2.1. Transport Equations

-2.1.1 from BTE to DDE(Drift Diffusion) Equation
-2.1.2 from Wigner function to Density Gradient*
-2.1.3 NEGF**

Goal;

To derive the current equation from the BTE (Boltzmann Transport Equation) and understand the terms affecting the carrier transport.

1.1. Boltzmann Transport Equation

Objective To understand BTE equation describing the collective carrier motion in the phase spce.

— We consider the carrier motion in the energy band as if the carriers are the carrier gas in the spce.

— Phase space: Consider a small volume in r space and k space as,

$$d^3 r = dx\,dy\,dz$$

$$d^3 k = dk_x\,dk_y\,dk_z$$

The volume in the phase space is large enough so that the number of carriers exist and small enough that the variation of physical quantities such as concentration of carriers, average velocity and so on.

— Define f as the distribution function (probability per unit phase volume). Then the number of carriers in the phase spce volume dN

and total number of carriers N can be writter as,

$$dN = f(\underline{r}, \underline{k}, t)\ d^3\underline{r}\ d^3\underline{k}$$

$$N = \int f(\underline{r}, \underline{k}, t) d^3\underline{r}\ d^3\underline{k}$$

Also, any mean value

$$\langle \phi(\underline{k}) \rangle = \frac{1}{n} \int \phi(\underline{k}) f(\underline{r}, \underline{k}, t)\ d^3\underline{k}$$

Here,

$$n = \int f(\underline{r}, \underline{k}, t)\ d^3\underline{k}$$

— Now consider time variation of $f(\underline{r}, \underline{k}, t)$ in a small time interval Δt

is large compared with the time taken during a scattering event τ_d (scattering time) but small compared with the free flight time τ.

If there is no collision during Δt,

$$\underline{r} \to \underline{r}' = \underline{r} + v_g \Delta t$$

$$\underline{k} \to \underline{k}' = \underline{k} + F \Delta t$$

so that

$$f(\underline{r}, \underline{k}, t)\ d^3\underline{r}\ d^3\underline{k} = f(\underline{r} + \underline{v}_g \Delta t, \underline{k} + \underline{F} \Delta t, t + \Delta t)\ d^3\underline{r}'\ d^3\underline{k}'$$

Liville theorem states that

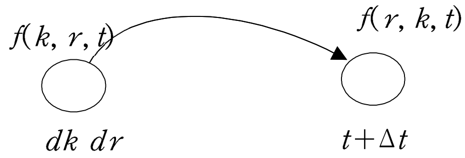
$$d^3\underline{r}\ d^3\underline{k} = d^3\underline{r}'\ d^3\underline{k}'$$

The f in RHS can be written as,

$$f(\underline{r}, \underline{k}, t) = f(\underline{r}, \underline{k}, t) + \left(\frac{\partial f}{\partial \underline{r}} \underline{v}_g + \frac{\partial f}{\partial \underline{k}} \underline{F} + \frac{\partial f}{\partial t} \right) \Delta t$$

so that

$$\frac{\partial f}{\partial \underline{r}} \cdot \underline{v}_g + \underline{F} \cdot \frac{\partial f}{\partial \underline{k}} + \frac{\partial f}{\partial t} = 0$$



1.2. The Moment Equation of BTE

Objective To find the moment equation of BTE up to the 4th moment and understand the physical quantities affecting the current under the external force F.

A. Formation

— Some background

Since the volume of each state in the k space is $4\pi^3/V$, the conversion from $\sum$ to $\int_k$ can be done as,

$$\sum_k \rightarrow \frac{V}{4\pi^3}\int_k d^3\underline{k}.$$

Summing all the states in conduction band in the Brillouine zone gives the total number of electrons, so that

$$\sum_k f(\underline{k}) = \frac{V}{4\pi^3}\int_k f(\underline{k})d^3\underline{k} = nV$$

Then the ensemble average of any quantity $\phi(\underline{k})$ can be written as

$$\langle\phi(\underline{k})\rangle = \frac{\int_k f(\underline{k})\phi(\underline{k})d^3\underline{k}}{\int f(\underline{k})d^3\underline{k}} = \frac{1}{4\pi^3 n}\int f(\underline{k})\phi(\underline{k})d^3\underline{k}$$

Generalized Moment equation for $\phi(\underline{k})$ can be found by integrating BTE in the Brillouine zone(k space) after multiplying each term of BTE by $\phi(\underline{k})$ as follows;

$$\phi(\underline{k})\frac{\partial f}{\partial t} = qE\frac{\partial f}{\partial \underline{k}} + \underline{v}_g\frac{\partial f}{\partial \underline{r}} + \left.\frac{\partial f}{\partial t}\right)_{coll}$$

$$\frac{\partial}{\partial t}(n\langle \phi\rangle) = -\frac{q\varepsilon}{\hbar} n\langle \frac{\partial \phi}{\partial \underline{k}}\rangle - \frac{\partial}{\partial \underline{r}} \cdot n\langle \phi \ \underline{v}_g\rangle + \frac{1}{4\pi^3}\int \phi(\underline{k})\frac{\partial f}{\partial t}\Big)_{coll} d^3\underline{k} \tag{1}$$

Then letting $\phi=1$, mv_i, E and Ev_i, we obtain up to 4th moment of BTE.

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x_j}(n\langle v_j\rangle) + \frac{1}{4\pi^3}\int \frac{\partial f}{\partial t}\Big)_{coll} d^3\underline{k} \tag{2a}$$

$$\frac{\partial(mnV_i)}{\partial t} = -q\varepsilon_j n\langle \frac{m}{m^*}\rangle_{ij} - \frac{\partial}{\partial x_j}(nk_BT_{ij}) + \frac{1}{4\pi^3}\int \frac{\partial f}{\partial t}\Big)_{coll} mv_i d^3\underline{k} \tag{2b}$$

$$\frac{\partial(nW)}{\partial t} = -q\varepsilon_j F_j - \frac{\partial}{\partial x_j} S_j + \frac{1}{4\pi^3}\int \frac{\partial f}{\partial t}\Big)_{coll} E d^3\underline{k} \tag{2c}$$

$$\frac{\partial(n\langle Ev_i\rangle)}{\partial t} = -q\varepsilon_j \frac{n}{\hbar}\langle \frac{\partial}{\partial k_j}(Ev_i)\rangle - \frac{\partial}{\partial x_j}\langle nEv_iv_j\rangle + \frac{1}{4\pi^3}\int \frac{\partial f}{\partial k}\Big)_{coll} Ev_i d^3\underline{k} \tag{2d}$$

In the above equations, small letter represents the physical quantity of interest and capital letter represents the averages of it taken in k space at some space point x.

v_i : ith component of the group velocity
V_j : jth component of average velocity
d/dx_j : summation for $j=1,2,3$ (Einstein convention)
$k_BT_{ij}=\langle mv_iv_j\rangle$ electron temperature
E : energy of electrons
W : average energy of electrons
Si : $\langle Ev_i\rangle$: ith component of energy flux
$F_j=nV_j$: jth component of carrier flux

— Another representation of the 1st moment can be made if $\phi = hK_i$ instead of mv_i;

$$\frac{\partial(nhK_i)}{\partial t} = -q\varepsilon_j n - \frac{\partial}{\partial x_j}(nk_BT_{ij}) + \frac{1}{4\pi^3}\int \frac{\partial f}{\partial t}\Big)_{coll} hK_i d^3\underline{k}$$

where $k_BT_{ij}=\langle hK_iK_j\rangle$. Notice that the carrier temperature is defined in a different way.

— The $\left.\frac{\partial}{\partial t}\right)_{coll}$ term represents the increase rate of the physical quantity due to collision(including interband scattering).

For convenience, the scattering integral is represented by "some average quantity" which can be connected to "measurable quantities" such as mobility, energy relaxation time and so on.

B. Conservation of momentum (2b) and average velocity V

Let $\phi = hk_i$

$$\frac{1}{4\pi^3}\int \left.\frac{\partial f}{\partial t}\right)_{coll} hk_i d^3\underline{k} = -\frac{nK_j}{\tau}\left(\frac{V_i}{V_j}\right) = -\frac{nV_i}{\tau}(\langle m^*\rangle_{ij}) \tag{B.3}$$

where

$$\frac{nK_j}{\frac{1}{4\pi^3}\int \left.\frac{\partial f}{\partial t}\right)_{coll} hK_i d^3\underline{k}} = \tau \ , \quad \frac{hK_j}{v_i} = \langle m^*\rangle_{ij}$$

Then,

$$V_i = -\frac{q\tau}{\langle m^*\rangle_{ij}}\varepsilon_j - \frac{\tau}{n\langle m^*\rangle_{ij}}\frac{\partial}{\partial x_j}(nk_B T_{ij}) = -\mu_{ij}\varepsilon_j - \frac{\mu_{ij}}{qn}\frac{\partial}{\partial x_j}(nk_B T_{ij}) \tag{B.4}$$

The above equation is a general equation for the ensemble average of electrons. Notice that it depends not only the electric field, but also gradient of n and temperature.

Thermoelectric effect can be modeled by the above equation, where the carrier flux is the function of the electron temperature, where the 'electron temperature' is defined above.

Also notice that the mobility and tau are definitions , not approximations.

C. Energy balance equation : Eq. (2c)

$$\frac{\partial(nW)}{\partial t} = -q\varepsilon_j F_j - \frac{\partial}{\partial x_j} S_j + \frac{1}{4\pi^3}\int \frac{\partial f}{\partial t}\Big)_{coll} E d^3\underline{k}$$

1st term of RHS: energy gain rate from E field per unit volume

3nd term of RHS: energy loss by heating lattice (by way of generating phonon)

Notice that for the uniform sample in the steady state, the energy balance equation in the above represent the Joule heating.

D. Energy flux equation : Eq. (2c)

Consider the 1st term of RHS.

$$\begin{aligned} \frac{n}{\hbar}\langle \frac{\partial}{\partial k_j}(Ev_i)\rangle &= \frac{n}{\hbar}\left(\langle \frac{v_i \partial E}{\partial k_j}\rangle + \langle \frac{E\partial v_i}{\partial k_j}\rangle\right) \\ &= \frac{n}{\hbar}\langle \frac{v_i \partial E}{\partial k_j} + \frac{E\partial v_i}{\partial k_j}\rangle \\ &= n\langle v_i v_j\rangle + n\langle \frac{E}{m^*_{ij}}\rangle \end{aligned} \qquad (B.5)$$

- 2nd term of RHS is the thermal diffusion term.
- 3rd term of RHS is the increase rate of energy flow by collision.

Defining a relaxation rate as $-\underline{S}/\tau_S$,

where $$\tau_s = -\frac{S}{4\pi^3 \int \frac{\partial f}{\partial \underline{k}}\Big)_{coll} E v_i d^3\underline{k}} \qquad (6)$$

Then the average energy flux can be written as,

$$S_i = -q\varepsilon_j \tau_s n\langle v_i v_j\rangle - q\varepsilon_j \tau_s n\langle \frac{E}{m^*_{ij}}\rangle - \tau_s \frac{\partial}{\partial x_j}(n\langle E v_i v_j\rangle) \qquad (7)$$

Usually, in practice, people prefers to use the simple form for S as the approximate form as,

$$\begin{aligned} S \;=\; & -\frac{q\varepsilon_j \tau_s n\langle m^*\rangle\langle v_i v_j\rangle}{\langle m^*\rangle} - q\varepsilon_j \tau_s n\langle \frac{E}{m^*} \rangle \\ & -\tau_s \frac{\partial}{\partial x_j} \frac{\langle m^*\rangle\langle nEv_i v_j\rangle}{\langle m^*\rangle} \\ \cong\; & -\varepsilon_j \mu_s n(k_B T_{ij} + \langle E\rangle) - \mu_s \frac{\partial}{\partial x_j} \frac{n\langle E\rangle k_B T_{ij}}{q} \end{aligned} \qquad (8)$$

where mobility for energy $\mu_s \equiv \frac{q\tau_S}{\langle m^*\rangle}$.

The last term is usually modeled by

$$\mu_s \frac{\partial}{\partial x_j}\left(\frac{n\langle E\rangle k_B T_{ij}}{q}\right) = \mu_s n k_B T_{ij} \frac{\partial}{\partial x_j}\langle E\rangle + \mu_s \langle E\rangle \frac{\partial}{\partial x_j} \frac{nk_B T_{ij}}{q} \qquad (9)$$

If the last term is coupled with the drift term in eq. (8),
S can be written as,

$$\begin{aligned} S \;=\; & -\varepsilon_j \mu_s n(k_B T_{ij} + \langle E\rangle) - \mu_s k_B \frac{T_{ij}}{q} \frac{\partial}{\partial x_j}(nk_B T_{ij}) \\ & -\mu_s \langle E\rangle \frac{\partial}{\partial x_j}\left(\frac{nk_B T_{ij}}{q}\right) - \mu_s n k_B T_{ij} \frac{\partial}{\partial x_j}\langle E\rangle + \mu_s \frac{k_B T_{ij}}{q} \frac{\partial}{\partial x}(nk_B T_{ij}) \\ =\; & nV(k_B T_{ij} + \langle E\rangle) - \mu_s n k_B T_{ij} \frac{\partial}{\partial x_j}\langle E\rangle \end{aligned} \qquad (10)$$

The above equation shows that the energy flux are dependent upon three terms; each is called as

- 1st term: thermal pressure term.
- 2nd term: convection term
- 3rd term: thermal diffusion term.

— Usually the thermal diffusion term is written as follows:

$$\textit{Thermal duffusion term} = (C + \frac{5}{2})\mu_s n k_B T_{ij} \frac{\partial}{\partial x_j}(k_B T_{ij}) \qquad (11)$$

From W.S.Choi, IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, VOL. 13, NO. 7. JULY 1994 =< reading material #3

$$\kappa_n = \left(\frac{5}{2} + c_n\right) \frac{k_B^2}{q} T_n \mu_n n.$$

$$\vec{S}_n = -\kappa_n \nabla T_n - (w_n + k_B T_n) \frac{\vec{J}_n}{q} \tag{8}$$

$$\vec{S}_p = -\kappa_p \nabla T_p + (w_p + k_B T_p) \frac{\vec{J}_p}{q}. \tag{9}$$

C is the correction parameter to include the approximations made in E = 1.5 kT (neglecting the contribution from V) and others. Usually, C =-0.5 in silicon.

1.3. Relaxation Time Approximation in BTE

Objective To find the current flux form from the relaxation time.

※Ref>

1. R. Stratton, "Semiconductor Current Flow Equations," IEEE TED, pp. 1288-1291, 1972.<= reading material #4

2. Ashkroft, Solid State Physics, pp. 310-319, Holt Rinehart Winston.
3. J. Mckelvey, Solid state and semiconductor physics, A Harper international, 1966, chaper 7

The increase rate of f due to collision is assumed to be

$$\left.\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f - f_0}{\tau}, \tag{1}$$

with τ as function of E^r with r varying according to scattering centers and f_0 is the equilibrium distribution function.

Equation (1) is called the relaxation time approximation and the rigorous discussion on the issue can be found, for example, in Ashkroft.

A. Approximation form for f

$$\underline{v}_g \cdot \nabla_r f - \frac{\underline{F}}{\hbar} \cdot \nabla_k f - \frac{f - f_o}{\tau} = 0 \tag{2}$$

Let the solution for BTE as $f = f_o + f_1$. Then f_1 can be written as,

$$\underline{v}_g \cdot \underline{\nabla}(f_o + f_1) - \frac{\underline{F}}{\hbar} \cdot \underline{\nabla}_k (f_o + f_1) = \frac{f}{\tau} \tag{3}$$

or

$$\begin{aligned} f_1 &= -\tau(\underline{v}_g \cdot \underline{\nabla} f_o + \frac{\underline{F}}{\hbar} \cdot \nabla_k f_o) \\ &\quad -\tau(\underline{v}_g \cdot \underline{\nabla} f_o + \frac{\underline{F}}{\hbar} \cdot \underline{\nabla}_k f_1) \end{aligned} \tag{4}$$

If the 2nd part of RHS is neglected as f_1 is much smaller than f_0,

$$f_1 \simeq -\tau(\underline{v}_g \cdot \underline{\nabla} f_o + \frac{\underline{F}}{\hbar} \cdot \nabla_k f_o) \tag{5}$$

If $\underline{F}$ is in Z direction,

$$\nabla_k f_o = \frac{\partial}{\partial \underline{k}_Z} f_o = \frac{\partial E}{\partial \underline{k}_Z} \frac{\partial}{\partial E} f_o \tag{6}$$

$$\left(= \frac{\hbar^2 \underline{k}_Z}{m} \frac{\partial}{\partial E} f_o \ : \text{ for apherical band}\right)$$

Since f_0 is known so the f, all the physical quantities of interest can be obtained from equations in §1.3.2. See Mckelvy(ref. 3 above) for derivation of thermal and electrical conductivity.

B. Current Equation Represented by Relaxation Approximation

reading #4> Stratton, 'Diffusion of hot and cold electrons in semiconductor barriers,' phys.Rev., vol. 126, no. 6, pp2002-2014, 1962

Let $f = f_o + f_1 \qquad f_o$: even $\qquad f_1$: odd function; (7)

Also let $\left.\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f - f_o}{\tau}$

Then $$f_o = f_o + \frac{q\varepsilon}{\hbar}\tau\frac{\partial f}{\partial \underline{k}} - \tau \underline{v}\cdot\frac{\partial f}{\partial \underline{r}} - \frac{\partial f}{\partial t} \tag{8}$$

$$\begin{aligned}\underline{V} &= \frac{1}{n}\cdot\frac{1}{4\pi^3}\int f\, \underline{v}_g d^3k \\ &= \frac{1}{n}\cdot\frac{1}{4\pi^3}\int\left[\left(\frac{q\varepsilon}{\hbar}\cdot\tau\frac{\partial f}{\partial \underline{k}}\right)\underline{v} - \left(\tau\,\underline{v}\cdot\frac{\partial f}{\partial \underline{r}}\right)\underline{v}\right]d^3\underline{k}\end{aligned} \tag{9}$$

Or $$\underline{F} = nV = \frac{1}{4\pi^3}\int[(a) - (b)]\,d^3\underline{k}$$

— 1st term (9a)

$$\begin{aligned}F_i &= \frac{1}{4\pi^3}\int\left(\frac{q\varepsilon_j}{\hbar}\cdot\tau\frac{\partial f}{\partial k_j}\right)v_i d^3k \\ &= \frac{q}{\hbar}\varepsilon_j\int\left(\tau\frac{\partial f}{\partial k_j}\right)v_i d^3k \\ &= \frac{q}{\hbar}\varepsilon_j[(f\tau v_i)]_{BZ} - \int f\frac{\partial}{\partial k_j}(\tau v_i)d^3k] \\ &= -\frac{q}{\hbar}\varepsilon_j n\left\langle\frac{\partial(\tau v_i)}{\partial k_j}\right\rangle\end{aligned} \tag{10a}$$

<Ex> Compare this with

$$-\frac{q\tau_p}{M_{ji}}n\varepsilon_j = -\frac{q}{\hbar}n\left\langle\frac{\partial(\tau v_i)}{\partial k_j}\right\rangle\varepsilon_j$$

$$\tau_p = \frac{M_{ji}}{\hbar}\left\langle\frac{\partial(\tau v_i)}{\partial k_j}\right\rangle \tag{10b}$$

This form is another representation of τ_p in terms of τ and effective mass and the < >.

— 2nd term : (9b)

$$\begin{aligned} F_i &= -\frac{1}{4\pi^3}\int\tau(v_j\frac{\partial f}{\partial x_j})v_i d^3\underline{k} \\ &= -\frac{1}{4\pi^3}\left[\int\frac{\partial}{\partial x_j}(\tau v_j v_i f)d^3\underline{k} - \int f\frac{\partial}{\partial x_j}(\tau v_j v_i)d^3\underline{k}\right] \\ &= -\frac{1}{4\pi^3}\left[\frac{\partial}{\partial x_j}\int\tau v_j v_i f d^3\underline{k} - \int f v_j v_i\frac{\partial}{\partial x_j}\tau d^3\underline{k}\right] \end{aligned}$$

Or

$$\underline{F} = -\frac{\partial}{\partial\underline{r}}\cdot[n\langle\tau\ \underline{v}\ \underline{v}\rangle] + n\langle\underline{v}\ \underline{v}\frac{\partial}{\partial\underline{r}}\tau\rangle \tag{11}$$

<Ex> Compare the carrier flux in §1.3.2.

Now consider again Eq.(11). How can we express terms in Eq.(11) as a more tractable, or physically meaningful form (such as $\underline{D}$, n, μ)?

$$\begin{aligned} \underline{F} &= -\frac{\partial}{\partial\underline{r}}\cdot[n\langle\tau\ \underline{v}\ \underline{v}\rangle] + n\langle\underline{v}\ \underline{v}\frac{\partial}{\partial r}\tau\rangle \\ &= -\frac{\partial}{\partial\underline{r}}\cdot[nD] + nU \end{aligned} \tag{12}$$

where

$$\begin{aligned} D &\equiv \langle\tau\ \underline{v}\ \underline{v}\rangle \\ U &\equiv \left\langle\underline{v}\ \underline{v}\frac{\partial}{\partial\underline{r}}\tau\right\rangle \end{aligned} \tag{12a}$$

ref. See the review paper on the HD issue and prediction capability of the related device characteristics can be found in ,

Reading material #5

A Review of Hydrodynamic and Energy-Transport Models for Semiconductor Device Simulation

TIBOR GRASSER, TING-WEI TANG, FELLOW, IEEE, HANS KOSINA, MEMBER, IEEE, AND

SIEGFRIED SELBERHERR, FELLOW, IEEE

PROCEEDINGS OF THE IEEE, VOL. 91, NO. 2, FEBRUARY 2003

HW> Verify that the ratio between the thermal conductivity and the electrical conductivity of the metal like material(where the conduction is decided by 'electrons' is the function of T only. Or

$L = (\text{®}_t / ,\text{®}_e) * (1/T) = 2k^2 / e^2$

.

Hint. See the McKelvy p 195