_n\left(\frac{T}{\theta_R}\right)$a transport integral (see [14]-[16]), which belong to the family of the Bloch - Grüneisen functions.

In the same context, not only resistivity that subject to BG function but also Phonons specific heat which derivative from thermal energy in solids. For all possible frequencies up to the maximum frequency (quantum Debye model), thermal energy given by [18]:

$$U_{phonons} = \int_0^{\omega_{\max}} \frac{V\omega^2}{2\pi^2\upsilon_s^3}\,\frac{\hbar\omega}{e^{\hbar\omega/K_BT}-1}d. \tag{5}$$

If $\upsilon_s$is identical for all three polarization, and suppose that:

$$\begin{aligned}&x \equiv \frac{\hbar\omega}{K_BT} \Rightarrow x_{\max} = \frac{\hbar\omega_{\max}}{K_BT} \Rightarrow x_D = \frac{\hbar\omega_D}{K_BT} \equiv \frac{\Theta}{T} \\ &\text{where } \Theta = \frac{\hbar\omega_D}{K_B} \Rightarrow U_{phonons} = 9NK_BT(\frac{T}{\Theta})^3 \int_0^{x_D} \frac{x^3}{e^x-1}\,dx.\end{aligned} \tag{6}$$

Where the Integral in equation (6) belong to the family of Debye functions. Derivative phonons energy will give specific heat as follows: [19, 20]

$$C_{phonons} = 9Nk_B \left(\frac{T}{\Theta}\right)^3 \int_0^{x_D} \frac{x^4 e^x}{(e^x-1)^2} dx, \tag{7}$$

where Integral in equation (7) belong to the family of BG functions.

Similarly, with phonons specific heat, fermions specific heat may be written as follows:

$$C_{v(fermions)} = AT^n \int_0^{\infty} \frac{x^{n+1}}{(e^x+1)^2}\, dx, \quad n=1. \tag{8}$$

3. Mathematical Integrals Results of Bloch-Grüneisen(BG) Function

In all equations log(x) is the natural logarithm and Li_s(x) = polylog (s, x) is the polylogarithm function given by:

$$Li_s(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^s} = x + \frac{x^2}{2^s} + \frac{x^3}{3^s} + \cdots, \tag{9}$$

where

$$Li_0(x) = \frac{x}{1-x} \qquad Li_1(x) = -\log(1-x).$$

When $e^y = x$, Then base e logarithm of x is $\ln(x) = \log e(x) = y$. In addition, Riemann zeta function describes by [21]:

$$\zeta(s) = \lim_{n\to\infty} \sum_{n=1}^{\infty} n^{-s} \quad or \quad \zeta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{x^{s-1}}{e^x - 1} dx, \tag{10}$$

where

$$Li_s(1) = \zeta(s), \quad \Gamma(s) \text{ is Gamma function}$$

The polylogarithm also arises in the closed form of the integrals of the Fermi-Dirac distribution and the Bose-Einstein Distribution:

$$\begin{aligned} \int_0^{\infty} \frac{\varepsilon^s}{e^{(\varepsilon-\mu)}-1}\, d\varepsilon &= \Gamma(s+1) Li_{1+s}(e^{\mu}) \quad \text{Bose-Einstein integrals},\\ \int_0^{\infty} \frac{\varepsilon^s}{e^{(\varepsilon-\mu)}+1}\, d\varepsilon &= -\Gamma(s+1) Li_{1+s}(-e^{\mu}) \quad \text{Ferml-Dirac integrals}. \end{aligned} \tag{11}$$

Many attempt was made to simplify BG functions [22]-[26], the integral formula for Debye specific heat function was treated by [27], [28] and written as follows:

$$
\begin{aligned}
C_v(3,x) =& \frac{3}{x^3}\int_0^x t^4 \frac{e^{-t}}{(1-e^{-t})^2}dt,\\
C_v(3,x) =& \frac{4\pi^4}{5x^5} + \frac{3xe^{-x}}{(e^{-x}-1)} + 12\left(\ln(1-e^{-x})\right) - \frac{36}{x}Li_2(e^{-x})\\
& - \frac{72}{x^2}Li_3(e^{-x}) - \frac{72}{x^3}Li_4(e^{-x}),
\end{aligned}
\tag{12}
$$

where

$$x = \frac{\theta_D}{T}.$$

In addition, Deutsch [29] was reported BG function for n=5 by the following equation:

$$
\begin{aligned}
J(5,x) = 120\zeta(5) - \sum_{n=1}^{\infty} e^{-nx}[x^5 + 5x^4/n + 20x^3/n^2 + 60x^2/n^3\\
+ 120x/n^4 + 120/n^5],
\end{aligned}
\tag{13}
$$

where

$$x = \frac{\theta_D}{T}.$$

However, mathematical programs may be simplify the problem to give solutions for all complicated functions as follows:

$$J(n,x) = \int_0^x t^n \frac{e^t}{(e^t-1)^2}dt, \tag{14}$$

$$J(1,x) = -x - \frac{x}{-1+e^x} + \text{Log}[1-e^x] + Constant,$$

$$Li_1(1) = \zeta(1) = \infty, \tag{15}$$

$$J(2,x) = x\left(\frac{e^x x}{1-e^x} + 2\text{Log}[1-e^x]\right) + 2\text{PolyLog}[2,e^x] - \frac{\pi^2}{3}.$$

$$Li_2(1) = \zeta(2) = \frac{\pi^2}{6} \simeq 1.645, \tag{16}$$

$$J(3,x) = x^2\left(\frac{e^x x}{1-e^x} + 3\text{Log}[1-e^x]\right) + 6x\text{PolyLog}[2,e^x] - 6\text{PolyLog}[3,e^x]$$

$$
\begin{aligned}
&- 7.212,\\
Li_3(1) =& \zeta(3) = 1.202, \qquad (17)\\
J(4,x) =& - x^4 - \frac{x^4}{-1+e^x} + 4x^3 \text{Log}[1-e^x] + 12x^2 \text{PolyLog}[2,e^x]\\
&- 24x\text{PolyLog}[3,e^x] + 24\text{PolyLog}[4,e^x] - \frac{24}{90}\pi^4,\\
Li_4(1) =& \zeta(4) = \frac{\pi^4}{90} \simeq 1.082, \qquad (18)\\
J(5,x) =& - x^5 - \frac{x^5}{-1+e^x} + 5x^4 \text{Log}[1-e^x] + 20x^3 \text{PolyLog}[2,e^x]\\
&- 60x^2\text{PolyLog}[3,e^x] + 120x\text{PolyLog}[4,e^x]\\
&- 120\text{PolyLog}[5,e^x] - 124.44,\\
Li_5(1) =& \zeta(5) = 1.037. \qquad (19)
\end{aligned}
$$

4. Results and Discussion

AL-Jalali [30] was analyzing noble metals experimental resistivity data as in figure (3).Figure (3) shows a general diagram between total noble metals resistivity as a function of low and high temperatures.

At low temperatures, the total theoretical resistivity in pure noble metals as expected may be written as:

$$
\rho = \rho_0 + AT^2 + BT^3 \int_0^{\frac{\theta}{T}} \frac{z^3}{(e^z-1)(1-e^{-z})} dz + CT^5 \int_0^{\frac{\theta}{T}} \frac{z^5}{(e^z-1)(1-e^{-z})} dz. \qquad (20)
$$

Whereas at high temperature, resistivity will become:

$$
\rho = \rho_0 + aT. \qquad (21)
$$

Table (1) show total resistivity for noble metals (Cu, Ag, Au) as a function of temperature. Precise mathematical analysis shows temperature dependence of total resistivity as a power series equation:

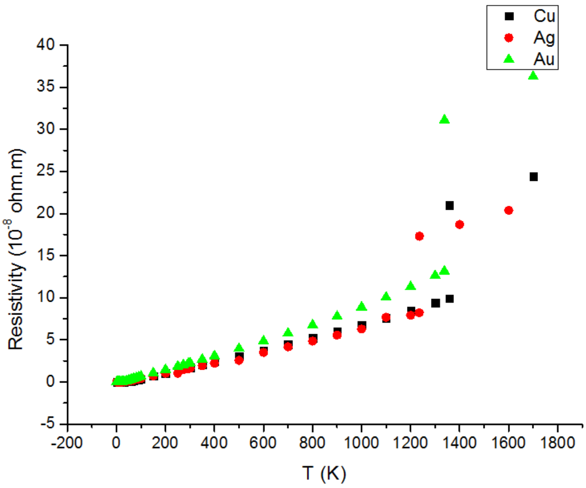

Figure 3: Noble metals resistivity as a function of low and high temperatures

$$\rho = (\rho_0 = a_0) + a_1T + a_2T^2 + a_3T^3 + a_4T^4 + a_5T^5 + a_6T^6 + a_7T^7 + \cdots = \sum_{n=0}^{\infty} a_nT^n, \quad (22)$$

Where the first term is residual resistivity, second and third terms belong to electron-electron resistivity, and remain terms belong to electron -phonon resistivity.

As for Debye temperature, a power series equation has got between Debye temperature in Cu, Ag, and Au (from Debye specific heat) as a function of temperature as follows:

$$\theta_D = a_0+a_1T+a_2T^2+a_3T^3+a_4T^4+a_5T^5+a_6T^6+a_7T^7+\cdots = \sum_{n=0}^{\infty} a_nT^n. \quad (23)$$

Table (2) shows temperature coefficients to Debye temperatures (θ_D) as a function of temperature.

Comparing between temperature coefficients in table (1, 2), theoretical equations (4, 20), and mathematical equation (19), Semi-empirical expression of phonons resistivity equation has investigated to graph or calculate the electron-lattice interaction constant C in equation (4) (constant of metal) numerically as a function of temperature.

Metal/ Temp.	a_0	a_1	a_2	a_3
Cu	0.0020072477	-6.59215 e-06	6.1465634e-07	1.9487627 e-07
Ag	0.0010727211	-8.5974242 e-05	2.3020238e-05	-2.3107606 e-06
Au	0.021514659	0.00057307547	-0.00015561305	1.5810016$e-$05

Metal/ Temp.	a_4	a_5	a_6	a_7
Cu	-3.7625358 e-08	2.396102 e-09	-4.5951453 e-11	2.9285589e-13
Ag	1.0165649 e-07	-2.2483697 e-10	-2.7065371 e-11	2.5129472 e-13
Au	-6.6902756 e-07	1.8891179 e-08	-2.8090806 e-10	1.6022257 e-12

Table 1: Coefficients of temperature in total experimental resistivity equation

Metal/ Temp.	a_0	a_1	a_2
Cu	346.9929	-0.69513111	0.13541134
Ag	227.22953	-1.0256429	0.45467396
Au	155.75443	3.4437989	-0.27512537

Metal/ Temp.	a_3	a_4	a_5	a_6
Cu	-0.015693188	0.00049115137	-4.4563378e-06	
Ag	-0.074871003	0.0045972012	-0.00012263238	1.210334e-06
Au	-0.0070253444	0.0015493054	-5.7678039e-05	6.797874e-07

Table 2: Temperature coefficients of equation (23)

In this way, Semi-empirical equation between electron-lattice interaction constant C (constant of the metal) and Debye temperature as a function of temperature has achieved as follows:

$$\rho^{N-process}_{electron-\text{phonon}}(T) = \frac{C}{M\theta_R}\left(\frac{T}{\theta_R}\right)^5 \int_0^{\frac{\theta}{T}} \frac{z^5}{(e^z-1)(1-e^{-z})}dz$$
$$= \frac{C}{M\theta_R}\left(\frac{T}{\theta_R}\right)^5 J_5\left(\frac{T}{\theta_R}\right) = a_5T^5,$$

$$C = \frac{a_5 M}{J_5\left(\frac{T}{\theta_R}\right)}$$

$$= a_5 M\theta_R^6 \left\{ \begin{array}{l} [-x^5 - \frac{x^5}{-1+\mathrm{e}^x} + 5x^4 \mathrm{Log}[1-\mathrm{e}^x] + 20x^3 \mathrm{PolyLog}[2,\mathrm{e}^x] \\ -60x^2 \mathrm{PolyLog}[3,\mathrm{e}^x] + 120x \mathrm{PolyLog}[4,\mathrm{e}^x] \\ -120 \mathrm{PolyLog}[5,\mathrm{e}^x] - 124.44] \end{array} \right\}^{-1}, \quad (24)$$

$$\rho^{U-process}_{electron-\mathrm{phonon}}(T) = BT^3 J_3\left(\frac{T}{\theta_R}\right) = a_3 T^3,$$

$$B = \frac{a_3}{J_3\left(\frac{T}{\theta_R}\right)}$$
$$= a_3 \left\{ \begin{array}{l} x^2\left(\frac{\mathrm{e}^x x}{1-\mathrm{e}^x} + 3\mathrm{Log}[1-\mathrm{e}^x]\right) + 6x \mathrm{PolyLog}[2,\mathrm{e}^x] \\ -6 \mathrm{PolyLog}[3,\mathrm{e}^x] - 7.212 \end{array} \right\}^{-1}, \quad (25)$$

a_3 and a_5 have been taken from table (1) for Cu, Ag, Au,and Debye temperature (θ_D) has been taken from equation(23) and table(2).

5. Conclusions

There are an excellent agreement between Grüneisen-Bloch function, and experimental results. Semi-empirical analysis shows that the metal constant is not constant, as well as the temperature of Debye, but they are dependent at temperature fluctuations.

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