



RESEARCH ARTICLE

THE SOLUTION OF THERMAL CONDUCTIVITY OF A FREE ELECTRON GAS BY BOLTZMANN TRANSPORT EQUATION IN NON-EQUILIBRIUM STATE

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ABSTRACT

The solution of the Boltzmann Transport equation for thermal conductivity is very difficult. In a large number of books the method given is very tedious. So Now , We have calculated a simple solution of the Boltzmann Transport equation for thermal conductivity assuming relaxation time is independent of temperature.

Key words:

Boltzmann Transport equation,  
Thermal conductivity,  
Relaxation time.

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INTRODUCTION

Statistical behavior of thermodynamic system is described by Boltzmann transport equation when the system is not in thermo-dynamical equilibrium. Boltzmann equation refers to any kinetic equation that describes the changes of a macroscopic quantity in a thermodynamic system. In macroscopic scales where the gas and fluid are regarded as a continuum, their motion is described by the macroscopic quantities such as macroscopic mass density, bulk velocity, temperature, pressure, stresses and heat flux. Boltzmann equation can be use to determine physical quantities like heat energy, momentum, thermal conductivity and electrical conductivity (Encyclopedia of Physics, 1991). These physical quantities depends on a distribution function which is defined as the average occupancy  $f(p, r, t)$  of a point in phase space is called distribution function. The distribution function may change as a result of the scattering, the flow of electron in real space determined by their velocity ( $v$ ) and the flow of electron in K-space, which is determined by the time derivatives, momentum (P) (Michael Shur, 1995). For the thermal conductivity of free electron, it is necessary to assume a sample in which there is no electric current but in which there exist a temperature gradient.

The distribution function at any point is characterized by the local temperature and must be regarded as a function of position as well as energy (John and Kelvey, 1966; Smith, 1961; Agarwal, 1998; Kittel, 1996). Let us consider a metallic specimen with temperature gradient  $dT/dx$  along x-axis. In the measurement of the thermal conductivity, the experimental conditions are such that the electric current in the metal is zero but not the electric field  $E_0$ . The temperature gradient produces a drift velocity of the electrons, and a small electric field is set up such that the electric current in the metal is zero. Thus the Boltzmann transport equation, besides thermal gradient  $dT/dx$ , includes a term containing an electric field  $E_0$ . The Boltzmann Transport equation is given by

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \text{grad}_{\vec{r}} f + \vec{F} \cdot \text{grad}_{\vec{p}} f = \left( \frac{\partial f}{\partial t} \right)_{coll} \dots \dots \dots (1)$$

In the relaxation approximation, the Boltzmann Transport equation is given by

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \text{grad}_{\vec{r}} f + \vec{F} \cdot \text{grad}_{\vec{p}} f = - \left( \frac{f - f_0}{\tau} \right) \dots \dots \dots (2)$$

Where  $f_0$  and  $f$  are equilibrium distribution function and non equilibrium distribution function respectively.  $\tau$  is

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momentum relaxation time. This relaxation time is assumed to be a function of wave vector or a function of the electron energy. This Boltzmann transport equation may be regarded as the continuity equation for the distribution function.

The Boltzmann transport equation along X-axis under the steady state and under the condition  $\left(\frac{f-f_0}{\tau}\right) \ll 1$ , is given by

$$f = f_0 + \frac{qE_0}{m} \tau \frac{\partial f_0}{\partial v_x} - \tau v_x \frac{\partial f_0}{\partial x} \quad \dots\dots\dots (3)$$

The electron gas in metals obey Fermi-Dirac distribution function and temperature gradient occurs along the x axis. If  $f_0$  is equilibrium Fermi-Dirac distribution function so this function is given by

$$f_0 = \frac{1}{\exp((\epsilon - \epsilon_F)\beta) + 1} \quad \dots\dots\dots (4)$$

Where  $\epsilon_F$  is Fermi energy and  $\beta$  is statistical temperature. Now

$$\frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial T} \frac{\partial T}{\partial x} = \frac{\partial}{\partial T} \left( \frac{1}{\exp((\epsilon - \epsilon_F)\beta) + 1} \right) \frac{\partial T}{\partial x}$$

$$\frac{\partial f_0}{\partial x} = \frac{\partial}{\partial T} \left\{ e^{(\epsilon - \epsilon_F)\beta} + 1 \right\}^{-1} \frac{\partial T}{\partial x}$$

$$\frac{\partial f_0}{\partial x} = \frac{1}{kT} \frac{e^{(\epsilon - \epsilon_F)\beta}}{\left\{ e^{(\epsilon - \epsilon_F)\beta} + 1 \right\}} \left( \frac{\epsilon - \epsilon_F}{T} \right) \frac{\partial T}{\partial x}$$

$$\frac{\partial f_0}{\partial x} = - \frac{\partial f_0}{\partial \epsilon} \left[ \frac{\epsilon - \epsilon_F}{T} \right] \frac{\partial T}{\partial x} \quad \dots\dots\dots (5)$$

And

$$\frac{\partial f}{\partial v_x} = m v_x \frac{\partial f_0}{\partial \epsilon} \quad \dots\dots\dots (6)$$

The values of equation (5) and (6) substitute in equation (3), we get

$$f = f_0 + \tau v_x \frac{\partial f_0}{\partial \epsilon} \left\{ \left( \frac{\epsilon - \epsilon_F}{T} \right) \frac{\partial T}{\partial x} + qE_0 \right\} \quad \dots\dots\dots (7)$$

In the presence of electric field and temperature gradient, the gas is in non-equilibrium state. Now the number of occupied electronic states per unit volume is given by

$$D(\epsilon) = 2 \frac{2\pi}{h^3} (2m)^{3/2} \epsilon^{1/2} \quad \dots\dots\dots (8)$$

The number of electrons at absolute zero temperature is given by

$$N = \frac{4\pi}{h^3} (2m)^{3/2} \frac{2}{3} \epsilon_F^{3/2} \quad \dots\dots\dots (9)$$

By the use of equation (8) and (9) we can write

$$D(\epsilon) = \frac{3}{2} N (\epsilon_F)^{-3/2} \epsilon^{1/2} \quad \dots\dots\dots (10)$$

The thermal current density  $Q_x$  along the x-axis with kinetic energy and velocity  $v_x$  of electrons is given by

$$Q_x = \int_{-\infty}^{\infty} v_x \epsilon f D(\epsilon) d\epsilon$$

By the use of equation (7), we get

$$Q_x = \int_{-\infty}^{\infty} v_x f_0 D(\epsilon) d\epsilon + \int_{-\infty}^{\infty} \left\{ \tau v_x^2 \epsilon \frac{\partial f_0}{\partial \epsilon} \left( \frac{\epsilon - \epsilon_F}{T} \right) \frac{\partial T}{\partial x} + qE_0 \right\} D(\epsilon) d\epsilon \quad \dots\dots (12)$$

Since, average of  $v_x^2$  is taken over the Fermi surface.

$$\left. \begin{aligned} v_x^2 &= \frac{v^2}{3} \\ v^2 &= \frac{2\epsilon}{m} \end{aligned} \right\} \quad \dots\dots\dots (13)$$

By the use of equation(13) we get from equation (12) as

$$Q_x = \frac{2}{3m} \int_0^{\infty} \left\{ \tau \epsilon^{3/2} \frac{\partial f_0}{\partial \epsilon} \left( \frac{\epsilon - \epsilon_F}{T} \right) \frac{\partial T}{\partial x} + qE_0 \right\} \frac{3}{2} N \epsilon_F^{-3/2} \epsilon^{1/2} d\epsilon \quad \dots\dots\dots (14)$$

$$Q_x = \frac{\epsilon_F^{-3/2} N}{m} \int_0^{\infty} \left\{ \tau \epsilon^{3/2} \frac{\partial f_0}{\partial \epsilon} \left( \frac{\epsilon - \epsilon_F}{T} \right) \frac{\partial T}{\partial x} + qE_0 \epsilon^{1/2} \right\} d\epsilon \quad \dots\dots (15)$$

Consider a general form of equation as

$$I_\nu = \frac{N}{m} \epsilon^{-3/2} \int_0^{\infty} \tau \epsilon^{\nu+1} \frac{\partial f_0}{\partial \epsilon} d\epsilon \quad \dots\dots\dots (16)$$

$\nu = 1, 2, 3.$

Then the solution of equation (16) is given by

$$I_\nu = \frac{N}{m} \epsilon^{-3/2} \left[ \tau \epsilon_F^{\nu+1/2} + \frac{\pi^2}{6} (kT)^2 \frac{\partial^2}{\partial \epsilon^2} \left( \tau \epsilon_F^{\nu+1/2} \right) \right] \quad \dots\dots\dots (17)$$

By the use of equation (15) and (16) we get

$$Q_x = \left( \frac{I_3}{T} - \frac{\epsilon_F}{T} I_2 \right) \frac{dT}{dx} + qE_0 I_2 \tag{18}$$

The electric current density along the x-axis is given by

$$J_x = \int_{-\infty}^{\infty} v_x q D(\epsilon) d\epsilon$$

By the use of equation (7), we get

$$J_x = \int_{-\infty}^{\infty} v_x q \left\{ f_0 + v_x \frac{\partial f_0}{\partial \epsilon} \left( \frac{\epsilon - \epsilon_F}{T} \right) \frac{\partial T}{\partial x} + qE_0 \right\} D(\epsilon) d\epsilon$$

$$J_x = 2 \int_0^{\infty} \left\{ v_x^2 q \frac{\partial f_0}{\partial \epsilon} \left[ \frac{\epsilon - \epsilon_F}{T} \right] \frac{\partial T}{\partial x} + qE_0 \right\} D(\epsilon) d\epsilon \tag{19}$$

By the use of equations (10),(13) and (19) we get

$$J_x = \frac{3}{2} N \frac{2q}{3m} \epsilon_F^{-3/2} \int_0^{\infty} \left\{ \tau \epsilon^{3/2} \frac{\partial f_0}{\partial \epsilon} \left[ \frac{\epsilon - \epsilon_F}{T} \right] \frac{\partial T}{\partial x} + qE_0 \right\} d\epsilon$$

$$J_x = \frac{Nq}{m} \epsilon_F^{-3/2} \int_0^{\infty} \left\{ \tau \epsilon^{3/2} \frac{\partial f_0}{\partial \epsilon} \left[ \frac{\epsilon - \epsilon_F}{T} \right] \frac{\partial T}{\partial x} + qE_0 \right\} d\epsilon \tag{20}$$

By the use of equation (16) and (20) we get

$$J_x = q \left( \frac{I_2}{T} - \frac{\epsilon_F}{T} I_1 \right) \frac{dT}{dx} + q^2 E_0 I_1 \tag{21}$$

But occurrence of temperature gradient the current density (J<sub>x</sub>) is zero

Thus we get from equation (21) as

$$E_0 = - \frac{1}{q} \left( \frac{I_2}{I_1 T} - \frac{\epsilon_F}{T} \right) \frac{dT}{dx} \tag{22}$$

Now on substituting E<sub>0</sub> in equation (18) we get

$$Q_x = - \frac{1}{T} \left( I_3 - \frac{I_2^2}{I_1} \right) \frac{dT}{dx} \tag{23}$$

And at Fermi surface,  $\epsilon = \epsilon_F$ , by the use of equation (17) we get

$$I_\nu = \frac{N}{m} \left[ T_F \epsilon_F^{\nu-1} + \frac{\pi^2}{6} (kT)^2 \epsilon_F^{-3/2} \frac{\partial^2}{\partial \epsilon^2} \left( \tau_F \epsilon^{\nu+1/2} \right) \right]_{\epsilon=\epsilon_F} \tag{24}$$

Now

$$\nu = 1, 2, 3, \dots$$

Then we get

$$I_1 = \frac{N}{m} \left[ T_F + \frac{\pi^2}{8} (kT)^2 \tau_F \epsilon_F^2 \right]$$

$$I_2 = \frac{N}{m} \left[ T_F \epsilon_F + \frac{5\pi^2}{8} (kT)^2 \tau_F \epsilon_F^{-1} \right]$$

Now

$$\frac{I_2^2}{I_1} = \frac{N}{m} T_F \epsilon_F^2 \left[ 1 + \frac{5}{4} \pi^2 \frac{(kT)^2}{\epsilon_F^2} \right] \left[ 1 + \frac{\pi^2}{8} \frac{(kT)^2}{\epsilon_f^2} \right]^{-1}$$

$$\frac{I_2^2}{I_1} = \frac{N}{m} T_F \epsilon_F^2 \left[ 1 + \frac{5}{4} \pi^2 \frac{(kT)^2}{\epsilon_F^2} \right] \left[ 1 - \frac{\pi^2}{8} \frac{(kT)^2}{\epsilon_f^2} \right]$$

$$\frac{I_2^2}{I_1} = \frac{N}{m} T_F \epsilon_F^2 \left[ 1 + \frac{5}{4} \pi^2 \frac{(kT)^2}{\epsilon_F^2} + \frac{5}{4} \pi^2 \frac{(kT)^2}{\epsilon_f^2} \right]$$

$$\frac{I_2^2}{I_1} = \frac{N}{m} T_F \epsilon_F^2 \left[ 1 + \frac{9}{8} \pi^2 \frac{(kT)^2}{\epsilon_F^2} \right] \tag{25}$$

Again

$$I_3 = \frac{N}{m} \left[ T_F \epsilon_F^2 + \frac{35\pi^2}{24} (kT)^2 \tau_F \right] \tag{26}$$

From equation (25) and (26)

$$I_3 - \frac{I_2^2}{I_1} = \frac{N}{m} \left[ T_F \epsilon_F^2 + \frac{35}{24} (kT)^2 \tau_F \right] - \frac{N}{m} T_F \epsilon_F^2 \left( 1 + \frac{9}{8} \pi^2 \frac{(kT)^2}{\epsilon_F^2} \right)$$

$$I_3 - \frac{I_2^2}{I_1} = \frac{N\pi^2 k^2 \tau_F T^2}{3m}$$

$$\left( I_3 - \frac{I_2^2}{I_1} \right) \frac{1}{T} = \frac{N\pi^2 k^2 \tau_F T}{3m} \tag{27}$$

By the use of equation (23) and (27)

$$Q_x = - \frac{N\pi^2 k^2 \tau_F T}{3m} \frac{dT}{dx} \tag{28}$$

By the definition of thermal conductivity

$$Q_x = -K \frac{dT}{dx} \tag{29}$$

From the equation (28) and (29) we get expression of thermal conductivity

$$K = \frac{N\pi^2 k^2 \tau_F T}{3m} \dots\dots\dots (30)$$

Where N is concentration of electron,  
This is the thermal conductivity.  
This derivation is derived on basis of constant relaxation time.

## RESULTS AND DISCUSSION

The Equation (30) is used for study of metals and semiconductors. Thermal conductivity depends on temperature. At very low temperatures impurities and defect scattering is dominant. In this study relaxation time is independent of temperature but, at high temperature the phonon scattering is dominant (7). The approach of Boltzmann transport equation is followed to describe the transport of charge and kinetic energy of electrons by a statistical distribution of mobile electrons behaves like an electron gas. Therefore, the behavior of the electronic contribution to the thermal conductivity of metals is depends on temperature. Thermal conductivity expression is also used in calculation of Lorentz number.

## Conclusion

In this study the relaxation time is kept constant. The equation (30) is valid for Fermi surface.

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