Balance Equation Approach to Electron Transport

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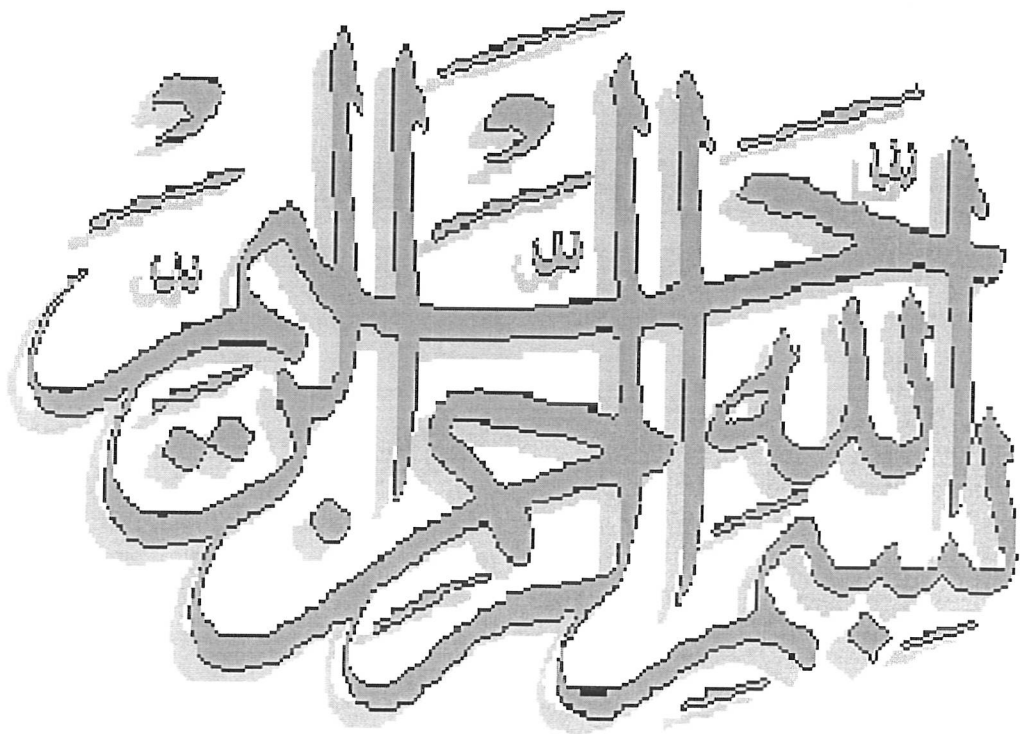This work is submitted as a dissertation on partial fulfillment for the award of the Degree of

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بِسْمِ اللهِ الرَّحْمٰنِ الرَّحِيمِ

IN THE NAME OF
ALLAH,
THE MOST GRACIOUS
&,
THE MERCIFUL

i

TO

MY SWEET PARENTS
&
UNCLE ALI HASSAN,
FROM WHOM I RECEIVED
UNBOUNED LOVE.

CERTIFICATE

It is certified that the work contained in this dissertation was carried out by **Mr. Muhammad Sharif** under my supervision.

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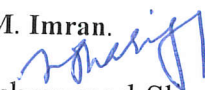Prof. Dr. S. K. Hasanain

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Acknowledgment

All praises and greatnesses to Almighty Allah alone, Whose bounties and favors are limitless - both spatially and temporally, which can never be described in words, measured with equipments, and comprehended by worldly minds. And Durud-o-Salam to the first and the last Prophet of Allah: Hazrat Muhammad (SAAWW), whom the whole universe has existed for.

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Muhammad Sharif

Abstract

In this work, the balance-equation approach formulated by X.L. Lei and C.S. Ting is studied which is extremely useful in analyzing nonlinear hot-carrier transport. This approach is well suited to treat interaction effects in electron transport.

The essential idea is to separate the center-of-mass motion from the relative motion of electrons. An electron temperature is introduced as a measure of the internal energy of the relative electrons. By allowing different temperatures for decoupled electrons and phonons in the initial state, we obtain the density matrix for the electron-lattice system to the first order of interaction but under arbitrarily strong electric field. The force- and energy-balance equations are obtained using this approach for the steady state dc transport in a 3D isotropic system. The scattering mechanism includes impurity and phonon interactions with nonlocal dynamic screening effects due to electron-electron interactions. Linear and nonlinear resistivities are discussed in the degenerate and non-degenerate statistical regime.

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Chapter 1

Background

Electron transport in submicron systems and specifically nano scale systems is an area of great interest in physics. It is not only an area rich in physics where ideas from various fields of physics come into play, but it also has practical implications for device physics.

In the following sections, we discuss the various approaches to electron transport in submicron systems. In the last section, of this chapter, Lei-Ting balance equation theory[1] is introduced which is the main focus of this thesis.

1.1   Different approaches to electron transport

1.1.1   Boltzmann Transport Equation

In a semi-classical theory of transport one can derive an equation of motion, known as the Boltzmann equation[2], for the non-equilibrium distribution function $f(\mathbf{r}, \mathbf{p}, t)$. To do this, consider first a set of N non-interacting particles subject to an external potential $V_{ext}(\mathbf{r}, t)$, and thus evolving according to the Hamiltonian

$$H = \sum_{i}^{N} \left(\frac{p_i^2}{2m} + V_{ext}(\mathbf{r}, t) \right).$$

(1.1)

By noninteracting, we mean that they do not experience any type of scattering. The Hamiltonian of Eq.(1.1) describes the dynamics of independent particles evolving under the same equation of motion. The phase space density $D(\mathbf{r}_1, \mathbf{p}_1; \ldots; \mathbf{r}_N, \mathbf{p}_N, t)$ factorizes into a prod-

uct of N one-particle reduced densities $f(\mathbf{r}, \mathbf{p}, t)$. Instead of working with the N-particle density we can thus work with the quantity $f(\mathbf{r}, \mathbf{p}, t)d\mathbf{r}d\mathbf{p}$, that gives the number of particles in $d\mathbf{r}d\mathbf{p}$.

Since the particles evolve under Hamiltonian dynamics, the Liouville theorem[3] guarantees that the phase-space volume $d\mathbf{r}d\mathbf{p}$ is conserved during time-evolution. In addition, no interactions are present among particles, therefore the number of particles in volume $d\mathbf{r}d\mathbf{p}$ remains constant during time-evolution under the above Hamiltonian. All of this implies that the single-particle density $f(\mathbf{r}, \mathbf{p}, t)$ must be conserved, namely

$$\frac{d}{dt}f(\mathbf{r}, \mathbf{p}, t) = 0. \tag{1.2}$$

The total time derivative of $f(\mathbf{r}, \mathbf{p}, t)$ is determined by all the terms that either implicitly or explicitly depend on time

$$\frac{\partial}{\partial t}f(\mathbf{r}, \mathbf{p}, t) + .\frac{d\mathbf{r}}{dt}.\nabla_\mathbf{r}f(\mathbf{r}, \mathbf{p}, t) + .\frac{d\mathbf{p}}{dt}.\nabla_\mathbf{p}f(\mathbf{r}, \mathbf{p}, t) = 0 \tag{1.3}$$

.We can use the Hamilton's canonical equations for the particles' conjugated variables $\{r_j, p_j\}$ (i.e., the jth component of the particle position and momentum, respectively)

$$\frac{dr_j}{dt} = \frac{\partial H}{\partial p_j}; \frac{dp_j}{dt} = -\frac{\partial H}{\partial r_j} \tag{1.4}$$

with the single-particle Hamiltonian $H = \frac{p^2}{2m} + V_{ext}(\mathbf{r}, t)$ to obtain

$$\frac{\partial}{\partial t}f(\mathbf{r}, \mathbf{p}, t) + \frac{\mathbf{p}}{m}.\nabla_\mathbf{r}f(\mathbf{r}, \mathbf{p}, t) - \nabla_\mathbf{r}V_{ext}(\mathbf{r}, t).\nabla_\mathbf{p}f(\mathbf{r}, \mathbf{p}, t) = 0. \tag{1.5}$$

Let us now allow the particles to interact via, say, a two-particle potential $W(\mid \mathbf{r} - \mathbf{r}' \mid)$ that depends on their relative distance (this could be, e.g., the mutual Coulomb interaction for charged particles), or via some other general potential that scatters particles. The presence of this interaction changes the particles' momenta via collisions, and the particles can scatter "in" and "out" of the phase-space volume $d\mathbf{r}d\mathbf{p}$. The distribution function $f(\mathbf{r}, \mathbf{p}, t)$ is no longer a conserved quantity and condition given by Eq.(1.2) is not satisfied. The change in time of the distribution function must thus be balanced by an equal amount of change due to collisions.

We write this as

$$\frac{d}{dt}f(\mathbf{r},\mathbf{p},t) = \left(\frac{\partial}{\partial t}f(\mathbf{r},\mathbf{p},t)\right)_{\text{col}} \equiv I\mid f\mid . \tag{1.6}$$

where the quatity $I\mid f\mid$ is called the collision integral(or scattering operator) and is a functional of the distribution function. It gives the net rate of change of number of particles with momentum $\mathbf{p}$, at position $\mathbf{r}$ and time t. For arbitrary interaction potentials, it contains information on the type of processes that drive the system to local equilibrium. These processes may be elastic or inelastic i.e., they may or may not change the energy of single particles. Equating Eq.(1.6) with Eq.(1.5), we obtain the Boltzmann equation :

$$\frac{\partial}{\partial t}f(\mathbf{r},\mathbf{p},t) + \frac{\mathbf{p}}{m}.\boldsymbol{\nabla}_{\mathbf{r}}f(\mathbf{r},\mathbf{p},t) - \boldsymbol{\nabla}_{\mathbf{r}}V_{ext}(\mathbf{r},t).\boldsymbol{\nabla}_{\mathbf{p}}f(\mathbf{r},\mathbf{p},t) = I\mid f\mid . \tag{1.7}$$

Given an interaction potential, the collision integral can be formally calculated exactly. For instance, for a two-body potential one finds

$$I\mid f\mid = \int d\dot{r}dp\boldsymbol{\nabla}_{\mathbf{r}}W(\mid \mathbf{r}-\mathbf{r}'\mid).\boldsymbol{\nabla}_{\mathbf{p}}f_2(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}',t). \tag{1.8}$$

Unfortunately, the above expression contains the two-particle reduced density f_2. We thus need an equation of motion for this quantity. Carrying out a derivation similar to that leading to Eq.(1.8), one can show that the equation of motion for f_2 contains the three-body reduced density f_3 . In turn, the equation of motion for f_3 depends on the four-body reduced density f_4 and so on. This generates an infinite hierarchy of coupled equations, known as the BBGKY hierarchy, thus making the problem practically unsolvable.

The collision integral can be expressed as

$$I\mid f\mid = -\int dp'\{W_{\mathbf{p},\mathbf{p}'}f(\mathbf{r},\mathbf{p},t)[1-f(\mathbf{r},\mathbf{p}',t)] - W_{\mathbf{p}',\mathbf{p}}f(\mathbf{r},\mathbf{p}',t)[1-f(\mathbf{r},\mathbf{p},t)]\} \tag{1.9}$$

where the quantity $W_{\mathbf{p},\mathbf{p}'}$ is the transition probabilty density per unit time that a particle with momentum p is scattered into a state with momentum p´. This probability density may depend on the distribution function itself. The term $f(\mathbf{r},\mathbf{p},t)$ that appears in Eq.(1.9) counts how many electrons are in the initial state $\mathbf{p}$, while the term $[1-f(\mathbf{r},\mathbf{p}',t)]$ counts the available states with momentum $\mathbf{p}'$ into which the electrons can scatter. Eq.(1.7) is now a nonlinear integro-

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differential equation for the distribution function. Therefore, approximations are required to solve the Boltzmann equation for $f(\mathbf{r}, \mathbf{p}, t)$.

According to the type and the strength of the scattering potential, the transition probability $W\mathbf{p}, \mathbf{p}'$ can be calculated using standard techniques of quantum mechanics, such as perturbation theory. An approximation, known as the relaxation-time approximation, can be employed that assumes the identity

$$\frac{1}{\tau(\mathbf{p})} = \int dp W \mathbf{p}, \mathbf{p}[1 - f(\mathbf{r}, \mathbf{p}', t)]. \tag{1.10}$$

where $\tau(\mathbf{p})$ is the relaxation time, i.e., the average time between successive collision. With this approximation we can rewrite the collision intergal as

$$I \mid f \mid = -\frac{[f(\mathbf{r}, \mathbf{p}, t) - f^{eq}(\mathbf{r}, \mathbf{p})]}{\tau}. \tag{1.11}$$

Here, $f^{eq}(\mathbf{r}, \mathbf{p})$ is the local equilibrium Fermi distribution function

$$f^{eq}(\mathbf{r}, \mathbf{p}) = \frac{1}{1 + e^{(E(\mathbf{p}) - \mu(\mathbf{r}))/k_B \theta(\mathbf{r})}}. \tag{1.12}$$

with position-dependent chemical potential and temperature.

Eq.(1.11) quantifies deviations from equilibrium, and contains the physical notion that once electrons reach local equilibrium, then further scattering will not modify their distribution ($I \mid f \mid = 0$ at local equilibrium).

Irrespective of the approximation employed for the collision integral, once the distribution function is known we can calculate the electron number density

$$n(\mathbf{r}, t) = \int d\mathbf{p} f(\mathbf{r}, \mathbf{p}, t). \tag{1.13}$$

and current density

$$j(\mathbf{r}, t) = e \int dp \frac{\mathbf{p}}{m} f(\mathbf{r}, \mathbf{p}, t). \tag{1.14}$$

Electron transport studies of sub-micron devices relies heavily on Boltzmann equation. In practice, solving the Boltzmann integro-differential equation is a very difficult task especially in the presence of electron-electron interactions.

1.1.2 Nonequilibrium Green's function approach (NEGF)

Another important approach to electron transport is the nonequilibrium Green's function approach (NEGF). When only the properties of the ground state are required, zero-temperature (single- and many-particle) Green's function together with its perturbation theory principally gives all the information. However, electron transport is essentially a nonequilibrium problem so the equilibriun Green's function technique needs to be generalized to the nonequilibrium situation. For certain applications it is advantageous to write the Boltzmann equation as an integral equation rather than an integro-differential equation. With this idea in mind, here, we will present the techniques of non-equilibrium Green's function, also known as the Keldysh Formalism[4]. Generally, we need to calculate the Green's function

$$G\left(x, t; x', t'\right) = -\frac{i}{\hbar} Tr \left(T \left\{ \psi_H\left(x, t\right) \psi_H^\dagger\left(x', t'\right) \right\} \rho_H \right) \tag{1.15}$$

where $\psi_H\left(x, t\right)$ is the annihilation field operator in the Heisenberg picture, and ρ is the density matrix, also in the Heisenberg picture. We have assumed that ρ is diagonal in the particle number basis, $[N, \rho] = 0$.

In order to understand Keldysh Formalism we must be aware of Dyson's equation. Consider an example with $V = \sum_{\alpha, \beta} M_{\alpha\beta} C_\alpha^\dagger C_\beta$. Then the first order perturbation gives,

$$G^+\left(\mu, t; \nu, t'\right) = G^{0,+}\left(\mu, t; \nu, t'\right) - \sum_{\alpha\beta} \int ds M_{\alpha\beta} Tr \left(T_c \left\{ C_\mu\left(t\right) C_\nu^\dagger\left(t'\right) C_\alpha^\dagger\left(s\right) C_\beta\left(s\right) \right\} \right) \tag{1.16}$$

The second term has one disconnected term and one non-zero connected term, which includes

$$\left\{ \sum_{\alpha\beta} \int ds M_{\alpha\beta} Tr \left(T_c \left\{ C_\mu\left(t\right) C_\nu^\dagger\left(t'\right) C_\alpha^\dagger\left(s\right) C_\beta\left(s\right) \right\} \right) = \sum_{\alpha\beta} \int_{-\infty}^{\infty} ds G^{0,c}\left(\mu, t; \alpha, s\right) M_{\alpha\beta} G^{0,+}\left(\beta, s; \nu, t'\right) \right.$$

$$\left. + \int_{\infty}^{-\infty} ds G^{0,+}\left(\mu, t; \alpha, s\right) M_{\alpha\beta} G^{0,\tilde{c}}\left(\beta, s; \nu, t'\right). \right\} \tag{1.17}$$

These expansion series can be represented by a matrix equation in the form

$$\widehat{G} = \widehat{G}^0 + \widehat{G}^0 \Sigma \widehat{G}^0 + \widehat{G}^0 \Sigma \widehat{G}^0 \Sigma \widehat{G}^0 + \ldots = \widehat{G}^0 \left(1 + \Sigma \widehat{G} \right) \tag{1.18}$$

which is the Dyson equation and this can be organised as

$$\widehat{G}(t,t') = \widehat{G}^0(t,t') + \int\int_{-\infty}^{\infty} dt_1 dt_2 \widehat{G}^0(t,t_1) \Sigma(t_1,t_2) \widehat{G}(t_2,t') \tag{1.19}$$

where $\widehat{G}(t,t')$ is the operator form of $G(x,t;x',t') = \langle x \mid G(t,t') \mid x' \rangle$; $\widehat{G}^0 = \widehat{D}$ is the free-field NEGF; and $\widehat{\Sigma}$ is the self-energy term coming from interaction. The calculation for the Green's function requires calculation of the self-energy if the last equation is expressed as

$$\widehat{G} = \widehat{G}^0 + \widehat{G}^0 \Sigma \widehat{G}. \tag{1.20}$$

NEGF has proven to be very effective tool to study transport phenomena. A wide range of electron transport phenomena have been successfully addressed using the NEGF technique. Several exact results, not obtained previously by conventional theoretical techniques have been obtained using NEGF.

1.1.3 Path Integral Formulation

The standard formulations of quantum mechanics was developed by Schrodinger, Heisenberg and others in the 1920's. In 1933, Dirac[5] published a paper where he suggested that $\exp(iS/\hbar)$ can be treated as the propagator, where S is the classical action, defined mathematically by

$$S[x(t)] = \int_{t_a}^{t_b} L\left(x', x, t\right) dt \tag{1.21}$$

and $L\left(x', x, t\right)$ is the classical Langrangian of the system. Here the prime ($'$) represents time-derivative.

Feynman developed this idea, taking into account paths other than only the classical one and published a third complete formulation of Quantum Mechanics which provides a much more intuitive introduction to the quantum theory.

Path Integral and the Wave Function

In order to perform the sum over all paths we divide the time interval $(t_a - t_b)$ into N intervals of length ϵ.For each path $x(t)$ we can write $x_i = x(t_i)$ $[N_\epsilon = t_b - t_a, \; \epsilon = t_{i+1} - t_i, \; t_0 = t_a, \; t_N = t_b, \; x_N = x_b]$

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and get a result for the sum over all paths:

$$K(b,a) = \lim_{\epsilon \to 0} \frac{1}{A} \int \int \cdots \int e^{(i/\hbar)S[b,a]} \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{N-1}}{A} \tag{1.22}$$

with some normalization factor A, which we need for the convergence of the whole expression, and, $K(b,a)$ is called the Kernel of the motion. We will write the above equation as

$$K(b,a) = \int_a^b e^{(i/\hbar)S[b,a]} Dx(t) \tag{1.23}$$

and call it in this notation the *configuration space path integral* or *Feynman path integral*.

For $K(b,a)$ there is a rule for combining amplitudes for events occuring in succession in time:

$$K(b,a) = \int_{x_c} K(b,c) K(c,a) \, dx_c, \, if \ \ t_a \langle t_c \langle t_b \tag{1.24}$$

[which follows from $S(b,a) = S(b,c) + S(c,b)$, which is true from the definition of the action. It holds for any point c lying on the path from a to b]. We can write the wave function in terms of the above kernel as

$$\Psi(x_2, t_2) = \int_{-\infty}^{\infty} K(x_2, t_2; x_1, t_1) \Psi(x_1, t_1) \, dx_1 \tag{1.25}$$

which means that the total amplitude to arrive at (x_2, t_2) is equal the sum over all possible values of x_1 (at a fixed time t_1) multiplied by the amplitude to go from 1 to 2.

Perturbation Theory

The idea of Perturbation theory in the path integral formalism is very simple but important. Inserting Eq.(1.21) in Eq.(1.23) and expanding the exponential, we have

$$K_V(2,1) = K_0(2,1) + K_1(2,1) + K_2(2,1) + \ldots \tag{1.26}$$

where,

$$K_0(2,1) = \int_1^2 \left[\exp\left(\frac{i}{\hbar} \int_{t_1}^{t_2} \frac{mx'^2}{2} dt \right) \right] Dx(t) \tag{1.27}$$

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$$K_1\left(2,1\right) = -\frac{i}{\hbar}\int_1^2\left[\exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}\frac{mx'^2}{2}dt\right)\right]\int_{t_1}^{t_2}V\left[x\left(s\right),s\right]ds Dx\left(t\right) \qquad (1.28)$$

$$K_2\left(2,1\right) = -\frac{1}{\hbar^2}\int_1^2\left[\exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}\frac{mx'^2}{2}dt\right)\right]\left[\int_{t_1}^{t_2}V\left[x\left(s\right),s\right]ds\right]^2 Dx\left(t\right) \qquad (1.29)$$

and so on. Here the prime ($'$) shows the time-derivative and $K_0\left(2,1\right)$ is just the free-particle kernel. If we interchange the order of integration over x and $x\left(t\right)$ we obtain for $K_1\left(2,1\right)$:

$$K_1\left(2,1\right) = -\frac{i}{\hbar}\int_{t_1}^{t_2}F\left(s\right)ds \qquad (1.30)$$

where

$$F(s) = \int_1^2\left[\exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}\frac{mx'^2}{2}dt\right)\right]\int_{t_1}^{t_2}V\left[x\left(s\right),s\right]Dx\left(t\right) \qquad (1.31)$$

which is interpreted as free propagation from t_1 until some intermediate time s and again from s to t_2, weighting each path with a characteristic factor $V\left[x\left(s\right),s\right]$. Consequently we can write $F(s)$ in the form

$$F(s) = \int_{-\infty}^{\infty}K_0\left(x_2,t_2;x_s,s\right)V(x_s,s)K_0\left(x_s,s;x_1,t_1\right)dx_s \qquad (1.32)$$

and with Eq.(1.30), the perturbation term gives

$$K_2\left(2,1\right) = -\frac{1}{\hbar^2}\int_{t_1}^{t_2}\int_{-\infty}^{\infty}K_0\left(x_2,t_2;x_s,s\right)V(x_s,s)K_0\left(x_s,s;x_1,t_1\right)dx_sds \qquad (1.33)$$

The interpretation is the following: $K_0\left(2,1\right)$ gives us the amplitude that the particle is propagating from 1 to 2 without being affected by $V\left(x,t\right)$ at all. $K_1\left(2,1\right)$ is the amplitude that the particle is scattered once at any time s between 1 to 2. $K_2\left(2,1\right)$ will then be scattered twice, and so on.

1.1.4   Scattering Matrix Approach

Scattering Matrix

This is one of the most widely used approaches in electron transport in nanostructures especially in the mesoscopic regime[6]. It is an important approach because at sufficiently low energies

any nanostructure can be regarded as a huge scatterer of electron waves coming from leads. Note that a nanostructure taking part in quantum transport is part of an electric circuit. It is connected to several leads(*reservoirs*), which are in thermal equilibrium and are characterized by a fixed voltage. Here we only consider the case when there are two reservoirs (referred to as left and right). Between the reservoirs is the *scattering region*. Let us start with a feature borrowed from quantum point contact model(QPC) - a system without potential barriers - ideal waveguides connect the reservoirs and the scattering region. This is convenient as scattering only takes place in a finite region, the reservoirs being far from this region. The wave functions may have very complicated form in the scattering region, but in the waveguides they can be treated as combination of plane waves. The left and the right waveguides do not have to have the same axis and the same cross-section. This is why it is convenient to introduce the separate coordinates $x_L < 0, y_L, z_L$ and $x_R > 0, y_R, z_R$ for the left and right waveguides,respectively.Generally, a wave function of fixed energy E can be presented as a linear combination of plane waves

$$\Psi(x_L, y_L, z_L) = \sum_n \frac{1}{\sqrt{2\pi\hbar v_n}} \phi_n(y_L, z_L)[a_{Ln} e^{ik_x^{(n)} x_L} + b_{Ln} e^{-ik_x^{(n)} x_L}] \tag{1.34}$$

and

$$\Psi(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m}} \phi_m(y_R, z_R)[a_{Rm} e^{ik_x^{(m)} x_R} + b_{Rm} e^{-ik_x^{(m)} x_R}]. \tag{1.35}$$

Here we label the transport channels in the left and right waveguides by the indices n and m, respectively.

The corresponding transverse wave functions are ϕ_n and ϕ_m, and the energies of the transverse motion are E_n, E_m. For any transverse channel n or m, be it in the left or the right waveguide, the energy E fixes the value of the wave vector $k_x^{(n)} = \sqrt{2m(E - E_n)}/\hbar$.Transport is due to propagating, not evanescent waves, and $k_x^{(n)}$ has to be real. Then, only a finite number of open channels, N_L to the left and N_R to the right, exist at a fixed energy E.

In Eqs.(1.34) and (1.35), the coefficients a_{Ln}, a_{Rm} are the amplitudes of the waves coming from the reservoirs, and b_{Ln}, b_{Rm} are the amplitudes of the waves transmitted through or reflected back from the scattering region. These coefficients are therefore not independent: the amplitude of the wave reflected from the obstacle linearly depends on the amplitude of incoming

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waves in all the channels:

$$b_{\alpha l} = \sum_{\beta=L,R} \sum_{l'} s_{\alpha l, \beta l'} \, a_{\beta l'}, \quad \beta = L, R, l = n, m. \tag{1.36}$$

The proportionality coefficients are combined into a $(N_L + N_R) \times (N_L + N_R)$ *scattering matrix* $\hat{s}$. It has the following block structure:

$$\hat{s} = \begin{pmatrix} \hat{s}_{LL} & \hat{s}_{LR} \\ \hat{s}_{RL} & \hat{s}_{RR} \end{pmatrix} \equiv \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix}. \tag{1.37}$$

The $N_L \times N_L$ *reflection matrix* $\hat{r}$ describes the reflection of the waves coming from the left. Thus, $r_{nn'}$ is the amplitude of the following process: the electron coming from the left in the transverse channel n is reflected to the channel n'. Consequently, $|r_{nn'}|^2$ is the probability of this process. The $N_R \times N_R$ *transmission matrix* $\hat{t}$ is responsible for the transmission through the scattering region.

An important condition on the scattering matrix is imposed by symmetry with respect to time reversal. If this symmetry holds, the scattering matrix is symmetric, $\hat{s} = \hat{s}^T$. So, the reflection matrices are summetric, and $\hat{t} = \hat{t}^T$.

Further, a scattering matrix satisfies the unitary condition, $\hat{s}^\dagger \hat{s} = \hat{1}$. The diagonal element is given by

$$\left(\hat{s}^\dagger \hat{s} \right)_{nn} = \sum_{n'} |r_{nn'}|^2 + \sum_m |t_{mn}|^2 = 1 \tag{1.38}$$

since it represents the total probability of an electron in channel n being either reflected or transmitted to any channel.

Transmission eigenvalues

Now we turn our attention to calculating the current. The current I can be expressed as

$$I = 2_s e \sum_n \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} v_x(k_x) f_n(k_x). \tag{1.39}$$

where $v_x(k_x) \, (= \hbar k_x / m)$ is the velocity and the factor 2_s reperesents spin-degeneracy. Let us calculate the current through a cross-section located in the left waveguide. The electrons

with $k_x > 0$ originate from the left reservoir, and their filling factor is therefore $f_L(E)$. Now, the electrons with $k_x < 0$ in a given channel n are coming from the scattering region. A fraction of these electrons originate from the left reservoir and are reflected; they carry the filling factor $f_L(E)$. This fraction is determined by the probability of being reflected to channel n from all possible starting channels n', $R_n(E) = \sum_{n'} | r_{nn'} |^2$. Other electrons are transmitted through the scattering region, their filling factor being $f_R(E)$. The resulting filling factor for $k_x < 0$ is therefore $R_n \, f_L(E) + (1 - R_n) \, f_R(E)$. For the current we write

$$I = 2_s e \sum_n \left(\int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) f_L(E) + \int_{-\infty}^0 \frac{dk_x}{2\pi} v_x(k_x) \left[R_n \, f_L(E) + (1 - R_n) f_R(E) \right] \right) \quad (1.40)$$

Replacing $-k_x$ by k_x in the second term of Eq.(1.40) we have the expression

$$I = 2_s e \sum_n \left(\int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) \left(1 - R_n(E) \right) \left[f_L(E) - f_R(E) \right] \right). \quad (1.41)$$

Eq.(1.38) can be written as

$$1 - R_n = \sum_m | t_{mn} |^2 = \left(\hat{t}^\dagger \hat{t} \right)_{nn} \quad (1.42)$$

changing variables from k_x to E, Eq.(1.41) can be expressed as

$$I = \frac{2_s e}{2\pi} \int_0^\infty dE Tr \left[\hat{t}^\dagger \hat{t} \right] \left[f_L(E) - f_R(E) \right]. \quad (1.43)$$

The trace can be represented as a sum of eigenvalues T_p of the Hermitian matrix $\hat{t}^\dagger \hat{t}$, the transmission eigenvalues. Because of the unitarity of the scattering matrix, T_p are real numbers between zero and one.

The transmission eigenvalues depend on energy. However, in the linear regime, when the applied voltage is much smaller than typical energy scale of this dependence, they can be evaluated at the Fermi surface, and we obtain the following expression for the conductance (using the left waveguide):

$$G = G_Q \sum_p T_p(\mu) \quad (1.44)$$

where $G_Q \equiv \frac{2e^2}{h}$ is the conductance quantum. Calculations of the current in the right waveguide gives the same result: current is conserved. Eq.(1.44) is known as the (two-terminal) *Landauer formula*.

The scattering matrix is the approach of choice when a simple intuitive approach is required to study coherent, linear transport of electrons in a nanostructures. In the presence of inelastic scattering or transport beyond linear regime, a better approach is required as the scattering matrix becomes unwieldly due to the large number of transport channels available.

1.1.5 Balance Equation Approach

Over the years, both classical and quantum transport theorists have studied transport phenomena using innovative techniques: superoperators, Feynman diagram expansions of equilibrim correlation functions and more recently non-equilibrium Green's functions, path integrals as well as Wigner distributions[7] and multi-particle density matrices. With the development of computational capacity, Monte Carlo techniques have been employed in transport calculations. These efforts have had great success, but also have some shortcomings. Some are formidable to deal with accurately even within linear regime and very hard to extend beyond linear conduction, others involve complicated analytic continuation, etc. Calculations are lengthy and difficult, and few of these seem to offer a simple vehicle for generating useful physical insight into transport dynamics on a systematic basis. Most often, because of technical difficulties, they also ignore electron-electron interaction effects which can be of vital importance.

Although the consideration of carrier-carrier (e-e) interaction introduces considerable complication, physically there is a substantial simplification in the situation when e-e interactions are large enough to induce rapid thermalization of the carriers about the drifted transport state. This opens a quasi-analytic description of transport, which is successfully addressed by Lei-Ting balance equation approach in developing a perturbation theory about a displaced drifted equilibrium state. As one would expect, the results differs from those analysis which ignore the role of e-e interactions. The quantum mechanical Lei-Ting balance equation, in the classical limit, exactly reproduce the successful gas plasma theory (develpoed by Spitzer et al.) which similarly cuts through the formidable difficulties of rigorous formal classical theory, particularly with the inclusion of e-e interactions which are germane to gas plasma dynamics. The results

offer considerable physical insight into the dynamics of both quantum and classical transport.

The object of the present work is to provide a comprehensive description of the quantum dynamical formulation of the Lei-Ting balance equation transport theory, clarifying approximations and to explore its advantages as a quasi-analytic approach to electron-transport[1].

The balance equation approach allows an analytically tractable analysis of transport problems even in the non-linear regime, taking electron-electron interaction into account. As an analytic theory, it provides physical insight beyond that provided by other methods which require extensive numerical work. In the earlier investigations of transport, the carrier-carrier Coulomb interactions were taken into account as static screening. On the contrary, the balance-equation approach incorporates the dynamic effects of the carrier-carrier interactions within the framework of the density-density correlation function $\Pi_2(q, \omega)$.

Chapter 2

Balance Equation Approach

2.1 Understanding Balance equations

As solving the Boltzmann transport equation for the electron-electron interaction is too difficult, simpler approaches are often adopted when analyzing, designing, and optimizing devices. The use of balance, or conservation, equations which are derived from the Boltzmann transport equation is a common approach. Balance equations have a very clear physical interpretation. For instance, the electron continuity equation[8]

$$\frac{\partial n}{\partial t} = -\nabla.\mathbf{F}_n + G_n - R_n \tag{2.1}$$

states that the net rate of increase of average carrier density at a specified location and time, $n(\mathbf{r}, t)$, is given by the rate per unit volume at which carriers are flowing in (negative divergence of the electron flux, $\mathbf{F}_n$) plus the rate per unit volume of electron creation, G_n (due to optical or avalanch generation, for example) minus the rate per unit volume at which electrons disappear (by recombining with the holes or defects). Balance equations for the average carrier momentum and energy density can also be formulated and expressed as continuity equations in the form of Eq.(2.1). Such equations find wide applications in device analysis. The familiar drift-diffusion equation, for instance, is a simplified form of the momentum balance equation. In the drift-diffusion approach, the unknowns are the average carrier density and velocity. When the average carrier density is required, another balance equation can be solved. Although the

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balance equations are conceptually sraightforwad, many different sets of balance equations can be formulated, depending upon the specific approach and the simplifying assumptions.

2.2 Center-of-mass and Relative Variables of Electron

We consider a system of N electrons under the influence of a uniform applied electric field $\mathbf{E}$. The electrons interact with each other through the Coulomb potential, and are coupled with phonons and scattered by N_i randomly distributed impurities.

The Hamiltonian of the system, for the single band effective-mass description of electrons, can be written as[9]

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_o \mid \mathbf{r}_i - \mathbf{r}_j \mid} + \sum_{i,a} u(\mathbf{r}_i - \mathbf{R}_a) - \sum_{i,j} \mathbf{u}_l . \boldsymbol{\nabla} v_l(\mathbf{r}_i - \mathbf{R}_l) - e \sum_i \mathbf{r}_i . \mathbf{E}. \quad (2.2)$$

Here $\mathbf{r}_i$ and $\mathbf{p}_i = -i\boldsymbol{\nabla}_i$ are the coordinate and momentum of the ith electron with effective mass $'m'$ and charge $'e'$. $v_l(\mathbf{r}_i - \mathbf{R}_l)$ denotes the potential by the lth ion at lattice site $\mathbf{R}_l$ and $\mathbf{u}_l$ is its displacement from the regular equilibrim position; $u(\mathbf{r} - \mathbf{R}_a)$ denotes the additional scattering potential due to an impurity at site $\mathbf{R}_a$ which is randomly located ; and the second term on the right hand side of Eq.(2.2) is the Coulomb interaction between electrons. The balance-equation theory proceeds from the separation of motion of centre-of-mass (c.m.)(ie. the motion of the system as an entity) from the relative motion of the electrons.

Denoting the centre-of-mass momentum and coordinate variables by $\mathbf{P}, \mathbf{R}$ and the relative electron momentum and coordinate variables by $\mathbf{p}'_i$, $\mathbf{r}'_i$, we have

$$\mathbf{P} = \sum_i \mathbf{p}_i, \quad \mathbf{R} = \frac{1}{N} \sum_i \mathbf{r}_i \quad (2.3)$$

$$\mathbf{p}'_i = \mathbf{p}_i - \frac{1}{N}\mathbf{P}, \quad \mathbf{r}'_i = \mathbf{r}_i - \mathbf{R}. \quad (2.4)$$

$\mathbf{P}, \mathbf{R}$ canonically conjugate variables:

$$[\mathbf{R}_\alpha, \mathbf{P}_\beta] = i\delta_{\alpha\beta} \quad (2.5)$$

$(\alpha, \beta = x, y, z)$, and they commute with $\mathbf{r}'_i, \mathbf{p}'_i$:

$$[\mathbf{r}'_i, \mathbf{P}] = [\mathbf{R}, \mathbf{p}'_i] = 0. \tag{2.6}$$

The N relative electron momenta and coordinates so defined are not completely independent, but subject to the constraints:

$$\sum_i \mathbf{p}'_i = 0, \qquad \sum_i \mathbf{r}'_i = 0 \tag{2.7}$$

and their commutation relations include a canonical $1/N$ term:

$$[\mathbf{r}'_{i\alpha}, \mathbf{p}'_{j\beta}] = i\delta_{\alpha\beta}(\delta_{ij} + \frac{1}{N}). \tag{2.8}$$

For a macroscopiclly large N system, we make a reasonable assumption that $1/N$ term in Eq.(2.8) is negligible, such that one can treat the relative momentum and coordinate as canonical variables:

$$[\,\mathbf{r}'_{i\alpha}, \mathbf{p}'_{j\beta}] \simeq i\delta_{\alpha\beta}\delta_{ij} \tag{2.9}$$

Although Eq.(2.9) is an approximation, the neglect of noncanonical $1/N$ term in Eq.(2.8) does not result in any error within the framework of balance-equation theory if the-center-of-mass coordinate $\mathbf{R}(t)$ is treated classically.

In terms of the-center-of-mass variables and the relative electron variables we can express Hamiltonian of Eq.(2.2) as

$$H = H_c + H_e + H_{ph} + H_{ei} + H_{ep} \tag{2.10}$$

$$H_c = \frac{P^2}{2Nm} - Ne\mathbf{E}.\mathbf{R} \tag{2.11}$$

$$H_e = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2\Omega} \sum_{\mathbf{q}} v_c(\mathbf{q})(\rho_{\mathbf{q}}\rho_{-\mathbf{q}} - N) \tag{2.12}$$

$$H_{ph} = \sum_{\mathbf{q},\lambda} \Omega_{\mathbf{q}\lambda} b^\dagger_{\mathbf{q}\lambda} b_{\mathbf{q}\lambda} \tag{2.13}$$

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$$H_{ei} = \frac{1}{\Omega} \sum_{\mathbf{q},a} u(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}_a)} \rho_{\mathbf{q}} \tag{2.14}$$

$$H_{ep} = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{q},\lambda} M(\mathbf{q},\lambda) \phi_{\mathbf{q}\lambda} \mathbf{q} e^{i\mathbf{q}\cdot\mathbf{R}} \rho_{\mathbf{q}} \tag{2.15}$$

where H_c is the centre of mass Hamiltonian, H_e is the relative electron Hamiltonian, H_{ph} is the non-interacting phonon Hamiltonian, H_{ei} is the electron-impurity interaction Hamiltonian, H_{ep} is the electron-phonon interaction Hamiltonian, Ω is the volume of the system, and $c^\dagger_{\mathbf{k}\sigma}$ ($c_{\mathbf{k}\sigma}$) are the creation(annihilation) operators for the relative electrons with wave-vector $\mathbf{k}$, spin σ, and energy $\varepsilon_{\mathbf{k}} = k^2/2m$, and $\rho_{\mathbf{q}}$ is the electron density operator defined as

$$\rho_{\mathbf{q}} \equiv \sum_{\mathbf{k}} \rho_{\mathbf{k}\mathbf{q}} = \sum_j e^{i\mathbf{q}\cdot\mathbf{r}j} = \sum_\sigma c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}, \tag{2.16}$$

$\phi_{\mathbf{q}\lambda} \equiv b^\dagger_{-\mathbf{q}\lambda} + b_{\mathbf{q}\lambda}$ is the phonon field operator with $b^\dagger_{\mathbf{q}\lambda}$ and $b_{\mathbf{q}\lambda}$ being creation and annihilation operators for phonons of wavevector $\mathbf{q}$ in branch λ with frequency $\Omega_{\mathbf{q}\lambda}$, $v_c(\mathbf{q}) = \frac{e2}{\varepsilon_o \kappa q^2}$ is the Coulomb potential (κ is the background dielectric constant), $u(\mathbf{q})$ and $M(\mathbf{q},\lambda)$ are respectively the electron–impurity potential and the electron-phonon-matrix element in the plane wave representation, satisfying $u(\mathbf{q}) = u^*(-\mathbf{q})$ and $M(\mathbf{q},\lambda) = M^*(-\mathbf{q},\lambda)$.

2.3 Center of mass treated as a classical particle

Because of its enormous mass, the motion of the centre-of -mass is essentially classical, and we can treat the c.m.-related operators classically, regarding $\mathbf{R}$ in H_{ei} and H_{ep} as real, time-dependent position of the center-of -mass. The relative electron system, which is composed of a large number of interacting particles and is treated fully quantum-mechanically, does not directly sense the electric field but is coupled to the centre-of-mass motion through the c.m. position $\mathbf{R}(t)$.

$$H_{It} = H_{ei} + H_{ep}. \tag{2.17}$$

Employing the Hamiltonian, it is apparent that the c.m. velocity V, or the time derivative of the c.m.position, is given by

$$\mathbf{V} \equiv \frac{d}{dt}\mathbf{R} = -i[\mathbf{R}, H] = \frac{\partial H}{\partial \mathbf{P}} = \frac{\mathbf{P}}{Nm}. \tag{2.18}$$

Note that the centre-of-mass, which is accelerated by the electric field and damped by the relative electron-phonon bath medium, is a Brownian particle due to the random force associated with the electron-impurity and electron-phonon interactions. Therefore the c.m. velocity $\mathbf{V}$ is composed of a drift part $\mathbf{v}$ and a fluctuation or random part $\delta\mathbf{V}$:

$$\mathbf{V} = \mathbf{v} + \delta\mathbf{V}. \tag{2.19}$$

We denote $\mathbf{v} = \langle\mathbf{V}\rangle$ or $\langle\delta\mathbf{V}\rangle = 0$,with the $\langle...\rangle$ symbol understood as an average either over an appropriate time period or over a statistical ensemble which eliminates the fluctuations. The forces experienced by the centre of mass are obtained by calculating the time-derivative of the c.m. momentum $\frac{d\mathbf{P}}{dt} = -i[\mathbf{P}, H] = -\frac{\partial H}{\partial \mathbf{R}}$, yielding

$$\frac{d\mathbf{P}}{dt} = Ne\mathbf{E} + \mathbf{F} \tag{2.20}$$

with $\mathbf{F} = \mathbf{F}_i + \mathbf{F}_p$, and

$$\mathbf{F}_i = -i\sum_{\mathbf{q},a} u(\mathbf{q})\mathbf{q}e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R_a})}\rho_{\mathbf{q}} \tag{2.21}$$

$$\mathbf{F}_p = -i\sum_{\mathbf{q},\lambda} M(\mathbf{q},\lambda)\mathbf{q}\phi_{\mathbf{q}\lambda}e^{i\mathbf{q}\cdot\mathbf{R}}\rho_{\mathbf{q}} \tag{2.22}$$

are frictional forces due to impurities and phonon scattering. Being quantum-mechanical operators in the relative-electron and phonon space, $\mathbf{F}_i$ and $\mathbf{F}_p$ also comprise an average part and a fluctuation part. The latter contributes a random force exerted on the center of mass. Eq.(2.20) can be regarded as an operator force balance equation.

We can calculate the rates of change of the energies of the phonon and relative electron system as

$$\frac{d}{dt}H_{ph} = -i[H_{ph}, H] = W \equiv -\sum_{\mathbf{q},\lambda} M(\mathbf{q},\lambda)\mathbf{q}(\frac{d}{dt}\phi_{\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}}\rho_{\mathbf{q}} \tag{2.23}$$

$$
\begin{aligned}
\frac{d}{dt}H_e &= -i[He, H] \equiv S = \left\{ -i\sum_{\mathbf{q},\lambda} M(\mathbf{q},\lambda)\mathbf{q}\phi_{\mathbf{q}\lambda}e^{i\mathbf{q}\cdot\mathbf{R}} \sum_{\mathbf{k}}(\varepsilon_{\mathbf{q}+\mathbf{k}} - \varepsilon_{\mathbf{k}})\rho_{\mathbf{kq}} \right.\\
&\quad \left. -i\sum_{\mathbf{q},a} u(\mathbf{q})\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{R}_a} \sum_{\mathbf{k}}(\varepsilon_{\mathbf{q}+\mathbf{k}} - \varepsilon_{\mathbf{k}})\rho_{\mathbf{kq}} \right\}
\end{aligned}
\tag{2.24}
$$

with

$$
\frac{d}{dt}\phi_{\mathbf{q}\lambda} \equiv -i[\phi_{\mathbf{q}\lambda}, H_{ph}] = -i\Omega_{\mathbf{q}\lambda}(b_{\mathbf{q}\lambda} - b^\dagger_{-\mathbf{q}\lambda}).
\tag{2.25}
$$

Energy balance for the electron system requires that the energy supplied per unit time by the field $\mathbf{E}$: $Ne\mathbf{E}.\mathbf{V}$, matches the sum of the energy increase rate of the center of mass, $d(\frac{1}{2}NmV^2)/dt$, the increase rate of the relative electron internal energy, $\frac{d}{dt}H_e$, and the energy loss rate of the electron system to the phonon system W:

$$
Ne\mathbf{E}.\mathbf{V} = Nm\mathbf{V}.\frac{d\mathbf{V}}{dt} + \frac{d}{dt}H_e + W
\tag{2.26}
$$

Eq.(2.26) states the energy balance for the relative electron system. All these equations are in operator form in the quantum number spaces of relative electrons and phonons.

The balance equations can also be derived by taking the ensemble averages of F and W over the density matrix of the relative electron and phonon systems. The statistical average of a dynamical variable Y at time t can be evaluated in the Schrodinger picture by

$$
\langle Y \rangle = Tr\{\rho Y\}.
\tag{2.27}
$$

Here Y is the operator (possibly time dependent) representing a dynamical variable in the Schrodinger picture and ρ is the density matrix satisfying the Liouville equation[10]

$$
i\frac{d\rho}{dt} = [H_e + H_{ph} + H_{It}, \rho]
\tag{2.28}
$$

subject to the initial condition at initial time t_0

$$
\rho\,|_{t_0} = \rho_0
\tag{2.29}
$$

where we will use $t_0 = -\infty$ or $t_0 = 0$ as initial time.

2.4   Initial Density matrix

As a parametrized theory, the balance-equation approach allows us to choose an initial state to have its major features resemble, as closely as possible, the real final state, such that the system, starting from its virtual initial state, can reach the real final state in a short evolution process. For the present work, we assume the relative electron system as an isolated system, will approach a thermodynamic equilibrium state with a fixed temperature $T_e(t)$, which is dependent on the system at time t. This value is then used for the initial state: $T_e = T_e(t)$. The phonon system that has been decoupled from the electron system, can also be considered to arrive at an equillibrium state jointly with the bath at the lattice temperature T. This is justified if phonons relax faster than electrons. The initial density matrix is thus chosen as:

$$\rho_{o=\frac{1}{Z}} e^{-H_e/T_e} e^{-H_{ph}/T} \tag{2.30}$$

where Z is a normalization coefficient and H_e is implicitly measured from the Fermi level corresponding to a grand canonical ensemble for the relative electron system. This initial density matrix depends on time t parametrically, $\rho_o = \rho_{ot}$.

It should be noted that there are at least two distinct time scales involved. The motion of the center-of-mass, the time variation of the applied electric field $E(t)$ and the temporal development of statistically averaged quantities such as $\mathbf{v}(t)$, $T_e(t)$, occur at a macroscopic time scale, which is assumed to be much larger than the microscpic relaxation time, or the evolution time scale of the Liouville equation.

2.5   Force- and Energy-Balance Equation to the Lowest Order in H_I

2.5.1   Density Matrix and Statistical Average to Linear Order in H_I

The statistical average of the time-independent dynamical variable Y is mathematically defined as

$$\langle Y \rangle = Tr\{\rho Y\}. \tag{2.31}$$

In analogy to Eq.(2.31), the statistical average of time-dependent dynamical Y can be written as[11]

$$\langle Y \rangle = Tr\left\{\rho(t)Y(t)\right\} \tag{2.32}$$

where we have defined

$$Y(t) \equiv e^{i(H_e+H_{ph})t}Ye^{-i(H_e+H_{ph})t} \tag{2.33}$$

and

$$\rho(t) \equiv e^{i(H_e+H_{ph})t}\rho e^{-i(H_e+H_{ph})t} \tag{2.34}$$

By differentiating Eq.(2.34), we can get the well-known Liouville's Equation which is written as

$$i\frac{d\rho(t)}{dt} = [H_{It}(t), \rho(t)] \tag{2.35}$$

and subject to the initial condition

$$\rho(t)\,|_{t=-\infty} = \rho_0 \tag{2.36}$$

Now integrating Eq.(2.35), we have

$$\rho(t) = \rho_0 - i\int^t dt'[H_{It'}(t'), \rho(t')]. \tag{2.37}$$

This integral equation facilitates perturbative expansion in the interaction H_l. The first order interation of Eq.(2.37) yields

$$\rho(t) = \rho_0 - i\int^t dt'[H_{It'}(t'), \rho_0]. \tag{2.38}$$

The statistical average for the dynamical variable Y, defined in Eq.(2.32), thus can be written as

$$\langle Y \rangle = \langle Y \rangle_0 - i\int^t \langle[H_{It'}(t'), Y(t)]\rangle_0\, dt' \tag{2.39}$$

where

$$\langle(...)\rangle_0 \equiv \mathbf{Tr}\left\{\rho_0(...)\right\}. \tag{2.40}$$

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Note that ρ_o may be dependent on time t.

2.6 Force Balance Equation

Taking the statistical average of Eq.(2.20) in the relative electron and phonon space to the lowest order in H_I in accordance with Eq.(2.39) and using expressions (2.14) and (2.15) for H_{ei} and H_{ep}, we have

$$nm\frac{d}{dt}\mathbf{v}(t) = ne\mathbf{E}(t) + \mathbf{f}_i + \mathbf{f}_p \tag{2.41}$$

which is written for unit volume of the system with n being the carrier number density. Here we have set $\langle \mathbf{f}_i \rangle_0$ and $\langle \mathbf{f}_p \rangle_0$ to be zero and have identified the average rate of change of c.m. momentum as

$$\left\langle \frac{d\mathbf{P}}{dt} \right\rangle = nm\frac{d}{dt}\mathbf{v}(t). \tag{2.42}$$

$\mathbf{v}(t)$ being the drift part of the c.m. velocity. The frictional forces $\mathbf{f}_i$ and $\mathbf{f}_p$ due to impurity scattering and due to electron-phonon interaction respectively, are given to lowest order by

$$\mathbf{f}_i = -in_i\sum_{\mathbf{q}}\mathbf{q}\mid u(\mathbf{q})\mid^2 \int_{-\infty}^{\infty}dt'A(\mathbf{q},t,t')\Pi(\mathbf{q},t-t') \tag{2.43}$$

$$\mathbf{f}_p = -i\sum_{\mathbf{q},\lambda}\mathbf{q}\mid M(\mathbf{q},\lambda)\mid^2 \int_{-\infty}^{\infty}dt'A(\mathbf{q},t,t')\Lambda(\mathbf{q},\lambda;t-t') \tag{2.44}$$

where n_i is the impurity density.

The correlation functions $\Pi(\mathbf{q},t-t')$ and $\Lambda(\mathbf{q},\lambda;t-t')$ are defined as

$$\Pi(\mathbf{q},t-t') = -i\theta(t-t')\left\langle [\rho_{\mathbf{q}}(t),\rho_{-\mathbf{q}}(t')] \right\rangle_0 \tag{2.45}$$

$$\Lambda(\mathbf{q},\lambda;t-t') = -i\theta(t-t')\left\langle [\phi_{\mathbf{q}\lambda}(t)\rho_{\mathbf{q}}(t),\phi_{-\mathbf{q}\lambda}(t')\rho_{-\mathbf{q}}(t')] \right\rangle_0 \tag{2.46}$$

Here

$$\rho_{\mathbf{q}}(t) = e^{iH_e t}\rho_{\mathbf{q}}e^{-iH_e t} = \sum_{\mathbf{k}}e^{i(\varepsilon_{\mathbf{q}+\mathbf{k}}-\varepsilon_{\mathbf{k}})}\rho_{\mathbf{k}\mathbf{q}} \tag{2.47}$$

and

$$\phi_{\mathbf{q}\lambda}(t) = e^{iH_{ph}t}\phi_{\mathbf{q}\lambda}e^{-iH_{ph}t} = b_{\mathbf{q}\lambda}e^{-i\Omega_{\mathbf{q}\lambda}t} + b_{\mathbf{q}\lambda}^{\dagger}e^{i\Omega_{-\mathbf{q}\lambda}t} \tag{2.48}$$

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have been obtained by using Baker-Hausdorff identity[13], and

$$A(\mathbf{q}, t, t') \equiv \exp[i\mathbf{q}.(\mathbf{R}(t) - \mathbf{R}(t'))] = \exp[i\mathbf{q}. \int_{t'}^{t} \mathbf{v}(s)ds]. \tag{2.49}$$

In writing the equality of Eq.(2.49), we have neglected effects due to velocity fluctuation.Eq.(2.42) is the time-dependent momentum (force) balance equation, or the equation of motion of the center of mass.

2.7 Energy Balance Equation

Let us take the statistical average of the right hand side of the operator equation (2.23) in the relative electron and phonon space to the lowest order in H_I to obtain

$$w = \langle W \rangle \equiv - \sum_{\mathbf{q}, \boldsymbol{\lambda}} \mid M(\mathbf{q}, \boldsymbol{\lambda}) \mid^2 \int_{-\infty}^{\infty} dt' A(\mathbf{q}, t, t') \Gamma(\mathbf{q}, \lambda; t - t') \tag{2.50}$$

with

$$\Gamma(\mathbf{q}, \lambda; t - t') = -i\theta(t - t') \left\langle [(\frac{d}{dt}\phi_{\mathbf{q}\lambda}(t))\rho_{\mathbf{q}}(t), \phi_{-\mathbf{q}\lambda}(t')\rho_{-\mathbf{q}}(t')] \right\rangle_0 \tag{2.51}$$

and

$$\frac{d}{dt}\phi_{\mathbf{q}\lambda}(t) = e^{iH_{ph}t}(\frac{d}{dt}\phi_{\mathbf{q}\lambda})e^{-iH_{ph}t}, \tag{2.52}$$

which can be written as

$$\frac{d}{dt}\phi_{\mathbf{q}\lambda}(t) = -i\Omega_{\mathbf{q}\lambda}(b_{\mathbf{q}\lambda}e^{-i\Omega_{\mathbf{q}\lambda}t} - b_{-\mathbf{q}\lambda}^{\dagger}e^{i\Omega_{-\mathbf{q}\lambda}t}). \tag{2.53}$$

w in Eq.(2.50) is the energy increase rate of phonon system due to electron-phonon interaction, i.e. the energy transfer rate from the electron system to the phonon system. The energy balance equation[12] results from the statistical average of the operator equation (2.26) if we retain only the drift part of c.m. velocity and identify $\left\langle \frac{d}{dt}H_e \right\rangle$ as the rate of change of relative electron internal energy, $dE_e/dt \equiv \frac{d}{dt}\langle H_e \rangle$:

$$ne\mathbf{E}.\mathbf{v} = nm\mathbf{v}.\frac{d\mathbf{v}}{dt} + \frac{d}{dt}E_e + w \tag{2.54}$$

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Using the first order perturbation expansion, Eq.(2.38), for the density matrix to calculate $E_e \equiv \langle H_e \rangle$, we find that only the ρ_o term in Eq.(2.38) contributes, leading to

$$E_e = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} f(\varepsilon_{\mathbf{k}}, T_e) \tag{2.55}$$

where

$$f(\varepsilon_{\mathbf{k}}, T_e) = \frac{1}{[\exp(\varepsilon_{\mathbf{k}} - \mu)/T_e + 1]} \tag{2.56}$$

is the Fermi distribution function at the electron temperature, and μ is the chemical potential. Thus we have

$$\delta \frac{dE_e}{dt} \equiv C_e \frac{dT_e}{dt} \tag{2.57}$$

with $C_e = \partial E_e / \partial T_e$ as the specific heat of the relative electron system. Eliminating $nm\mathbf{v}.\frac{d\mathbf{v}}{dt}$ by means of the force balance equation (2.42), we can write the energy balance equation as

$$-C_e \frac{dT_e}{dt} = \mathbf{v}.\mathbf{f} + w. \tag{2.58}$$

Eq.(2.54) or Eq.(2.58) are the time-dependent energy balance equation of the system.

It should be noted that the energy balance equation can also be obtained by taking the average of operator equation (2.24) and identifying $\langle \frac{d}{dt} H_e \rangle = dE_e/dt$, such that

$$\frac{dE_e}{dt} = \langle S \rangle . \tag{2.59}$$

The balance equation thus obtained is equivalent to Eq.(2.54) for steady state transport and for time-dependent drift motion involving negligible memory effects.

Chapter 3

Applications of Balance Equation Approach

In this chapter, we will apply the balance equation approach to study electron transport phenomena. We will employ the force- and energy-balance equations developed in chapter (2) to the examination of steady state dc transport in a 3D isotropic system. We take $\hbar = 1$ in all the equations that follow.

3.1 Steady-State DC Transport in a 3D System

3.1.1 Balance Equation for Steady-State Transport

In an externally applied uniform electric field, the system approaches a steady state with a constant drift velocity $\mathbf{v}_d$ and a contant electron temperature T_e, after transients die out. For steady state transport we can take $\mathbf{v}(s) = \mathbf{v}_d$ in Eq.(2.49) to obtain

$$A(\mathbf{q}, t, t') \equiv \exp[i\mathbf{q}.\int_{t'}^{t} \mathbf{v}_d ds] = \exp\left[i\mathbf{q}.\mathbf{v}_d(t - t')\right] \tag{3.1}$$

which can also be written as

$$A(\mathbf{q}, t, t') = e^{i\omega_0(t-t')} \tag{3.2}$$

where $\omega_0 \equiv i\mathbf{q}.\mathbf{v}_d$.

Now using Eq.(3.2) in Eqs.(2.43), (2.44) and (2.50), we obtain

$$\mathbf{f}_i = -in_i \sum_{\mathbf{q}} \mathbf{q} \mid u(\mathbf{q}) \mid^2 \int_{-\infty}^{\infty} dt' e^{i\omega_0(t-t')} \Pi(\mathbf{q}, t - t') \tag{3.3}$$

$$\mathbf{f}_p = -i \sum_{\mathbf{q},\lambda} \mathbf{q} \mid M(\mathbf{q}, \boldsymbol{\lambda}) \mid^2 \int_{-\infty}^{\infty} dt' e^{i\omega_0(t-t')} \Lambda(\mathbf{q}, \lambda; t - t') \tag{3.4}$$

and

$$w = \langle W \rangle \equiv - \sum_{\mathbf{q},\lambda} \mid M(\mathbf{q}, \boldsymbol{\lambda}) \mid^2 \int_{-\infty}^{\infty} dt' e^{i\omega_0(t-t')} \Gamma(\mathbf{q}, \lambda; t - t'). \tag{3.5}$$

Fourier transforming Eqs.(3.3),(3.4), and(3.5) followed by a change of variables i.e. replacing $(t - t')$ by t' we obtain the steady state force- and energy-balance equations:

$$ne\mathbf{E} + \mathbf{f} = 0 \tag{3.6}$$

$$\mathbf{v}_d.\mathbf{f} + w = 0 \tag{3.7}$$

where $\mathbf{f} = \mathbf{f}_i + \mathbf{f}_p$, with

$$\mathbf{f}_i = n_i \sum_{\mathbf{q}} \mathbf{q} \mid u(\mathbf{q}) \mid^2 \Pi_2(\mathbf{q}, \omega_0) \tag{3.8}$$

$$\mathbf{f}_p = 2 \sum_{\mathbf{q},\lambda} \mathbf{q} \mid M(\mathbf{q}, \boldsymbol{\lambda}) \mid^2 \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda} + \omega_0) \left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} + \omega_0}{T_e}\right) \right] \tag{3.9}$$

and

$$w = 2 \sum_{\mathbf{q},\lambda} \Omega_{\mathbf{q}\lambda} \mid M(\mathbf{q}, \boldsymbol{\lambda}) \mid^2 \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda} + \omega_0) \left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} + \omega_0}{T_e}\right) \right] \tag{3.10}$$

where $n(x) \equiv \frac{1}{e^x-1}$ is the Bose distribution function, and $\Pi_2(\mathbf{q}, \omega_0)$ is the imaginary part of the Fourier transform of the density-density correlation function:

$$\Pi(\mathbf{q}, \omega) = \int_{-\infty}^{\infty} e^{i\omega t} \Pi(\mathbf{q}, t) dt \tag{3.11}$$

The function $\Pi(\mathbf{q}, t)$, defined in 2.45, is the density-density correlation function in a thermody-

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namic equilibrium state with temperature T_e for the relative electron system described by the Hamiltonian

$$H_e = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2\Omega} \sum v_c(\mathbf{q})(\rho_{\mathbf{q}}\rho_{-\mathbf{q}} - N). \tag{3.12}$$

Let's introduce the field operators[11]

$$\psi_\sigma^\dagger(\mathbf{r},t) = \frac{1}{\Omega} \sum_{\mathbf{p}} e^{-i[(\mathbf{p}\cdot\mathbf{r})-(\epsilon_{\mathbf{p}}t)]/\hbar} a_{\mathbf{p}\sigma}^\dagger \tag{3.13}$$

and

$$\psi_\sigma(\mathbf{r},t) = \frac{1}{\Omega} \sum_{\mathbf{p}} e^{-i[(\mathbf{p}\cdot\mathbf{r})+(\epsilon_{\mathbf{p}}t)]/\hbar} a_{\mathbf{p}\sigma}. \tag{3.14}$$

The density operator is

$$\widehat{n}(\mathbf{r},t) = \psi_\sigma^\dagger(\mathbf{r},t)\psi_\sigma(\mathbf{r},t). \tag{3.15}$$

The density-density correlation function $\Pi(\mathbf{q},t)$ is defined as

$$\Pi(\mathbf{q},t) = [\widehat{n}(\mathbf{r},t), \widehat{n}(\mathbf{r}',t)]. \tag{3.16}$$

Using Eq.(3.15) along with (3.13)and (3.14), the density-density correlation function $\Pi(\mathbf{q},\omega)$ (for a 3D single parabolic band system in the absence of the Coulomb interaction between carriers) turns out to be

$$\Pi_0(\mathbf{q},\omega) = 2 \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}}, Te) - f(\varepsilon_{\mathbf{k}}, Te)}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \omega + i\delta} \tag{3.17}$$

followed by Fourier transformation[14] and application of Wick's theorem[15]. The real part $\Pi_{01}(\mathbf{q},\omega)$ and the imaginary part $\Pi_{02}(\mathbf{q},\omega)$ of this function are, respectively, given by

$$\Pi_{01}(\mathbf{q},\omega) = -2 \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}}, Te) \left[\frac{1}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \omega} - \frac{1}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \omega} \right] \tag{3.18}$$

$$\Pi_{02}(\mathbf{q},\omega) = 2\pi \sum_{\mathbf{k}} [f(\varepsilon_{\mathbf{k}}, Te) - f(\varepsilon_{\mathbf{k}+\mathbf{q}}, Te)] \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \omega). \tag{3.19}$$

Changing the sum into an integral and solving for a parabolic band $(i.e.\varepsilon_{\mathbf{k}} = k^2/2m)$, the real

part gives

$$\Pi_{01}(\mathbf{q},\omega) = -\frac{mk_F^2}{4\pi^2 q}\left\{\left[1-\left(\mu-\frac{\nu}{\mu}\right)^2\right]\ln\left|\frac{1+\left(\mu-\frac{\nu}{\mu}\right)}{1-\left(\mu-\frac{\nu}{\mu}\right)}\right|+\right.$$
$$\left.\left[1-\left(\mu-\frac{\nu}{\mu}\right)^2\right]\ln\left|\frac{1+\left(\mu-\frac{\nu}{\mu}\right)}{1-\left(\mu-\frac{\nu}{\mu}\right)}\right|\right\} \tag{3.20}$$

and shifting the momentum of the second term $f(\varepsilon_{\mathbf{k+q}},Te)$ by $f(\varepsilon_{\mathbf{k}},Te)$, the last equation reads

$$\Pi_{02}(\mathbf{q},\omega) = 2\pi\int\frac{d\mathbf{k}}{(2\pi)^3}f(\varepsilon_{\mathbf{k}},Te)\left[\delta\left(-\varepsilon_{\mathbf{k+q}}+\varepsilon_{\mathbf{k}}+\omega\right)-\delta\left(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k-q}}+\omega\right)\right]. \tag{3.21}$$

For the case of a parabolic band, $\varepsilon_{\mathbf{k}}=k^2/2m$, the last equation can be written as

$$\Pi_{02}(\mathbf{q},\omega) = 2\pi\int\frac{d\mathbf{k}}{(2\pi)^3}f(\varepsilon_{\mathbf{k}},Te)\left[\delta\left(\omega-\frac{k^2}{2m}-\frac{\mathbf{p.k}}{m}\right)-\delta\left(\frac{k^2}{2m}+\frac{\mathbf{p.k}}{m}+\omega\right)\right]$$
$$\equiv I_\omega - I_{-\omega} \tag{3.22}$$

and will contain a single Fermi distribution function. We now transform to spherical coordinates and obtain

$$I_\omega = \frac{1}{\pi}\int_0^{p_F}k^2 dk\int_{-1}^1 dx\,\delta\left(\omega-\frac{k^2}{2m}-\frac{\mathbf{p.k}}{m}\right)$$
$$= \frac{m}{\pi k}\left[p_F^2-\left(\frac{m}{q}\left(\omega-\frac{k^2}{2m}\right)\right)^2\right]\times\theta\left(p_F-\frac{m}{q}\left|\omega-\frac{k^2}{2m}\right|\right). \tag{3.23}$$

Substituting I_ω in Eq.(3.22) we obtain

$$\Pi_{02}(\mathbf{q},\omega) = -\frac{m^2 T_e}{2\pi q}P_2(\mathbf{q},\omega) \tag{3.24}$$

where

$$P_2(\mathbf{q},\omega) = \ln\left\{\frac{1+\exp\left[-\frac{1}{2mT_e}\left(\frac{q}{2}-\frac{m\omega}{q}\right)^2+\frac{\mu}{T_e}\right]}{1+\exp\left[-\frac{1}{2mT_e}\left(\frac{q}{2}+\frac{m\omega}{q}\right)^2+\frac{\mu}{T_e}\right]}\right\}. \tag{3.25}$$

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For the case of a degenerate system at low temperature, we have the expression $(T = 0K)$

$$\Pi_{02}(\mathbf{q}, \omega) = -\frac{mk_F^2}{4\pi q}\left\{\left[1 - \left(\mu - \frac{\nu}{\mu}\right)^2\right]\theta\left(1 - \left(\mu - \frac{\nu}{\mu}\right)^2\right) - \left[1 - \left(\mu + \frac{\nu}{\mu}\right)^2\right]\theta\left(1 - \left(\mu + \frac{\nu}{\mu}\right)^2\right)\right\} \quad (3.26)$$

where $\theta(x)$ is the Heaviside unit step function, k_F is the Fermi wavevector, $v_F = k_F/m$ is the Fermi velocity, ε_F is the Fermi level from band bottom at $T = 0K$, and $\mu \equiv q/2k_F$, $\nu \equiv \omega/4\varepsilon_F$.

Within the random phase approximation the density-density correlation function including Coulomb interactions is given by

$$\Pi(\mathbf{q}, \omega) = \frac{\Pi_0(\mathbf{q}, \omega)}{\mid \epsilon(\mathbf{q}, \omega) \mid^2} \quad (3.27)$$

where

$$\epsilon(\mathbf{q}, \omega) = 1 - v_c(\mathbf{q})\Pi_0(\mathbf{q}, \omega) \quad (3.28)$$

is the dielectric function. Here the factor $\mid \epsilon(\mathbf{q}, \omega) \mid^2$ is the dynamical screening by carriers of the electron-impurity potential $\mid u(\mathbf{q}) \mid^2$ and of the electron-phonon matrix element $\mid M(\mathbf{q}, \boldsymbol{\lambda}) \mid^2$. The frictional forces $\mathbf{f}_i$ and $\mathbf{f}_p$, and energy transfer rate w may be written in terms of screened potentials

$$u(\mathbf{q})/\epsilon(\mathbf{q}, \omega_0) \quad (3.29)$$

and

$$M(\mathbf{q}, \boldsymbol{\lambda})/\epsilon(\mathbf{q}, \Omega_{\mathbf{q}\lambda} + \omega_0) \quad (3.30)$$

together with the Π_{02} function. This screening is dynamic in that the dielectric functions appearing in these equations are at the frequency $\omega_0 \equiv i\mathbf{q}.\mathbf{v}_d$ or at frequency $\Omega_{\mathbf{q}\lambda} + \omega_0$, which depend on the drift velocity $\mathbf{v}_d$. For an isotropic system the total electrical resistivity ρ is defined as

$$\rho = (\mathbf{E}.\mathbf{v}_d)/(\mathbf{J}.\mathbf{v}_d) \quad (3.31)$$

where

$$\mathbf{J} = ne\mathbf{v}_d \quad (3.32)$$

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is the current density. The force balance equation (3.6) can be written as

$$\mathbf{v}_d.\left(ne\mathbf{E} + \mathbf{f}\right) = 0 \tag{3.33}$$

or

$$ne\mathbf{v}_d.\mathbf{E} + \mathbf{v}_d.\mathbf{f} = 0. \tag{3.34}$$

Dividing by $n^2e^2v_d^2$ and using $\mathbf{f} = \mathbf{f}_i + \mathbf{f}_p$, we have

$$\frac{ne\mathbf{v}_d.\mathbf{E}}{n^2e^2v_d^2} + \frac{\mathbf{v}_d.\left(\mathbf{f}_i + \mathbf{f}_p\right)}{n^2e^2v_d^2} = 0 \tag{3.35}$$

which can be written as

$$\rho = \rho_i + \rho_p \tag{3.36}$$

where

$$\rho = \left(\mathbf{E}.\mathbf{v}_d\right)/\left(\mathbf{J}.\mathbf{v}_d\right), \tag{3.37}$$

$$\rho_i = -\frac{\mathbf{v}_d.\mathbf{f}_i}{n^2e^2v_d^2} \tag{3.38}$$

and

$$\rho_p = -\frac{\mathbf{v}_d.\mathbf{f}_p}{n^2e^2v_d^2}. \tag{3.39}$$

The last two equations are, respectively, the resistivities due to impurity and phonon scatterings.

The energy balance equation(3.34) can also be written as

$$\rho - \rho_E = 0 \tag{3.40}$$

in terms of an equivalent resistivity related to the electron energy loss rate:

$$\rho_E = w/n^2e^2v_d^2. \tag{3.41}$$

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3.1.2 Weak Current Ohmic Resistivity

Let's propose a solution to the energy balance equation(3.7) as

$$T_e = T. \tag{3.42}$$

Using the expression for $\mathbf{f}_i$ from Eq.(3.8) in Eq.(3.38) we get

$$\rho_i = -\frac{n_i}{n^2 e^2} \sum \frac{\mathbf{v}_d \cdot \mathbf{q}}{v_d^2} \mid \overline{u(\mathbf{q})} \mid^2 \Pi_2(\mathbf{q}, \omega_0) \tag{3.43}$$

which with $\mathbf{v}_d \cdot \mathbf{q} = \omega_0 = v_d q \cos\theta = v_d q_x$, can be written as

$$\rho_i = -\frac{n_i}{n^2 e^2} \sum_q q_x^2 \mid \overline{u(\mathbf{q})} \mid^2 \Pi_2(\mathbf{q}, \omega_0)/\omega_0. \tag{3.44}$$

Now we expand $\Pi_{02}(\mathbf{q}, \omega_0 = v_d q_x)$ in a Taylor series to obtain

$$\Pi_{02}(\mathbf{q}, v_d q_x) = \Pi_{02}(\mathbf{q}, 0) + v_d q_x \left[\frac{\partial}{\partial \omega} \Pi_{02}(\mathbf{q}, \omega) \right] |_{\omega=0} + ... \tag{3.45}$$

and also we see that with respect to ω the real part of $\Pi(\mathbf{q}, \omega)$ is even while the imaginary part is odd, i.e.,

$$\Pi_{01}(\mathbf{q}, \omega) = \Pi_{01}(\mathbf{q}, -\omega) \tag{3.46}$$

and

$$\Pi_{02}(\mathbf{q}, \omega) = -\Pi_{02}(\mathbf{q}, -\omega). \tag{3.47}$$

Therefore, for $\omega = 0$, we have

$$\Pi_{02}(\mathbf{q}, 0) = -\Pi_{02}(\mathbf{q}, 0) \tag{3.48}$$

or

$$\Pi_{02}(\mathbf{q}, 0) = 0 \tag{3.49}$$

which can be used in Eq.(3.45) to obtain

$$\Pi_{02}(\mathbf{q}, v_d q_x)/\omega_0 \simeq \left[\frac{\partial}{\partial \omega} \Pi_{02}(\mathbf{q}, \omega) \right] |_{\omega=0}. \tag{3.50}$$

Substituting Eq.(3.50) in Eq.(3.44)

$$\rho_i = -\frac{n_i}{n^2 e^2} \sum_q q_x^2 \mid \overline{u(\mathbf{q})} \mid^2 \left[\frac{\partial}{\partial \omega} \Pi_{02}(\mathbf{q}, \omega) \right] \mid_{\omega=0} \tag{3.51}$$

with

$$\mid \overline{u(\mathbf{q})} \mid^2 \equiv \mid u(\mathbf{q})/\epsilon(\mathbf{q}, 0) \mid^2 \tag{3.52}$$

which is the screened electron-impurity potential.

Using Eq.(3.9) in Eq.(3.39) and taking $T_e = T$, we get

$$\rho_p = \frac{-2}{n^2 e^2 v_d^2} \sum_{\mathbf{q}, \lambda} \mathbf{q} \mid M(\mathbf{q}, \lambda) \mid^2 \Pi_{02}\left(\mathbf{q}, \Omega_{\mathbf{q}\lambda} + \omega_0\right) \left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} + \omega_0}{T}\right) \right]. \tag{3.53}$$

in which $n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} + \omega_0}{T}\right)$ can be expressed using Taylor's expansion as

$$\begin{aligned}
\left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} + \omega_0}{T}\right) \right] &= n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - \frac{\omega_0}{T} n'\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) \\
&= -\frac{\omega_0}{T} n'\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right)
\end{aligned} \tag{3.54}$$

where prime (´) represents derivative w.r.t $\frac{\Omega_{\mathbf{q}\lambda}}{T}$. With Eq.(3.54), (3.53) becomes

$$\rho_p = \frac{-2}{n^2 e^2} \sum_{\mathbf{q}, \lambda} q_x^2 \mid \overline{M(\mathbf{q}, \lambda)} \mid^2 \Pi_{02}(\mathbf{q}, \Omega_{\mathbf{q}\lambda}) \left[-\frac{1}{T} n'\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) \right] \tag{3.55}$$

where we have defined $q_x \equiv \frac{\omega_0}{v_d}$. Also, the screened electron-phonon interaction matrix element is

$$\mid \overline{M(\mathbf{q}, \lambda)} \mid^2 \equiv \mid M(\mathbf{q}, \lambda)/\epsilon(\mathbf{q}, \Omega_{\mathbf{q}\lambda}) \mid^2 . \tag{3.56}$$

For the degenerate case $k_B T \ll \varepsilon_F$ (and $v_d \longrightarrow 0$), we have

$$\frac{\Pi_{02}(\mathbf{q}, \omega)}{\omega_0} \simeq \frac{\partial}{\partial \omega} \Pi_{02}(\mathbf{q}, \omega) \tag{3.57}$$

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and

$$\Pi_{02}(\mathbf{q}, \omega) \simeq -\frac{m^2}{2\pi q}\theta\left(1 - (q/2k_F)^2\right)\omega. \tag{3.58}$$

Using Eq.(3.58) in Eq.(3.51) and changing the sum of latter into integral as $\sum_{\mathbf{q}} = \left(\frac{1}{2\pi}\right)^3 \int_\Omega d\overrightarrow{\mathbf{q}}$, we obtain

$$\rho_i = \frac{m^2 n_i}{12\pi^3 n^2 e^2} \int_0^{2k_F} dq q^3 \mid \overline{u(\mathbf{q})} \mid^2, \tag{3.59}$$

where the result

$$\int_0^\infty dq f(q)\, \theta\left(1 - (q/2k_F)^2\right) = \int_0^{2k_F} dq f(q), \tag{3.60}$$

along with Eq.(3.57) have been used.

For the evaluation of phonon-induced resistivity at low temperature, we consider long wavelength longitudinal acoustic phonons with a Debye-type spectrum

$$\Omega_{\mathbf{q}} = v_s q. \tag{3.61}$$

We use Eq.(3.61) in Eq.(3.58) and obtain

$$\Pi_{02}(\mathbf{q}, \Omega_{\mathbf{q}}) \simeq -\frac{m^2}{2\pi q}\theta\left(1 - (q/2k_F)^2\right)v_s q. \tag{3.62}$$

Now substituting Eq.(3.62) in Eq.(3.55) & using Eq.(3.60) we arrive at

$$\rho_p(v_d \longrightarrow 0) \equiv \rho_{p0} = \frac{m^2 v_s}{6\pi^3 n^2 e^2} \int_0^{2k_F} dq q^4 \mid \overline{M(\mathbf{q}, \boldsymbol{\lambda})} \mid^2 \left[-\frac{1}{T}n'\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right)\right] \tag{3.63}$$

which is the Bloch-Gruneissen[16][17] formula. Assuming a deformation potential of the type

$$\mid \overline{M(\mathbf{q}, \boldsymbol{\lambda})} \mid^2 = \eta \times q, \tag{3.64}$$

where η is a constant of proportionality, Eq(3.63) can also be expressed as

$$\rho_{p0} = \rho^* g(t_F), \tag{3.65}$$

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where ρ^* is a resistivity-dimension coefficient given by

$$\rho^* \equiv \frac{16m^2\eta k_F^5}{3\pi^3 n^2 e^2},$$
(3.66)

$t_F \equiv T/\Theta_F$ with $\Theta_F \equiv 2k_F$, and

$$g(t) = \frac{1}{t}\int_0^1 dy \frac{y^5}{\left(e^{y/t} - 1\right)\left(1 - e^{-y/t}\right)}.$$
(3.67)

All of these formulae for impurity- and phonon-induced dc steady-state resistivities are known as isothermal force-balance equation results, in contrast to those obtained from conventional adiabatic transport theories.

3.1.3 Nonlinear Zero-Lattice-Temperature Limit

It is also interesting to discuss the zero-lattice-temperature limit. When $T \to 0$, the terms with $n\left(\frac{\Omega_{q\lambda}}{T}\right)$ in force- and energy-balance equations vanish and only the electron tempearture T_e is involved in these balance equations. We find that the electron temperature T_e approaches a finite value T^* which depends on the electric field and impurity resistivity. We assume $M(\mathbf{q}, \lambda)$ to be the deformation potential type, Eq.(3.64). The energy balance Eq.(3.40) can be rearranged as

$$\rho_i = \rho_E - \rho_p.$$
(3.68)

Using the expressions for ρ_E and ρ_p from Eqs(3.41) & (3.39), respectively, in Eq.(3.68) we obtain

$$\rho_i = \frac{w}{n^2 e^2 v_d^2} + \frac{\mathbf{v}_d \cdot \mathbf{f}_p}{n^2 e^2 v_d^2}.$$
(3.69)

Substituting the expressions for w and $\mathbf{f}_p$ in the above Eq(3.69) we have

$$\rho_i = \frac{2}{n^2 e^2 v_d^2}\sum_{\mathbf{q}}(\Omega_{\mathbf{q}} + \omega_0)^2 \eta q \frac{m^2}{2\pi q}\theta\left(1 - (q/2k_F)^2\right) n\left(\frac{\Omega_{\mathbf{q}} + \omega_0}{T^*}\right)$$
(3.70)

where Eq(3.64) and (3.62) have been used to eliminate$|\overline{M(\mathbf{q}, \lambda)}|^2$and $\Pi_{02}(\mathbf{q}, \Omega_{\mathbf{q}\lambda} + \omega_0)$, respectively. Note that we have omitted the subscript λ in the above Eq(3.70) since we are dealing with a single branch (long wavelength acoustic phonons), substituted $\Omega_{\mathbf{q}} = v_s q$, and consider-

ing $v_s \ll v_F$. Changing the sum into integral, letting $x = \cos\theta$ & $\frac{\Omega_\mathbf{q}}{T^*} = \frac{y}{t_F}$, Eq(3.70) simplifies to

$$\frac{\rho_{i0}}{\rho^*} = \frac{3}{2}\left(\frac{v_s}{v_d}\right)^2 \int_0^1 dy \int_{-1}^1 dx y^4 \left(1 + \frac{v_d}{v_s}x\right)^2 n\left[\frac{y}{t_F}\left(1 + \frac{v_d}{v_s}x\right)\right]. \tag{3.71}$$

Eq(3.53) can be expressed as

$$\rho_p = \frac{-2}{n^2 e^2} \sum_{\mathbf{q},\lambda} \left(\frac{\mathbf{v}_d \cdot \mathbf{q}}{v_d^2}\right) \mid M(\mathbf{q},\lambda)\mid^2 \Pi_{02}(\mathbf{q},\Omega_{\mathbf{q}\lambda} + \omega_0)\left[-n\left(\frac{\Omega_{\mathbf{q}\lambda} + \omega_0}{T}\right)\right] \tag{3.72}$$

where we have used the zero-lattice temperature limit as $n(\frac{\Omega_{\mathbf{q}\lambda}}{T}) \longrightarrow 0$ and $T_e \longrightarrow T^*$. Eliminating $\Pi_{02}(\mathbf{q},\Omega_{\mathbf{q}\lambda} + \omega_0)$ from the above expression by means of Eq(3.62) and following the usual procedure we followed to derive Eq.(3.71), we get

$$\frac{\rho_p}{\rho^*} = -\frac{3}{2}\left(\frac{v_s}{v_d}\right)\int_0^1 dy \int_{-1}^1 dx y^4 x \left(1 + \frac{v_d}{v_s}x\right) n\left[\frac{y}{t_F}\left(1 + \frac{v_d}{v_s}x\right)\right]. \tag{3.73}$$

For $\frac{v_d}{v_s} < 1$, the integrations in Eqs.(3.71) and (3.73) are easily carried out, yielding

$$t_F^5 \equiv \left[\frac{T^*}{\Theta_F}\right]^5 = 0.0134\frac{\rho_{p0}}{\rho^*}\frac{(v_d/v_s)^2}{\left[1 - (v_d/v_s)^2\right]^2} \tag{3.74}$$

and

$$\frac{\rho_p}{\rho^*} = \frac{4}{3}\frac{\rho_{i0}}{\rho^*}\frac{(v_d/v_s)^2}{\left[1 - (v_d/v_s)^2\right]^2}. \tag{3.75}$$

Now

$$\frac{E}{E^*} = \frac{(\rho_p + \rho_i)\, nev_d}{\rho^* nev_s}. \tag{3.76}$$

Since the impurity resistivity ρ_i is almost equal to its weak field value ρ_{i0}, so the last expression becomes

$$\frac{E}{E^*} = \left(\frac{\rho_p}{\rho^*} + \frac{\rho_{i0}}{\rho^*}\right)\frac{v_d}{v_s}. \tag{3.77}$$

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Using (3.75) in (3.77), the electric field can be expressed as

$$\frac{E}{E^*} = \frac{\rho_{i0}}{\rho^*} \frac{v_d}{v_s} \left[1 + \frac{4}{3} \frac{(v_d/v_s)^2}{\left[1 - (v_d/v_s)^2 \right]^2} \right] \tag{3.78}$$

where $E^* = \rho^* n e v_s$. Eliminating the factor $(v_d/v_s)^2 / \left[1 - (v_d/v_s)^2 \right]^2$ from Eq.(3.74) and using it in Eq.(3.75), we have

$$\frac{T^*}{\Theta_F} = 0.416 \left(\frac{\rho_{i0}}{\rho^*} \right)^{-1/5} \left(\frac{E}{E^*} \right)^{2/5} \tag{3.79}$$

and similarly

$$\frac{\rho_p}{\rho^*} = \frac{4}{3} \frac{\rho^*}{\rho_{i0}} \left(\frac{E}{E^*} \right)^2 . \tag{3.80}$$

Eq(3.79) is in agreement with the result obtained by Arai[18]. It should be noted that Eqs.(3.79) and (3.80) are valid only in a narrow electric field range, depending on the impurity resistivity ρ_{p0}/ρ^*, but they are completely invalid when $\rho_{i0} = 0$. The calculated results of $\frac{T^*}{\Theta_F}$ and the phonon-induced resistivity ρ_p/ρ^* have been plotted in Figure (3.1) and Figure (3.2), respectively, as functions of the electric field for different values of impurity scattering.

3.1.4 Nondegenerate (Maxwell-Boltzmann) Case - Acoustic Phonon Scattering

Many experimental investigations have been carried out with nondegenerate semiconductors, in which carriers in thermal equilibrium obey Maxwell-Boltzmann distribution even at low temperatures. In this case the chemical potential is negative and $|\mu|/T_e \gg 1$, such that the function $P_2(\mathbf{q}, \omega)$ (Eq.(3.25)) reduces to

$$P_2(\mathbf{q}, \omega) = e^{-|\mu|/T_e} \left\{ \exp\left[-\frac{1}{2mT_e} \left(\frac{q}{2} - \frac{m\omega}{q} \right)^2 \right] - \exp\left[-\frac{1}{2mT_e} \left(\frac{q}{2} + \frac{m\omega}{q} \right)^2 \right] \right\}. \tag{3.81}$$

We assume that acoustic phonons are the only scatterers and $M(\mathbf{q})$ is of the deformation potential type given by Eq.(3.64). For convenience, we introduce a temperature-dimension parameter
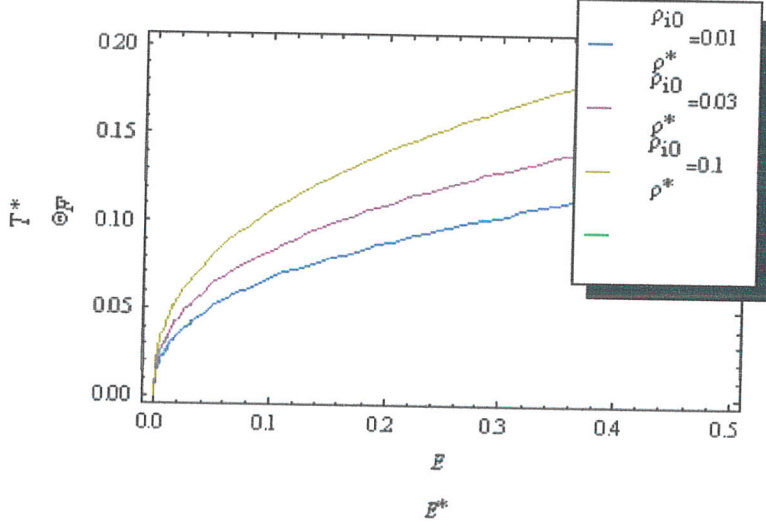
$$\Theta_s = m v_s^2 \tag{3.82}$$

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Figure 3-1: The electron temperature T^* in the limit $T \longrightarrow 0$ is shown as a function of dimensionless electric field E/E^* for several impurity resistivities in a degenarate electron system with acoustic phonon and impurity scatterings. Here, $\rho_{i0}/\rho^* = 0.01$, 0.03 and 0.1.

Figure 3-2: The dimensionless phonon–induced resistivity ρ_p/ρ^* is shown as a function of dimensionless electric field E/E^* in the limit $T \to 0$ for several impurity resistivities in a degenarate electron system with acoustic phonon and impurity scatterings. Here, $\rho_{i0}/\rho^* = 001$, 0.03 and 0.1, while, ρ_p stands for ρ.
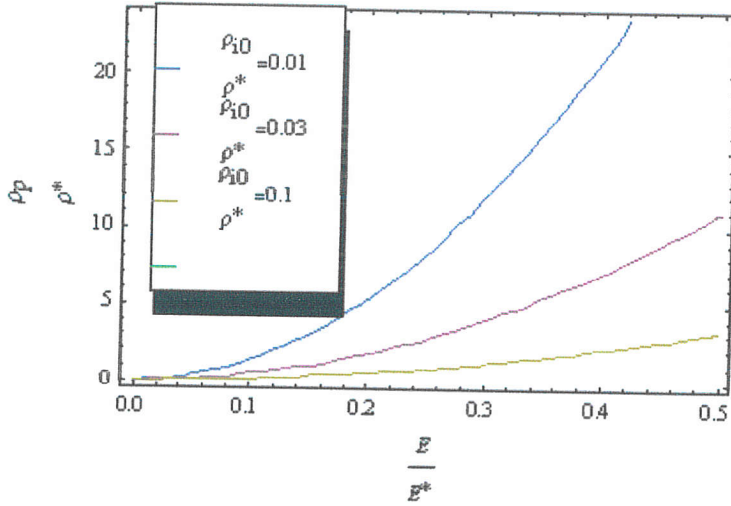
which is about $1K$ for $v_s = 5 \times 10^5 cm/s$ and the electron's effective mass $m = 0.6 m_e (m_e$ is the free-electron mass), and denote $\alpha \equiv T_e/T$ and $t_s = T/\Theta_s$. The energy balance equation (3.40) can be written in the form of Eq.(3.69) which is

$$\rho_i = \frac{w}{n^2 e^2 v_d^2} + \frac{\mathbf{v}_d.\mathbf{f}_p}{n^2 e^2 v_d^2}. \tag{3.83}$$

We use the values of w and $\mathbf{f}_p$ from Eqs.(3.10) and (3.9), respectively, in Eq(3.83). Following the same procedure (as we did earlier to derieve the expressions (3.74) and (3.75)), but, now using Eq.(3.24) instead of Eq.(3.50) for the density-density correlation function. The solution to the energy balance equation thus obtained for $\alpha t_s \gg 1$: to the lowest order of the power expansion in $(\alpha t_s)^{-1}$, is

$$\left(\frac{v_d}{v_s}\right)^2 = \frac{6\alpha^3 t_s^3}{S(\alpha, t_s)} - 3 \tag{3.84}$$

where

$$S(\alpha, t_s) = \int_0^\infty e^{-y^2/2\alpha t_s} y^4 \coth\left(\frac{y}{t_s}\right) dy. \tag{3.85}$$

With $\coth\left(\frac{y}{t_s}\right) \approx 1$ for $\alpha/t_s \gg 1$, Eq.(3.85) becomes

$$S(\alpha, t_s) \simeq 3 \frac{\sqrt{\pi}}{\sqrt{2}} (\alpha t_s)^{5/2}. \tag{3.86}$$

Using Eq.(3.86) in (3.84) we can write,

$$\alpha = \frac{\pi}{8ts} \left(\frac{v_d}{v_s}\right)^4. \tag{3.87}$$

The dimensionless resistivity ρ_p/ρ_{p0} for $\alpha t_s \gg 1$ can be expressed as

$$\frac{\rho_p}{\rho_{p0}} = \frac{S(\alpha, t_s)}{2\alpha^{2/3} g_s(t_s)} \tag{3.88}$$

where

$$g_s(t_s) = \int_0^\infty \exp\left[-\frac{(y-1)^2}{2t_s}\right] [-n'(2y/t_s)] \, dy, \tag{3.89}$$

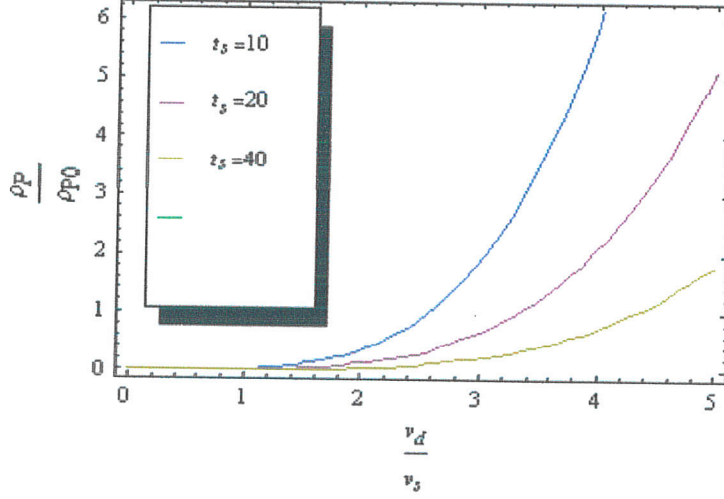which, for $t_s \gg 1$, reduces to

$$g_s(t_s) \simeq t_s^3. \tag{3.90}$$

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Figure 3-3: The dimensionless phonon–induced resistivity ρ_p/ρ_{p0} is shown as a function of v_d/v_s at several lattice temperatures. The scattering is solely because of acoustic phonons, i.e., $\rho = \rho_p$.

Substituting the expressions of $S(\alpha, t_s)$ and $g_s(t_s)$ from Eqs.(3.86) & (3.90), respectively, the expression for ρ_p/ρ (3.88) becomes,

$$\frac{\rho_p}{\rho_{p0}} \simeq 1.88 \frac{\alpha}{t_s^{1/2}}, \tag{3.91}$$

which can be combined with the expression of α to obtain a relationship between $\alpha \equiv T_e/T$ and the electric field $E = \rho_p n e v_d$:

$$\frac{T_e}{T} = 0.5 \left(\frac{T}{\Theta_s}\right)^{1/5} \left(\frac{E}{E_o}\right)^{4/5} \tag{3.92}$$

which is valid for $t/\Theta_s \gg 1$ and $E/E_0 \gg 1$. Here $E_0 = \rho_{p0} n e v_s = v_s/\mu_0$, μ_0 being the carrier mobility in the zero-field limit.Both the temperature ratio T_e/T and the dimensionless resistivity have been plotted as functions of $\frac{v_d}{v_s}$ in Figures(3.2) and (3.3), respectively. The result, Eq.(3.92), differs from the result of the carrier temperature model analysis obtained
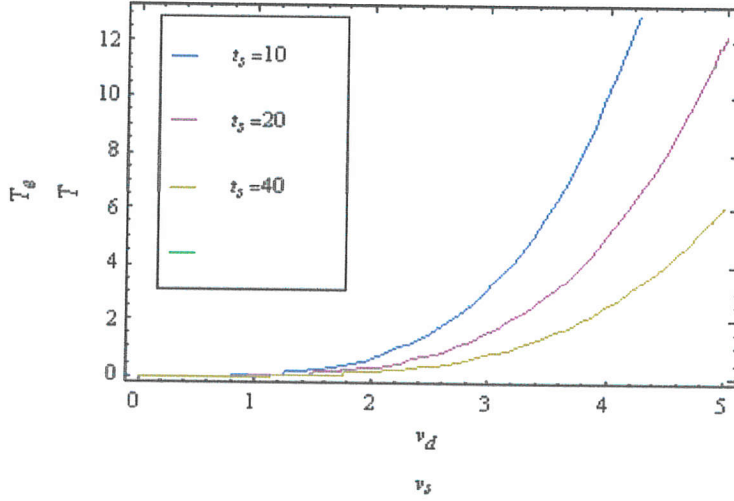
Figure 3-4: The temperature ratio T_e/T is shown as a function of v_d/v_s at several lattice temperatures.

by Seeger[19]. The latter predicts a linear dependence of T_e/T on the electric field with a temperature-independent coefficient.

3.1.5 Optic Phonon Scattering

Now we discuss an interesting case in which the optic phonon scattering dominates. As is usually done in discussing optic-phonon scattering, we employ the Einstein model for the optic phonon spectrum: $\Omega_{\mathbf{q}\lambda} = \Omega_{\mathbf{o}}$, and assume $| \overline{M(\mathbf{q},\boldsymbol{\lambda})} |^2$ to be a constant (nonpolar optic deformation potential).

In describing optic phonon scattering it is convenient to introduce temperature and velocity parameters $\Omega_{\mathbf{o}}$ and v_0, respectively, defined by

$$mv_0^2 \equiv \Omega_{\mathbf{o}} ,\qquad (3.93)$$

where m is the effective mass of the charge carriers. Also, denote

$$t_0 \equiv T/\Omega_{\mathbf{o}} .\qquad (3.94)$$

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Let's define the matrix element of electron-nonploar optic phonon interaction[20]

$$| \overline{M(\mathbf{q}, \boldsymbol{\lambda})} |^2 = \frac{D^2}{2\Omega_o d},$$ (3.95)

where D is the shift of the band edge per unit relative displacement of the two sublattices relative to the optical mode and d is the mass density of the lattice.

The electric resistivity ρ and the equivalent resistivity ρ_E due to optic phonon scattering, respectively, are

$$\rho = \left\{ \rho_0^* \alpha t_o \left(\frac{v_s}{v_d} \right) \int_0^\infty d \left(\frac{q}{mv_0} \right) \left(\frac{q}{mv_0} \right)^2 \int_{-1}^1 dx\, x\, P_2\, (q, \omega_0 + \Omega_o) \right.$$
$$\left. \times \left[n \left(\frac{\Omega_o}{T} \right) - n \left(\frac{\omega_0 + \Omega_o}{\alpha T} \right) \right] \right\}.$$ (3.96)

and

$$\rho_E = \left\{ -\rho_0^* \alpha t_o \left(\frac{v_s}{v_d} \right)^2 \int_0^\infty d \left(\frac{q}{mv_0} \right) \left(\frac{q}{mv_0} \right) \int_{-1}^1 dx\, P_2\, (q, \omega_0 + \Omega_o) \right.$$
$$\left. \times \left[n \left(\frac{\Omega_o}{T} \right) - n \left(\frac{\omega_0 + \Omega_o}{\alpha T} \right) \right] \right\}.$$ (3.97)

where

$$\rho_0^* = \frac{m^5 v_s^2 D^2}{8\pi^3 dn^2 e^2}$$ (3.98)

Assuming the optic phonons to be the dominent scatterers, the energy-balance equation will be the same as Eq.(3.40)

$$\rho - \rho_E = 0$$ (3.99)

The important feature of optic-phonon scattering is the saturation of the current density at high electric fields. That is, the solution of the energy-balance equation exists only when $v_d <$

v_m with a saturation maximum v_m. We examine the asymptotic behavior of the energy-balance equation at large αt_0, to determine the saturation value of the drift velocity. To the leading order of its expansion in $(\alpha t_0)^{-1}$, the energy-balance equation yields

$$\left(\frac{v_d}{v_0}\right)^2 = 3\left[2 - \frac{K_1'(1/2\alpha t_0)}{\alpha t_0 K_1(1/2\alpha t_0)}\right]^{-1} \tanh\left(\frac{1}{2t_0}\right) \qquad (3.100)$$

where $K_1(x)$ and $K_1'(x)$ are the modified Bessel functions and their derivatives. The saturation value v_m can be obtained by letting $\alpha t_0 \longrightarrow \infty$ in Eq (3.100), whence

$$\left(\frac{v_m}{v_0}\right)^2 = \frac{3}{4} \tanh\left(\frac{1}{2t_0}\right) \qquad (3.101)$$

which is temperature dependent, having a maximum at $v_m = 0.866 v_0$. The velocity ratio $\frac{v_d}{v_0}$ as a function of T_e/T can be obtained from Eq.(3.100) and has been plotted in Figure (3.5). In the limit $E \longrightarrow \infty$, the above result.(3.100) is the same as the one obtained from the Boltzmann equation. It is also consistent with the result of Thornber and Feynman[21] in regard to saturation at high field. Figure (3.5) shows the electron temperature calculated as a function of drift velocity for the case of pure nonpolar optic phonon scattering.

3.1.6

3.1.7 Electron Cooling

One of the most interesting consequences of the force- and energy-balance equations is the possible cooling of the relative electrons, in that the electron temperature T_e may be lower than the lattice temperature T in the presence of a finite drift v_d. Such a lowering of the electron temperature below the lattice temperature occurs in low-impurity samples. At low lattice temperature, when acoustic phonons dominate the scattering, the maximum cooling occurs at a current density for which the electron drift velocity is near the sound velocity. In this case, cooling is most likely to occur at much higher drift velocities in the range $v_d = 0.3 - 0.5 v_0$. The problem of the electron cooling was further examined in GaAs/AlGaAs systems[22]. It was found that in these selectively high doped high-mobility systems, in which polar optic phonon

q-integration region. Therefore, the contribution from very large ω should be equivalent to that without screening. This is a high-field descreening effect.

The other dynamic screening effect comes from plasmon contributions. It is seen from the RPA expression for $\Pi_{02}(\mathbf{q}, \omega)$, Eq(3.27), that significant contribution to the frictional forces and energy transfer rate may occur in the region where both $[1 - v_c(\mathbf{q})\Pi_{01}(\mathbf{q}, \omega)]$ and $\Pi_{02}(\mathbf{q}, \omega)$ nearly vanish, the region of the plasmon excitation. This effect on dc steady state transport is significant in the impurity-induced resistivity at low temperature for a degenerate 3D system [22].

3.2 Summary and Results

In chapter(1), both classical and quantum mechanical approaches to electron transport in semi-conductors are presented. It is realized that in any realistic study of electron transport, electron-electron interactions need to be taken into account in order to explain a number of experimental results. Lei-Ting balance equation approach[1] allows us to include the effects of interactions between electrons in an analytically tractable manner. At the end of Chapter (1) Lei-Ting balance equation approach was introduced, which is the main focus of this thesis.

In chapter(2), the basic formalism behind the balance equation approach is introduced. This approach to electronic transport is suitable for systems where electron-electron interaction, electron-phonon interaction and electron-impurity scattering need to be considered. As the starting point of this method, the center-of-mass variables were separated from the relative variables of the electrons in the Hamiltonain. This separation allowed us to separate the thermal motion of the electron system from its drift motion. The fact that the electric field acts only on the center-of-mass and the relative electrons were coupled with the center-of-mass and with phonons only via the electron-impurity and electron-phonon interaction made it possible to introduce an electron temperature T_e for the nonequilibrium electron system, which was in a steady transport state in the presence of an electric field, as a measurement of its internal energy. This temperature (T_e) was defined as the thermodynamic temperature of an isolated system, which was obtained form the electrons in relative coordinates by turning off the electron-phonon and electron-impurity interactions after the system had reached the steady state. Thus, these

decoupled electrons and phonons had different temperatures[23] (T_e and T, respectively), and this was used as the initial condition of the density matrix describing relative electrons and phonons. Unlike the conventional Boltzmann theory of phonon-induced resistivity where the phonon system is assumed to be in an equilibrium state, the phonon temperture T (which is a measure of its internal energy) can be determined in the same way as we did for relative electrons. To the first order of electron-impurity and electron-phonon interaction, the solution of the Liouville equation for the density matrix was obtained and the force- and energy-balance equations were derived.

In chapter(3), we discussed the applications of the balance equation approach. There, we performed the calculations for an isotropic electron system with parabolic band, assuming the simplest phonon dispersion and electron-phonon matrix elements. For convenience, we presented the results only for the systems with fixed carrier density n. They can be easily modified to be applicable to, for example, semiconductors where the carrier density is temperature dependent, if the temperature dependence of the carrier density $n(T_e)$ is included in the calculation.

Our first two plots (Figure (3.1) and Figure (3.2)) show the behaviour of the electron temperature T_e and phonon resistivity ρ_p, respectively, as functions of the dimensionless electric field E/E^* for several impurity resistivities in a degenerate electron system with acoustic phonons and impurity scatterings. We take $\rho_{i0}/\rho^* = 0.01$, 0.03 and 0.1. We see that the electron temperature T_e/Θ_F varies as $(E/E^*)^2$ which initially increases rapidly then tends to move towards saturation (tends to be uniform). It should be so because as the electric field increases, the electron temperature increases rapidly, as expected. While, initially the phonon resistivity remains almost constant for low electric field but surges at once as the electric field is increased which is because of the fact that the electric field accelerates the electrons thereby gaining energy which increases the phonon resistivity (energy- and momentum-trasfer occur because of electron-phonon interaction).

Figure (3.3) shows that the phonon-induced resistivity ratio ρ_p/ρ_{p0}, which has been plotted against v_d/v_s, increases very rapidly (with $\rho_p/\rho_{p0} \sim .(v_d/v_s)^4$). The temperature ratio T_e/T plotted against the same function (v_d/v_s); shows the same behavior i.e., $T_e/T \sim (v_d/v_s)^4$. This is illustrated in Figure (3.4). Which means that the acoustic phonon scattering causes both the electron temperature and phonon-induced resistivity to increase rapidly as the drift velocity of

electrons increases.

Figure (3.5) reflects the behavior of v_d/v_0 when plotted against T_e/T, for the case of optic phonons. For small fields, i.e., for small electron temperature T_e the drift velocity increases rapidly in the absence of optic phonons (and dilute impurities affects very little). Once optic phonons appear, for large fields and thus large T_e, they resist the electron motion so the drift velocity tends to get a saturation value. This fact that drift velocity saturation at large fields is consistent with the result of Thornber and Feynman[21]. They quantum-mechanically analyze the expectation value of the steady state velocity acquired by an electron interacting with the longitudinal optic phonons of polar crystals in a finite electric field for arbitrary coupling strength, field strength, and temperature. They present numerical calculations which show a decreasing rate of energy loss with velocity for very fast electrons. They conclude that optic phonon scattering can indeed produce the high rate of energy loss that is present in tunnel-cathode structures.

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