ORIGINAL PAPER

ANALYTICAL CALCULATION OF TEMPERATURE DEPENDENCE OF THE LORENZ NUMBER IN SEMICONDUCTORS

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Abstract. *In this study, a complete analytical method of the evaluation and temperature behavior of the Lorenz number for non-degenerate and degenerate semiconductors has been proposed. Based on the quantum theory of kinetic effects, the Lorenz number formula of semiconductors in terms of two parameter Fermi functions has been formulated analytically. In spite of the long history of thermoelectric effect and its significant role in semiconductor phenomena, the analytical studies of two parameter Fermi function are very limited in the literature. By using an efficient algorithm for the calculation of two parameters Fermi function, the temperature dependence of Lorenz number has been evaluated analytically. The suggested method is useful for determination of Wiedemann-Franz law that provides connection between the thermal and electrical conductivity which is important for thermoelectric materials.*

Keywords*: Nondegenerated semiconductor, Wiedemann-Franz law, Lorenz number; thermal conductivity, electric conductivity*

1. INTRODUCTION

Thermoelectric properties of materials have played a crucial role in development of the electric and electronic industry since their conductivities are closely related to the temperature [1-10]. The sequential theory of kinetic effects in semiconductors with nonstandard zone was constructed in the works [10-13]. The theoretical assessment of Lorenz number, occurring in the Wiedemann-Franz law, is an important parameter to characterize the thermoelectric matters and the experimental evaluation of the lattice thermal conductivity [14-29]. The fact that the temperature and pressure dependences of Lorenz number are still the subject of current researches and many studies carried out to date [26]. In the study [27], the authors have proposed a new algorithm for providing an effective solution for determination of discrepancies of the Lorenz number from the observed nondegenerate, degenerate semiconductors and metals. The authors in work [28] have been proposed the remarkable review about recent progress of assessment thermoelectric properties of semiconductors and materials. In [29], an efficient approach has been developed for predicting the lattice thermal conductivity through a new Lorenz number equation. Besides, this study also leads to the defination of Lorenz number with Seedbeck coefficient.

An efficient expression for the Lorenz numbers is of great significance for the evaluation of thermoelectric properties of semiconductors and materials. In this paper, a new analytical algorithm of computing the Lorenz number for semiconductors and materials is

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presented. The efficiancy of the proposed algorithm for calculation Lorenz number is analyzed.

2. DEFINITION AND GENERAL ANALYTICAL EXPRESSIONS

The Wiedemann-Franz law for semiconductors in the absence of an external magnetic field is generally determined by the formula [10]:

$$\frac{\kappa}{\sigma} = A(r,\eta,\beta)\left(\frac{k_B}{e}\right)^2 T = L(r,\eta,\beta)T \tag{1}$$

where $L(r,\eta,\beta)$ is Lorenz number, κ is thermal conductivity, σ is electric conductivity, k_B is Boltzmann coefficient, e is charge electron, T is absolute temperature and the quantity $A(r,\eta,\beta)$ is defined as:

$$A(r,\eta,\beta) = \frac{I^2_{r+1,2}(\eta,\beta)}{I^0_{r+1,2}(\eta,\beta)} + \left(\frac{I^1_{r+1,2}(\eta,\beta)}{I^0_{r+1,2}(\eta,\beta)}\right)^2 . \tag{2}$$

From Eq. (1), the Lorenz number satisfies the general equation:

$$L(r,\eta,\beta) = A(r,\eta,\beta)\left(\frac{k_B}{e}\right)^2 . \tag{3}$$

Note that in the case of scattering of acoustic phonons $r=0$ and in the case of scattering on optical phonons at high temperatures $r=1$. In Eq.(2) the quantity $I^m_{n,k}(\eta,\beta)$ is two-parameter Fermi integral defined as [10, 30]:

$$I^m_{nk}(\eta,\beta) = \int_0^\infty \frac{x^m (x+\beta x^2)^n e^{x-\eta}}{(1+e^{x-\eta})^2 (1+2\beta x)^k} dx . \tag{4}$$

where $\eta = \frac{\zeta}{k_B T}$ is the reduced chemical potential, the quantity $\beta = \frac{k_B T}{\varepsilon_g}$ characterizes the band nonparabolicity and ε_g is energy gap. In Eq. (3), for the strong degenerate semiconductors, the quantity $A(r,\eta,\beta)$ equals to $\frac{\pi^2}{3}$. Note that, in the parabolic and nonparabolic zones the Lorenz number does not depend on the scattering mechanism r [10]. Then, in the special case of strong degenerate semiconductors and most metals, the Lorenz number formula (Eq.(3)) takes the following basic form:

$$L = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \approx 2.44x10^{-8}\, W\Omega K^{-2} \tag{5}$$

In the recent papers [31, 32], the authors have presented an analytical method for the two parameter Fermi integrals that it is suitable for applications of the thermoelectric effects of semiconductors. The series analytical relation for the two parameter Fermi integrals of the paper [32] is as follows:

for $n \neq 0,\ k \neq 0, m \neq 0$

$$I_{nk}^{m}(\eta,\beta) = e^{-\eta} \lim_{N\to\infty} \sum_{i=0}^{N} f_i(-k) \begin{cases} \sum_{j=0}^{n} f_j(n) \left[\beta^{i+j} 2^i P_{m+n+i+j}\left(\eta, \frac{1}{2\beta}\right) \right. \\ \left. \quad + \beta^{j-k-i} 2^{-k-i} Q_{m+n-k-i+j}\left(\eta, \frac{1}{2\beta}\right) \right] \quad for \quad n \text{ integer} \\ \lim_{N\to\infty} \sum_{j=0}^{N} f_j(n) \left[\beta^{i+j} 2^i P_{m+n+i+j}\left(\eta, \frac{1}{2\beta}\right) \right. \\ \left. \quad + \beta^{n-j-k-i} 2^{-k-i} Q_{m+2n-k-i+j}\left(\eta, \frac{1}{2\beta}\right) \right] \quad for \quad n \text{ noninteger} \end{cases} \tag{6}$$

for $n = 0,\ k = 0$ *and* $m \neq 0$

$$I_{00}^{m}(\eta,\beta) = e^{-\eta} \begin{cases} \lim_{N\to\infty} \sum_{i=0}^{N} \frac{f_i(-2)}{(1+i)^{m+1}} [e^{i\eta}(-1)^{m+1}\gamma(m+1,-(1+i)\eta) \\ \quad + e^{\eta(2+i)}\Gamma(m+1,(1+i)\eta)] \quad for \quad \eta > 0 \\ \lim_{N\to\infty} \sum_{i=0}^{N} f_i(-2) \frac{e^{\eta(2+i)}\Gamma(m+1)}{(1+i)^{m+1}} \quad for \quad \eta < 0 \end{cases} \tag{7}$$

for $n \neq 0,\ k = 0,\ m = 0$ *and* $\eta > 0$

$$\mathrm{I}_{n0}^{0}(\eta,\beta) = e^{-\eta} \begin{cases} \sum_{i=0}^{n} f_i(n)\beta^i L_{n+i}(\eta) \quad for\ n \text{ integer} \\ \lim_{N\to\infty} \sum_{i=0}^{N} f_i(n)(\beta^i P_{n+i}(\eta, 1/\beta) + \beta^{n-i} Q_{2n-i}(\eta, 1/\beta)) \quad for\ n \text{ noninteger} \end{cases} \tag{8}$$

for $n \neq 0,\ k = 0,\ m = 0$ *and* $\eta < 0$

$$\mathrm{I}_{n0}^{0}(\eta,\beta) = e^{-\eta} \begin{cases} \sum_{i=0}^{n} f_i(n)\beta^i \lim_{N\to\infty} \sum_{j=0}^{N} f_j(-2) \frac{e^{(2+j)\eta}\Gamma(n+i+1)}{(1+j)^{n+i+1}} \quad for\ n \text{ integer} \\ \lim_{N\to\infty} \sum_{i=0}^{N} f_i(n) \sum_{j=0}^{N} f_j(-2) e^{(2+j)\eta} \left[\frac{\beta^i \gamma(n+i+1,(1+j)/\beta)}{(1+j)^{n+i+1}} \right. \\ \left. \quad + \frac{\beta^{n-i}\Gamma(2n-i+1,(1+j)/\beta)}{(1+j)^{2n-i+1}} \right] \quad for\ n \text{ noninteger} \end{cases} \tag{9}$$

for $n=0,\ k<0,\ m=0$

$$\mathrm{I}_{0k}^{0}(\eta,\beta)=e^{-\eta}\begin{cases}\sum_{i=0}^{k} f_i(k)(2\beta)^i \lim_{N\to\infty}\sum_{j=0}^{N} f_j(-2)\left(\dfrac{e^{-i\eta}(-1)^{i+1}\gamma(i+1,-(1+j)\eta)}{(1+j)^{i+1}}\right. & \\ \left. +\dfrac{e^{(2+j)\eta}\Gamma(i+1,(1+j)\eta))}{(1+j)^{i+1}}\right) & for\ \eta>0 \\ \sum_{i=0}^{k} f_i(k)(2\beta)^i \lim_{N\to\infty}\sum_{j=0}^{N} f_j(-2)\dfrac{e^{(2+i)\eta}\Gamma(i+1)}{(1+j)^{i+1}} & for\ \eta<0\end{cases} \tag{10}$$

for $n\neq 0,\ k<0,\ m=0$

$$\mathrm{I}_{nk}^{0}(\eta,\beta)=e^{-\eta}\begin{cases}\sum_{i=0}^{n} f_i(n)\beta^i \sum_{j=0}^{k} f_j(k)(2\beta)^j \lim_{N\to\infty}\sum_{l=0}^{N} f_l(-2)\left(\dfrac{e^{-l\eta}(-1)^{n+i+j+1}}{(1+l)^{n+i+j+1}}\right. & \\ \left.\times\gamma(n+i+j+1,-(1+l)\eta)+\dfrac{e^{(2+l)\eta}\Gamma(n+i+j+1,(1+l)\eta))}{(1+l)^{n+i+j+1}}\right) & for\ \eta>0 \\ \sum_{i=0}^{n} f_i(n)\beta^i \sum_{j=0}^{k} f_j(k)(2\beta)^j \lim_{N\to\infty}\sum_{l=0}^{N} f_l(-2)\dfrac{e^{(2+l)\eta}\Gamma(n+i+j+1)}{(1+l)^{n+i+j+1}} & for\ \eta<0\end{cases} \tag{11}$$

where N is upper limit of summations, $\Gamma(\alpha)$, $\Gamma(\alpha,x)$ and $\gamma(\alpha,x)$ are the incomplete Gamma functions defined by [33]

$$\Gamma(\alpha)=\int_0^{\infty} t^{\alpha-1}e^{-t}dt\,. \tag{11}$$

$$\Gamma(\alpha,x)=\int_x^{\infty} t^{\alpha-1}e^{-t}dt \tag{12}$$

and

$$\gamma(\alpha,x)=\int_0^{x} t^{\alpha-1}e^{-t}dt\,. \tag{13}$$

See Ref. [31] for the exact definition of the auxiliary functions $P_n(p,q)$, $Q_n(p,q)$ and $L_n(p)$ occurring in the Eqs. (6)-(11). Note that a new approximation has been developed for the calculation of incomplete Gamma functions [34].

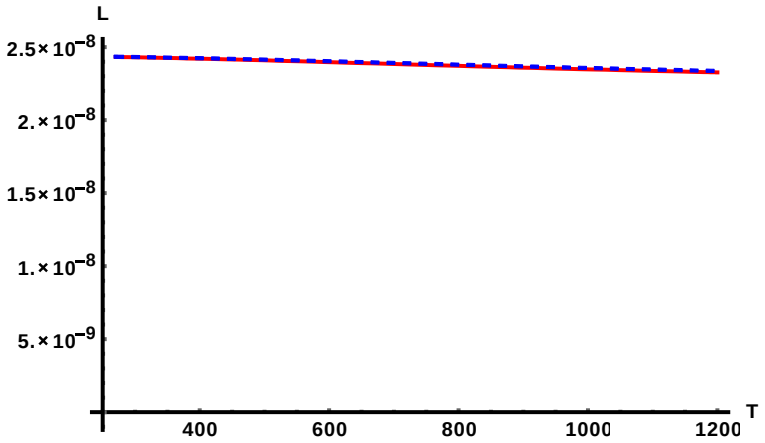

Figure 1. The temperature dependence of Lorenz number of *Si*
(Solid red line- Mathematica numerical results; Blue dashed line- results of this study).

3. NUMERICAL RESULTS AND DISCUSSION

A convenient analytical method has been proposed for calculation of the Lorenz number of non-degenerate and degenerate semiconductors through suitable expression of two parameter Fermi functions. It is well known that analytical approximations for the two parameter Fermi functions are important in the study of thermoelectric effects of semiconductors and materials. Unfortunately, the studies on analytical evaluation formulas of the two-parameter Fermi function are very limited in the literature. To show the effectiveness of this method, a computer program based on Mathematica 10.0 compiler is applied to the calculation of Lorenz number for Si semiconductor. It is clear that determining the variation of Lorenz number with respect to the temperature is very important for the exact calculation of thermoelectric properties of metals. With this purpose, we have obtained calculation results with respect to the wide temperature ranges. As seen from Figure 1, the results for the Lorenz number of Si have been successfully compared with Mathematica 10.0 numerical simulation software over a wide temperature range. The results show that the Lorenz number decreases with increasing temperature. All calculations have been performed for Si semiconductor with the following characteristics: $\varepsilon_g = 1.12eV$, $r = 1$, $\varepsilon_F = 0.56eV$, $k = 1.3806504E-23JK^{-1}$ and $e = 1.6021766C$. The advance of this work is to suggest a consistent approach for the evaluations of Lorenz number and related thermoelectric quantities according to the variation of temperature.

4. CONCLUSION

In this research we presented an analytical method to evaluate the Lorenz number of non-degenerate and degenerate semiconductors. Can be concluded that the analytical approach is general and it can be used to analyze all the kinetic effects of semiconductors and materials. All calculations have been done in SI unit systems.

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