

Chapter 1

Main Physical Considerations and Transport Balance Equations

1.1 Center-of-Mass and Relative Variables of Electrons

We consider a semiconductor system under the influence of a uniform electric field \mathbf{E} . The system consists of ions vibrating around their individual equilibrium positions in the lattice and numerous mobile carriers having total number N , which, in most cases, will be simply called “electrons” without distinguishing their charge type. These electrons, interacting with each other through the Coulomb potential, are coupled with lattice vibrations and scattered by randomly distributed impurities. Assuming a single-band effective-mass description for electrons, we can write the Hamiltonian of this electron–ion system as

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{e^2}{4\pi\epsilon_0\kappa} \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - e \sum_i \mathbf{r}_i \cdot \mathbf{E} + \sum_{i,a} u(\mathbf{r}_i - \mathbf{r}_a) - \sum_{i,l} \mathbf{u}_l \cdot \nabla v_l(\mathbf{r}_i - \mathbf{R}_l) + H_{\text{ph}}. \quad (1.1)$$

Here, \mathbf{r}_i and $\mathbf{p}_i = -i\nabla_i$ ($i = 1, \dots, N$) are the coordinate and momentum of the i th electron with effective mass m and charge e . The first term on the right-hand-side of Eq. (1.1) is the kinetic energy of electrons; the second term is the Coulomb interaction between electrons in the host semiconductor having a dielectric constant κ ; the third term is the potential energy of electrons in the uniform electrical field \mathbf{E} ; $v_l(\mathbf{r} - \mathbf{R}_l)$ denotes the potential produced by the l th ion on the lattice site \mathbf{R}_l , and \mathbf{u}_l is its displacement from the regular (equilibrium) position; $u(\mathbf{r} - \mathbf{r}_a)$ denotes the additional scattering potential due to an impurity located at \mathbf{r}_a , which is assumed randomly distributed; and the last term H_{ph} represents the Hamiltonian of lattice vibration itself (phonons).

To deal with the electronic transport in semiconductors we first focus our attention on electrons. The initial starting point of the balance equation approach is the separation of the motion of the center of mass, i.e. the motion of all electrons as an integrity, from the relative motion of the electrons in this many-particle system. We define (Ting, Ying and Quinn, 1976a; Lei and Ting, 1984) the center-of-mass momentum and coordinate of the electron system, \mathbf{P} and \mathbf{R} , by

$$\mathbf{P} = \sum_i^N \mathbf{p}_i, \quad \mathbf{R} = \frac{1}{N} \sum_i^N \mathbf{r}_i, \quad (1.2)$$

and the momentum and coordinate of the i th electron relative to the center of mass, \mathbf{p}'_i and \mathbf{r}'_i , by

$$\mathbf{p}'_i = \mathbf{p}_i - \frac{1}{N}\mathbf{P}, \quad \mathbf{r}'_i = \mathbf{r}_i - \mathbf{R}. \quad (1.3)$$

For brevity, we will simply call \mathbf{p}'_i and \mathbf{r}'_i the relative momentum and coordinate of the i th electron, or the momentum and coordinate of the i th relative electron. It is easily seen that \mathbf{P}, \mathbf{R} are canonical conjugate variables:

$$[R_\alpha, P_\beta] = i \delta_{\alpha\beta} \quad (1.4)$$

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

$$[\mathbf{r}'_i, \mathbf{P}] = [\mathbf{R}, \mathbf{p}'_i] = 0. \quad (1.5)$$

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

$$\sum_i^N \mathbf{p}'_i = 0, \quad \sum_i^N \mathbf{r}'_i = 0, \quad (1.6)$$

and their commutation relations involve an noncanonical $1/N$ term:

$$[r'_{i\alpha}, p'_{j\beta}] = i \delta_{\alpha\beta} (\delta_{ij} - \frac{1}{N}). \quad (1.7)$$

The original derivation of the balance equation theory (Lei and Ting, 1984, 1985a,b) proceeds with a reasonable assumption that the $1/N$ term in Eq. (1.7) is negligible for a macroscopic large N system, such that one can essentially treat the relative-electron momenta and coordinates as canonical conjugate variables:

$$[r'_{i\alpha}, p'_{j\beta}] \simeq i \delta_{\alpha\beta} \delta_{ij}. \quad (1.8)$$

While the approximate equality (1.8) is very useful and justifiable in dealing with most macroscopic transport problems, it is an approximation. Therefore, care must be taken to avoid using it in a way that can result in a macroscopic error. For example, the summation of the right-hand-side of (1.7) over index j for all N particles is zero, while that of (1.8) yields a nonzero value $i\delta_{\alpha\beta}$. This indicates that it is impossible to construct a translation generator of the system by summing the individual momenta of relative electrons \mathbf{p}'_j over all particles, since this sum is zero rather than the total momentum of the system. Nevertheless, it has been shown (Lei, 1990a), that the neglect of the noncanonical $1/N$ term in Eq. (1.7) induces no error within the framework of balance equation theory if the center-of-mass coordinate $\mathbf{R}(t)$ is treated classically.

The system, consisting of N independent particles (relative electrons) which are characterized by the set of canonical conjugate variables \mathbf{p}'_i and \mathbf{r}'_i ($i = 1, \dots, N$), is called the relative electron system. In the second quantization representation of plane wave basis, the relative electron system can be described by means of the creation and annihilation operators $c_{\mathbf{k}\sigma}^\dagger$ and $c_{\mathbf{k}\sigma}$ for a relative electron having wave vector \mathbf{k} , spin σ , and energy $\varepsilon_{\mathbf{k}} = k^2/2m$. In terms of the center-of-mass variables and the relative-electron variables we can separate the Hamiltonian (1.1) of the electron-ion system into a center-of-mass part H_{cm} , a relative-electron part H_{er} , a phonon part H_{ph} , together with electron-impurity and electron-phonon interactions H_{ei} and H_{ep} :

$$H = H_{\text{cm}} + H_{\text{er}} + H_{\text{ph}} + H_{\text{ei}} + H_{\text{ep}}, \quad (1.9)$$

$$H_{\text{cm}} = \frac{P^2}{2Nm} - Ne\mathbf{E} \cdot \mathbf{R}, \quad (1.10)$$

$$H_{\text{er}} = \sum_i \frac{\mathbf{p}'_i{}^2}{2m} + \frac{e^2}{4\pi\epsilon_0\kappa} \sum_{i<j} \frac{1}{|\mathbf{r}'_i - \mathbf{r}'_j|} \quad (1.11)$$

$$= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \frac{1}{2} \nu_c(q) (\rho_{\mathbf{q}} \rho_{-\mathbf{q}} - N), \quad (1.12)$$

$$H_{\text{ph}} = \sum_{\mathbf{q},\lambda} \Omega_{\mathbf{q}\lambda} b_{\mathbf{q}\lambda}^\dagger b_{\mathbf{q}\lambda}, \quad (1.13)$$

$$H_{\text{ei}} = \sum_{\mathbf{q},a} u(\mathbf{q}) e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{r}_a)} \rho_{\mathbf{q}}, \quad (1.14)$$

$$H_{\text{ep}} = \sum_{\mathbf{q},\lambda} M(\mathbf{q}, \lambda) \phi_{\mathbf{q}\lambda} e^{i\mathbf{q} \cdot \mathbf{R}} \rho_{\mathbf{q}}. \quad (1.15)$$

Here, $\rho_{\mathbf{q}}$ is the density operator of the relative electrons,

$$\rho_{\mathbf{q}} = \sum_i e^{i\mathbf{q}\cdot\mathbf{r}'_i} = \sum_{\mathbf{k}} \rho_{\mathbf{k}\mathbf{q}}, \quad \rho_{\mathbf{k}\mathbf{q}} = \sum_{\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} c_{\mathbf{k}\sigma}, \quad (1.16)$$

$\phi_{\mathbf{q}\lambda} \equiv b_{\mathbf{q}\lambda} + b_{-\mathbf{q}\lambda}^{\dagger}$ is the phonon field operator with $b_{\mathbf{q}\lambda}^{\dagger}$ and $b_{\mathbf{q}\lambda}$ being creation and annihilation operators for a phonon of wavevector \mathbf{q} in branch λ having frequency $\Omega_{\mathbf{q}\lambda}$, $\nu_c(q) = e^2/\epsilon_0\kappa q^2$ is the Coulomb potential (κ is the background dielectric constant), and $u(\mathbf{q})$ 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 $M(\mathbf{q}, \lambda) = M^*(-\mathbf{q}, \lambda)$.

1.2 Center-of-Mass Treated as a Classical Particle

As is seen from Hamiltonian (1.9), our system comprises three parts: the center of mass, relative electrons and phonons. The center of mass (CM), described by the canonical conjugate variables \mathbf{R} and \mathbf{P} (\mathbf{R} is the average position of all electrons and \mathbf{P} is the total momentum of all electrons) and considered as a single particle having mass Nm and charge Ne , is moving under the influence of the acceleration due to the applied electric field \mathbf{E} and the damping due to electron–impurity and electron–phonon interactions H_{ei} and H_{ep} . Because of its enormous mass, the motion of the center of mass is essentially classical, and we can treat the CM-related operators classically, regarding the coordinate variable \mathbf{R} in H_{ei} and H_{ep} as the real, time-dependent expectation position of the center of mass, $\mathbf{R}(t)$. The relative electron system, which is composed of a large number of interacting particles and described by the set of canonical conjugate variables \mathbf{r}'_i and \mathbf{p}'_i , or by creation and annihilation operators $c_{\mathbf{k}\sigma}^{\dagger}$ and $c_{\mathbf{k}\sigma}$, is treated fully quantum-mechanically. The significance is that the relative electron system does not directly sense the electric field but it is coupled to the center-of-mass motion through the time-varying CM position $\mathbf{R}(t)$ appearing in both H_{ei} and H_{ep} . In the following we will denote

$$H_{\text{It}} = H_{\text{ei}} + H_{\text{ep}} \quad (1.17)$$

as a time-dependent interaction containing $\mathbf{R}(t)$ as a time-dependent classical parameter. Note that the error arising from treating $\mathbf{R}(t)$ as a classical variable, i.e. from neglecting the noncommutability of the CM coordinate operators at different times, $\mathbf{R}(t)$ and $\mathbf{R}(t')$, is of order of $1/N$, and has

been shown (Lei, 1990a) to be exactly canceled by that arising from the neglect of the noncanonical $1/N$ terms in the commutation relations of the relative electron variables, Eq.(1.7). Therefore, the two major approximations made above in formulating the balance equation theory, i.e. treating relative electrons as an unconstrained canonical system and treating the center of mass as a classical single particle, induce no error save in regard to the intracollisional field effect (see Sec.10.1). In accordance with this Hamiltonian, it is apparent that the CM velocity \mathbf{V} , or the time derivative of the CM position, is given by

$$\mathbf{V} \equiv \dot{\mathbf{R}} = -i[\mathbf{R}, H] = \frac{\partial H}{\partial \mathbf{P}} = \frac{\mathbf{P}}{Nm}. \quad (1.18)$$

Note that the center 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 CM velocity \mathbf{V} is composed of a drift or average part \mathbf{v} and a fluctuation or random part $\delta\mathbf{V}$:

$$\mathbf{V} = \mathbf{v} + \delta\mathbf{V}. \quad (1.19)$$

Here we denote $\mathbf{v} = \langle \mathbf{V} \rangle$ or $\langle \delta\mathbf{V} \rangle = 0$, with the $\langle \dots \rangle$ 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 center of mass are obtained by calculating the time derivative of the CM momentum $\dot{\mathbf{P}} = -i[\mathbf{P}, H] = -\partial H/\partial \mathbf{R}$, yielding

$$\dot{\mathbf{P}} = Ne\mathbf{E} + \hat{\mathbf{F}}, \quad (1.20)$$

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

$$\hat{\mathbf{F}}_i = -i \sum_{\mathbf{q}, a} u(\mathbf{q}) \mathbf{q} e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}_a)} \rho_{\mathbf{q}}, \quad (1.21)$$

$$\hat{\mathbf{F}}_p = -i \sum_{\mathbf{q}, \lambda} M(\mathbf{q}, \lambda) \mathbf{q} \phi_{\mathbf{q}\lambda} e^{i\mathbf{q} \cdot \mathbf{R}} \rho_{\mathbf{q}}, \quad (1.22)$$

are identified as forces respectively due to impurity and phonon scatterings. Being quantum-mechanical operators in the relative-electron and phonon space, $\hat{\mathbf{F}}_i$ and $\hat{\mathbf{F}}_p$ also comprise an average part and a fluctuating part. The latter contributes a random force exerting on the center of mass. Eq.(1.20) is an operator force balance equation of the system.

Similarly, we can obtain the rate of change of the energy of the phonon system and that of relative electron systems from the Heisenberg equation

of motion:

$$\dot{H}_{\text{ph}} = -i[H_{\text{ph}}, H] = \hat{W} \equiv - \sum_{\mathbf{q}, \lambda} M(\mathbf{q}, \lambda) \dot{\phi}_{\mathbf{q}\lambda} e^{i\mathbf{q}\cdot\mathbf{R}} \rho_{\mathbf{q}}, \quad (1.23)$$

$$\begin{aligned} \dot{H}_{\text{er}} = -i[H_{\text{er}}, H] = \hat{S} \equiv & -i \sum_{\mathbf{q}, \lambda} M(\mathbf{q}, \lambda) \phi_{\mathbf{q}\lambda} e^{i\mathbf{q}\cdot\mathbf{R}} \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \rho_{\mathbf{k}\mathbf{q}} \\ & -i \sum_{\mathbf{q}, a} u(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}_a} \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \rho_{\mathbf{k}\mathbf{q}}, \end{aligned} \quad (1.24)$$

with

$$\dot{\phi}_{\mathbf{q}\lambda} \equiv -i[\phi_{\mathbf{q}\lambda}, H_{\text{ph}}] = -i\Omega_{\mathbf{q}\lambda}(b_{\mathbf{q}\lambda} - b_{-\mathbf{q}\lambda}^\dagger). \quad (1.25)$$

Energy balance for the electron system requires that the energy supplied per unit time by the electric field, $Ne\mathbf{E}\cdot\mathbf{V}$, 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, \dot{H}_{er} , and the energy loss rate of the electron system to the phonon system \dot{W} :

$$Ne\mathbf{E}\cdot\mathbf{V} = Nm\mathbf{V}\cdot\frac{d\mathbf{V}}{dt} + \dot{H}_{\text{er}} + \dot{W}. \quad (1.26)$$

Eq. (1.26) is an energy balance equation of the electron system in operator form. Of course, Eq. (1.24) which states the energy balance for the relative electron system, is also an operator energy balance equation. All these equations are in operator form in the relative electron and phonon spaces.

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

$$\langle \mathcal{O} \rangle = \text{tr}\{\hat{\rho}\mathcal{O}\}. \quad (1.27)$$

Here $\text{tr}\{\cdot\}$ indicates the trace of the operator in the bracket, \mathcal{O} is the operator (possibly time dependent) representing the dynamical variable in the Schrödinger picture and $\hat{\rho}$ is the density matrix satisfying the Liouville equation

$$i\frac{d\hat{\rho}}{dt} = [H_{\text{er}} + H_{\text{ph}} + H_{\text{It}}, \hat{\rho}] \quad (1.28)$$

subject to an initial condition at the initial time t_0

$$\hat{\rho}|_{t_0} = \hat{\rho}_0. \quad (1.29)$$

We will use $t_0 = -\infty$ or $t_0 = 0$ as the initial time.

1.3 Initial Density Matrix

Physically, we expect that external conditions (the applied electric field, magnetic field, bath temperature, etc) uniquely determine the final steady state of a system in transport. This means that the final steady state to which the system evolves under the influence of a given electric field, for instance, does not depend on the particulars of the initial condition. After a sufficiently long time the system will arrive at a unique steady state no matter what an initial state it starts from. However, the time required for the system to go from an initial state to the final state does depend strongly on the initial state. As a parametrized theory, the balance equation approach allows us to choose an initial state, which should be simple enough to handle easily and has its major features resemble, as closely as possible, the final state, such that the system, starting from this virtual initial state, can reach the real final state through a short evolution process. When dealing with a time-independent (steady) problem, the final state is of course the steady transport state we are seeking for. When dealing with a time-dependent problem, the “final” state can be the transport state at a time t during the transport process. To figure out the key features of the final state we image to turn off the electron–impurity and electron–phonon interactions H_I together with the electric field \mathbf{E} at a certain time t suddenly during the temporal development of the transport process (but keep the electron–electron interaction intact). Then the center of mass, the relative electrons and phonons are decoupled from each other. Being a free particle, the center of mass moves inertially with the constant velocity \mathbf{v} equal to the drift velocity $\mathbf{v}(t)$ of the transporting electron system at time t . The relative electron system, as an isolated object, will approach a thermal equilibrium state after a certain relaxation time τ_{th} , having a well-defined thermodynamic temperature $T_e(t)$. This temperature apparently depends on the state of relative electrons at time t , and will be called the electron temperature of this transport state, even though it may not be possible to define a thermodynamic temperature directly with a transport state (it is not a thermal equilibrium state). In the same vein, the phonon system, which has been decoupled from the electron system, can also be considered to reach a thermal equilibrium state jointly with the bath at the lattice temperature T . This is justifiable if phonons relax faster than electrons. If

this is not the case one may need to consider that during the time period after turning off the interactions when relative electrons have arrived at an equilibrium state, phonons only reach a quasi-equilibrium state with a mode $\mathbf{q}\lambda$ - and time-dependent temperature $T_{\mathbf{q}\lambda}(t)$. Further discussion of this will be given in Chapter 5 (Nonequilibrium and Confined Phonons). For the most part in this book, we assume the former case for phonons and correspondingly choose the initial state as the one in which the center of mass moves with constant velocity $\mathbf{v} = \mathbf{v}(t)$, the relative electrons are in a thermal equilibrium state with temperature $T_e = T_e(t)$ and phonons are in its thermal equilibrium state with lattice temperature T . The initial density matrix for the relative-electron-phonon system is then (Lei and Ting, 1985a; Xing and Ting, 1987)

$$\hat{\rho}_0 = \frac{1}{Z} e^{-H_{\text{cr}}/T_e} e^{-H_{\text{ph}}/T}, \quad (1.30)$$

where Z is a normalization coefficient and H_{cr} 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, $\hat{\rho}_0 \equiv \hat{\rho}_{0t}$.

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 $\mathbf{E}(t)$ and the temporal development of statistically averaged quantities such as $\mathbf{v}(t)$ and $T_e(t)$, occur on a macroscopic time scale, which is assumed to be much larger than the microscopic relaxation time, or the evolution time scale of the Liouville equation. In other words, we assume that the evolution from the initial state to the final state in accordance with the Liouville equation is a fast microscopic process, whereas the temporal development of the transport quantities is a slow macroscopic process. The latter is included in the parametric time-variation of the initial density matrix $\hat{\rho}_{0t}$ and the center-of-mass velocity $\mathbf{v}(t)$.

The initial state described by Eq. (1.30) is one in which the electrons are characterized as being in thermal equilibrium with respect to their center of mass which is moving at a velocity equal to their average drift velocity in the presence of the electric field. Such a selection of the initial state is significant (Lei, 1990b). Since the final state bears the same center-of-mass velocity as the initial state, the time evolution from the initial state to the final state is solely a thermalization process with no need for momentum relaxation. This process involves not only impurity and phonon scatterings, but in most cases, it is determined mainly by intercarrier scatterings.

For systems in which there exists a strong carrier–carrier scattering the microscopic relaxation is very fast, lending validity to the time-dependent description of transport. Even for steady state transport in a constant electric field, a short thermalization time τ_{th} also plays a key role in making it possible to develop a simple perturbative expansion (Lei, 1990b). The underlying phenomenology is that the strong intercarrier scattering promotes a tendency towards rapid thermalization of the electrons in their drifting frame, such that the final steady state is only “a small perturbation away” from the thermal equilibrium state of relative electrons as given by (1.30). We will return to this matter in Chapter 7.

1.4 Density Matrix and Statistical Averages to Linear Order in H_{I}

The statistical average of a dynamical variable \mathcal{O} at time t , Eq. (1.27), can alternatively be written in the interaction picture as

$$\langle \mathcal{O} \rangle = \text{tr} \{ \hat{\rho}(t) \mathcal{O}(t) \}, \quad (1.31)$$

where the operators in the interaction picture are defined as

$$\mathcal{O}(t) \equiv e^{i(H_{\text{er}}+H_{\text{ph}})t} \mathcal{O} e^{-i(H_{\text{er}}+H_{\text{ph}})t}, \quad (1.32)$$

$$\hat{\rho}(t) \equiv e^{i(H_{\text{er}}+H_{\text{ph}})t} \hat{\rho} e^{-i(H_{\text{er}}+H_{\text{ph}})t}. \quad (1.33)$$

In view of the Liouville equation (1.28) and the initial condition (1.30), $\hat{\rho}(t)$ satisfies the equation

$$i \frac{d}{dt'} \hat{\rho}(t') = [H_{\text{I}t'}(t'), \hat{\rho}(t')] \quad (1.34)$$

and is subject to the initial condition

$$\hat{\rho}(t') \Big|_{t'=-\infty} = \hat{\rho}_0. \quad (1.35)$$

Or, equivalently, it obeys the integral equation

$$\hat{\rho}(t') = \hat{\rho}_0 - i \int_{-\infty}^{t'} dt'' [H_{\text{I}t''}(t''), \hat{\rho}(t'')]. \quad (1.36)$$

This integral equation facilitates a perturbative expansion in orders of the interaction H_I . The first order iteration of Eq. (1.36) yields

$$\hat{\rho}(t') = \hat{\rho}_0 - i \int_{-\infty}^{t'} dt'' [H_{I t''}(t''), \hat{\rho}_0]. \quad (1.37)$$

The statistical average of a dynamical variable \mathcal{O} , Eq. (1.31), can thus be written, to the linear order in H_I , as

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} \rangle_0 - i \int_{-\infty}^t dt' \langle [\mathcal{O}(t), H_{I t'}(t')] \rangle_0, \quad (1.38)$$

where

$$\langle \cdots \rangle_0 \equiv \text{tr} \{ \hat{\rho}_0(\cdots) \}. \quad (1.39)$$

Note that $\hat{\rho}_0$, and the average $\langle \cdots \rangle_0$, may be dependent on time t .

Eq. (1.38), containing only to the linear order of impurity and phonon scatterings, is the formula mostly often used for calculating the statistical averages of physical quantities in the balance equation approach. Of course, one can continue to iterate Eq. (1.36) to obtain an expansion series with arbitrarily higher order terms of H_I . In principle, a perturbation treatment is valid when the resultant expansion series converges. In this case it is reasonable to take the partial sum of the first finite-number terms or to sum over a partial array of infinite terms as an approximation for the full series, even we are not able to sum over the entire series. On the contrary, if the resultant series of the iterative expansion does not converge or contains divergent high order terms, the perturbative treatment will generally no longer work. Even if a renormalization through summing up the divergent terms seems possible, the physical nature of the issue may be changed completely.

1.5 Force Balance Equation

Taking the statistical average of operator equation (1.20) in the relative electron and phonon space to the lowest order in H_I in accordance with (1.38), and using expressions (1.14) and (1.15) for H_{ei} and H_{ep} , we obtain the equation of motion of the center of mass, or the time-dependent momentum or force balance equation of the system (Lei and Ting, 1984,

1985a; Xing and Ting, 1987)

$$Nm \frac{d}{dt} \mathbf{v}(t) = Ne \mathbf{E}(t) + \tilde{\mathbf{f}}_i + \tilde{\mathbf{f}}_p, \quad (1.40)$$

by identifying the average rate of the CM momentum change as

$$\langle \dot{\mathbf{P}} \rangle = Nm \frac{d}{dt} \mathbf{v}(t), \quad (1.41)$$

$\mathbf{v}(t)$ being the drift part of the center-of-mass velocity. In Eq. (1.40), $\tilde{\mathbf{f}}_i$ and $\tilde{\mathbf{f}}_p$, the frictional forces experienced by the center of mass respectively due to electron-impurity and electron-phonon interactions, are given by

$$\tilde{\mathbf{f}}_i = -i n_i \sum_{\mathbf{q}} \mathbf{q} |u(\mathbf{q})|^2 \int_{-\infty}^{\infty} dt' A(\mathbf{q}, t, t') \Pi(\mathbf{q}, t - t'), \quad (1.42)$$

$$\tilde{\mathbf{f}}_p = -i \sum_{\mathbf{q}, \lambda} \mathbf{q} |M(\mathbf{q}, \lambda)|^2 \int_{-\infty}^{\infty} dt' A(\mathbf{q}, t, t') \Lambda(\mathbf{q}, \lambda, t - t'). \quad (1.43)$$

In this, n_i is the impurity density, and the retarded correlation functions are defined as

$$\Pi(\mathbf{q}, t - t') = -i \theta(t - t') \langle [\rho_{\mathbf{q}}(t), \rho_{-\mathbf{q}}(t')] \rangle_0, \quad (1.44)$$

$$\Lambda(\mathbf{q}, \lambda, t - t') = -i \theta(t - t') \langle [\phi_{\mathbf{q}\lambda}(t) \rho_{\mathbf{q}}(t), \phi_{-\mathbf{q}\lambda}(t') \rho_{-\mathbf{q}}(t')] \rangle_0, \quad (1.45)$$

with

$$\rho_{\mathbf{q}}(t) = e^{i H_{\text{er}} t} \rho_{\mathbf{q}} e^{-i H_{\text{er}} t} = \sum_{\mathbf{k}} e^{i(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})t} \rho_{\mathbf{k}\mathbf{q}}, \quad (1.46)$$

$$\phi_{\mathbf{q}\lambda}(t) = e^{i H_{\text{ph}} t} \phi_{\mathbf{q}\lambda} e^{-i H_{\text{ph}} t} = b_{\mathbf{q}\lambda} e^{-i \Omega_{\mathbf{q}\lambda} t} + b_{-\mathbf{q}\lambda}^\dagger e^{i \Omega_{\mathbf{q}\lambda} t}, \quad (1.47)$$

and the step function $\theta(t) = 1$ for $t \geq 0$ and $\theta(t) = 0$ for $t < 0$.

The expressions (1.42) and (1.43) of frictional forces $\tilde{\mathbf{f}}_i$ and $\tilde{\mathbf{f}}_p$ have important physical connotation. Firstly, the center-of-mass motion enters (1.42) and (1.43) through the function

$$A(\mathbf{q}, t, t') \equiv \exp[i \mathbf{q} \cdot (\mathbf{R}(t) - \mathbf{R}(t'))], \quad (1.48)$$

which plays a crucial role in the balance equation theory. Since the CM velocity relates to its position by $\mathbf{V} \equiv \dot{\mathbf{R}}$, when neglecting effects associated with the velocity fluctuation $\delta \mathbf{V}$ of the center of mass in (1.19), the CM

velocity \mathbf{V} can be approximated by its average part \mathbf{v} and $A(\mathbf{q}, t, t')$ function is determined only by the drift velocity $\mathbf{v}(t)$ of the electron system:

$$A(\mathbf{q}, t, t') = \exp \left[i\mathbf{q} \cdot \int_{t'}^t \mathbf{v}(s) ds \right]. \quad (1.49)$$

In this way the frictional forces $\tilde{\mathbf{f}}_i$ and $\tilde{\mathbf{f}}_p$ depend on the time-dependent average velocity of the center of mass, i.e. the time-dependent drift velocity of the electron system, $\mathbf{v}(t)$. This indicates that the behavior of the frictional forces (thus the major transport properties) of the system is directly affected by the drift motion of carriers rather than by the electric field, which shows up only as a force acting on the center-of-mass in the force balance equation (1.40). The functional dependence involving in Eqs. (1.42) and (1.43), however, is rather complicated and generally hard to handle. Approximations can be made in different cases to simplify the treatment.

The second point connoted in the expressions (1.42) and (1.43) is related to the correlation functions $\Pi(\mathbf{q}, t - t')$ and $\Lambda(\mathbf{q}, \lambda; t - t')$ given by (1.44) and (1.45), which involve the statistical average $\langle \dots \rangle_0$ with respect to the initial density matrix $\hat{\rho}_0$ given by (1.30) containing the electron temperature $T_e(t)$ as a parameter. Thus, the frictional forces $\tilde{\mathbf{f}}_i$ and $\tilde{\mathbf{f}}_p$ expressed in Eqs. (1.42) and (1.43) also depend on the time-dependent electron temperature $T_e(t)$ of the system.

1.6 Energy Balance Equation

Taking the statistical average of the right hand side of the operator expression (1.23) in the relative electron and phonon space to the lowest order in H_I , we obtain the energy increase rate of the phonon system due to electron-phonon interaction, i.e. the energy transfer rate from the electron system to the phonon system:

$$\tilde{\omega} = \langle \hat{W} \rangle = - \sum_{\mathbf{q}\lambda} |M(\mathbf{q}, \lambda)|^2 \int_{-\infty}^{\infty} dt' A(\mathbf{q}, t, t') \Gamma(\mathbf{q}, \lambda, t - t'), \quad (1.50)$$

with

$$\Gamma(\mathbf{q}, \lambda, t - t') = -i\theta(t - t') \langle [\dot{\phi}_{\mathbf{q}\lambda}(t) \rho_{\mathbf{q}}(t), \phi_{-\mathbf{q}\lambda}(t') \rho_{-\mathbf{q}}(t')] \rangle_0 \quad (1.51)$$

and

$$\dot{\phi}_{\mathbf{q}\lambda}(t) = e^{iH_{\text{ph}}t} \dot{\phi}_{\mathbf{q}\lambda} e^{-iH_{\text{ph}}t} = -i\Omega_{\mathbf{q}\lambda} \left(b_{\mathbf{q}\lambda} e^{-i\Omega_{\mathbf{q}\lambda}t} - b_{-\mathbf{q}\lambda}^\dagger e^{i\Omega_{\mathbf{q}\lambda}t} \right). \quad (1.52)$$

This energy-transfer rate \tilde{w} also functionally depends on the CM drift velocity $\mathbf{v}(t)$ through the $A(\mathbf{q}, t, t')$ function and on the electron temperature $T_e(t)$ through the statistical average of the correlation function $\Gamma(\mathbf{q}, \lambda, t - t')$ with respect to the initial density matrix $\hat{\rho}_0$.

An energy balance equation is derived from the statistical average of the operator equation (1.26). Retaining only the drift part of the center-of-mass velocity (i.e. neglecting the contribution from the CM velocity fluctuation) and identifying $\langle \dot{H}_{\text{er}} \rangle$ as the rate of increase of the internal energy of relative electrons,

$$\langle \dot{H}_{\text{er}} \rangle = \frac{dU}{dt} \quad (1.53)$$

with $U \equiv \langle H_{\text{er}} \rangle$, we have

$$Ne\mathbf{E} \cdot \mathbf{v} = Nm\mathbf{v} \cdot \frac{d\mathbf{v}}{dt} + \frac{dU}{dt} + \tilde{w}. \quad (1.54)$$

Eliminating the term $Nm\mathbf{v} \cdot d\mathbf{v}/dt$ by means of the force balance equation (1.40), we can write the energy balance equation (1.54) in the form

$$-\frac{dU}{dt} = \mathbf{v} \cdot \tilde{\mathbf{f}} + \tilde{w}, \quad (1.55)$$

where $\tilde{\mathbf{f}} = \tilde{\mathbf{f}}_i + \tilde{\mathbf{f}}_p$. Eq. (1.54) or Eq. (1.55) is the time-dependent energy balance equation of the system (Lei and Ting, 1984, 1985a; Xing and Ting, 1987).

It should be noted that energy balance equation can also be derived by taking the statistical average of the operator expression (1.24) to the lowest order in H_I (Lei and Ting, 1984, 1985a),

$$\begin{aligned} \langle \hat{S} \rangle = & -i n_i \sum_{\mathbf{q}} |u(\mathbf{q})|^2 \int_{-\infty}^{\infty} dt' A(\mathbf{q}, t, t') \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \Pi(\mathbf{k}, \mathbf{q}, t - t') \\ & -i \sum_{\mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 \int_{-\infty}^{\infty} dt' A(\mathbf{q}, t, t') \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \Lambda(\mathbf{k}, \mathbf{q}, \lambda, t - t'), \end{aligned} \quad (1.56)$$

with

$$\Pi(\mathbf{k}, \mathbf{q}, t - t') = -i\theta(t - t') \langle [\rho_{\mathbf{k}\mathbf{q}}(t), \rho_{-\mathbf{q}}(t')] \rangle_0, \quad (1.57)$$

$$\Lambda(\mathbf{k}, \mathbf{q}, \lambda; t - t') = -i\theta(t - t') \langle [\phi_{\mathbf{q}\lambda}(t)\rho_{\mathbf{k}\mathbf{q}}(t), \phi_{-\mathbf{q}\lambda}(t')\rho_{-\mathbf{q}}(t')] \rangle_0, \quad (1.58)$$

$$\rho_{\mathbf{k}\mathbf{q}}(t) = e^{iH_{\text{er}}t} \rho_{\mathbf{k}\mathbf{q}} e^{-iH_{\text{er}}t}, \quad (1.59)$$

and identifying $\langle \dot{H}_{\text{er}} \rangle = dU/dt$. This results in another energy balance equation:

$$\frac{dU}{dt} = \langle \hat{S} \rangle. \quad (1.60)$$

This equation is equivalent to Eq. (1.54) for steady state transport (Lei and Ting, 1985a) and for time-dependent drift motion involving negligible memory effects (Chapter 3). However, there may be some differences when discussing nonlinear processes in which memory effects are significant, or discussing processes involving effects of velocity fluctuations in higher orders (see Chapter 4).

Using the perturbation expansion (1.38) to calculate the relative electron internal energy $\langle H_{\text{er}} \rangle$, we find that only the $\hat{\rho}_0$ term contributes, i.e.

$$U = \langle H_{\text{er}} \rangle_0, \quad (1.61)$$

which depends on the electron temperature T_e . Expressing the rate of change of the relative electron internal energy in terms of its specific heat $C_e = \partial U / \partial T_e$ and the rate of change of the electron temperature, we can write

$$\frac{dU}{dt} = C_e \frac{dT_e}{dt}. \quad (1.62)$$