

## Chapter 2

# Drift-Diffusion and Ballistic Transport

As the thermoballistic approach is devised to unify the drift-diffusion and ballistic (thermionic) descriptions of carrier transport, we present in this chapter a detailed exposition of the standard formulations of these two limiting cases. We consider one-dimensional transport in three-dimensional, “plane-parallel” semiconducting samples and disregard spin degrees of freedom. In the ballistic case, effects of carrier tunneling and degeneracy are taken into account. The ranges of validity of the drift-diffusion and ballistic models are indicated. With a view towards the thermoballistic description of transport, we comment on the role of interface resistances and on the chemical potential in the ballistic description.

## 2.1 Drift-Diffusion Transport

The drift-diffusion model is an extension of the transport model of Drude, so that we begin here with an account of the latter. Drude’s model is far from being able to describe transport properties of semiconductors quantitatively; nevertheless, its exposition provides us with the opportunity to introduce and discuss the basic notions on which classical and semiclassical transport theories rely, and which will appear ubiquitously throughout this book.

### 2.1.1 Drude’s Model

In the transport model of Drude [1–4], one considers a (three-dimensional) homogeneous classical gas of non-interacting electrons in thermodynamic equilibrium at temperature  $T$ , which is subjected to an externally applied, constant electric field  $\mathbf{E}$ . The electrons collide with randomly distributed, spatially fixed scattering centers (“impurities”). The collisions are assumed to cause the electrons to return instantaneously to complete thermodynamic equilibrium. The average vectorial velocity of

the electrons emerging from this equilibration is equal to zero. Their mean speed  $u$ , i.e., the thermal average of the magnitude of the electron velocity as derived from the three-dimensional Maxwell-Boltzmann velocity distribution function, is given by

$$u = \left( \frac{8}{\pi m^* \beta} \right)^{1/2}, \quad (2.1)$$

where  $m^*$  is the effective electron mass, and  $\beta = 1/k_B T$ , with  $k_B$  the Boltzmann constant. (Note that in Drude's original papers [1, 2], the mean electron speed was derived from Boltzmann's equipartition theorem; the Maxwell-Boltzmann velocity distribution was introduced into the description of electron transport in metals by Lorentz [5].)

### 2.1.1.1 Drift Current

Defining the *mean free path* (or *momentum relaxation length*)  $l$  as the average distance (measured along the transport direction) traveled by the electrons between two collisions, one finds for the *collision time* (or *relaxation time*)  $\tau$ , defined as the average time-of-flight between successive collisions,

$$\tau = \frac{l}{u}. \quad (2.2)$$

The mean free path  $l$  characterizes a set of collision-free *ballistic intervals* of average length  $l$ , across which electrons move ballistically under the influence of the external field  $\mathbf{E}$ . On average, they acquire a velocity, the *drift velocity*  $\mathbf{v}_{dr}$ , given by the acceleration  $-e\mathbf{E}/m^*$  times their average time-of-flight across the ballistic intervals, i.e., times the collision time  $\tau$ ,

$$\mathbf{v}_{dr} = -\frac{e\mathbf{E}}{m^*} \tau \equiv -\nu \mathbf{E}, \quad (2.3)$$

where

$$\nu \equiv \frac{e}{m^*} \tau = \frac{e}{m^*} \frac{l}{u} = e \left( \frac{\pi \beta}{8 m^*} \right)^{1/2} l \quad (2.4)$$

is the electron mobility.

In the picture of Drude, the charge current density  $\mathbf{j}$  (current, for short) is a *drift current*,  $\mathbf{j}_{dr}$ , driven by the external electric field  $\mathbf{E}$ ,

$$\mathbf{j} \equiv \mathbf{j}_{dr} = -en\mathbf{v}_{dr} = en\nu \mathbf{E}, \quad (2.5)$$

where  $n$  is the electron density. Since, in Drude's model,  $n$  as well as the field  $\mathbf{E}$  are independent of position,  $\mathbf{j}$  is constant. In terms of the electron conductivity

$$\sigma = e\nu n, \quad (2.6)$$

the current  $\mathbf{j}$  is expressed as

$$\mathbf{j} = \sigma \mathbf{E}, \quad (2.7)$$

i.e., in the form of Ohm's law.

The transport mechanism in Drude's model can be elucidated [4] by noting that Eq. (2.3), when written as

$$-e\mathbf{E} - \frac{m^*}{\tau} \mathbf{v}_{dr} = 0, \quad (2.8)$$

states that the effect of the external force  $-e\mathbf{E}$  is balanced, on average, by that of a *friction force*  $-\gamma \mathbf{v}_{dr}$ , with the friction coefficient  $\gamma$  given by

$$\gamma = \frac{m^*}{\tau} = \frac{e}{\nu}. \quad (2.9)$$

The friction force reflects the reset to zero, on average, of their individual velocities when, subsequent to their acceleration through the external field, the electrons are thermally equilibrated due to impurity scattering.

### 2.1.1.2 Range of Validity

Limits on the range of validity of Drude's model are set by the requirement that the perturbation of the electron gas due to the external field is sufficiently small such that the gas stays close to thermodynamic equilibrium. This condition can be met by requiring the magnitude of the drift velocity to be very small as compared with the mean speed of the electrons,

$$|\mathbf{v}_{dr}| \ll u. \quad (2.10)$$

Using Eqs. (2.1), (2.3) and (2.4), condition (2.10) can be re-expressed in a form that restricts, for given mean free path  $l$ , the magnitude of the electric-field vector  $\mathbf{E}$ ,

$$|\mathbf{E}| \ll \frac{8}{\pi\beta el}. \quad (2.11)$$

For a homogeneous sample of length  $S$  subjected to an externally applied voltage  $V$ , so that  $|\mathbf{E}| = |V|/S$ , one has

$$|V| \ll \frac{8S}{\pi\beta el}. \quad (2.12)$$

Reversely, for given  $V$ , the ratio of mean free path to sample length is restricted by the condition

$$\frac{l}{S} \ll \frac{8}{\pi\beta e|V|}. \quad (2.13)$$

For room temperature, i.e.,  $1/\beta \approx 0.025$  eV, and values of  $e|V|$  of a few tens of meV, which are typical for semiconducting devices, the right-hand side of condition (2.13) is of order unity. Hence, one may use the condition

$$\frac{l}{S} \ll 1 \quad (2.14)$$

as a rough criterion for delimiting the range of validity of Drude's model. The value of  $l$  remains small if the density of impurities is sufficiently high.

### 2.1.2 Drift-Diffusion Model

Electron transport in inhomogeneous semiconductors is outside of the scope of Drude's model. The non-uniformity of the donor density in inhomogeneous samples entails a position dependence of the electron density,  $n = n(x)$ , and gives rise to an  $x$ -dependent internal ("built-in") electrostatic potential [3, 6, 7]. [Throughout this book, we consider *one-dimensional* transport in *three-dimensional*, "plane-parallel" semiconducting samples, i.e., samples whose parameters do not vary in the directions perpendicular to the transport direction, which is taken as the  $x$ -direction (for a discussion of this assumption, see Sect. 4.4.2). Further, the temperature  $T$  is assumed to be constant across the sample.]

#### 2.1.2.1 Local Thermodynamic Equilibrium

Transport in inhomogeneous systems near thermodynamic equilibrium can be described in terms of a *local* thermodynamic equilibrium [3] characterized by a *local chemical potential*  $\mu(x)$ <sup>1</sup> Disregarding spin degrees of freedom and adopting the effective-mass approximation [3, 6], we have for the equilibrium electron density  $n(x)$  in a nondegenerate system

$$n(x) = 4\pi \left(\frac{m^*}{h}\right)^3 \int_{-\infty}^{\infty} dv_x \int_0^{\infty} dw w f^{MB}(E(v; x) - \mu(x)). \quad (2.15)$$

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<sup>1</sup> Throughout this book, we use the term "chemical potential" as defined in Ref. [3].

Here,  $h$  is Planck's constant, and we have introduced cylindrical coordinates in three-dimensional velocity space (with Cartesian coordinates  $v_x, v_y, v_z$ ) such that

$$v = (v_x^2 + w^2)^{1/2}, \quad (2.16)$$

with  $w^2 = v_y^2 + v_z^2$ . The function

$$f^{MB}(E) = e^{-\beta E} \quad (2.17)$$

is the Maxwell-Boltzmann energy distribution function, and

$$E(v; x) = \epsilon(v) + E_c(x) \quad (2.18)$$

is the total electronic energy at the equilibrium point  $x$ , with the kinetic energy

$$\epsilon(v) = \frac{m^*}{2} v^2. \quad (2.19)$$

The potential energy profile  $E_c(x)$ , here assumed to be a prescribed function, comprises the conduction band edge potential (which includes the position-dependent internal potential) and the external electrostatic potential. In general,  $E_c(x)$  exhibits a “multiple-barrier” shape associated with local maxima of the profile. Evaluation of the integrals in Eq. (2.15) results in the standard form for the density,

$$n(x) = N_c e^{-\beta[E_c(x) - \mu(x)]}, \quad (2.20)$$

where

$$N_c = 2 \left( \frac{2\pi m^*}{\beta h^2} \right)^{3/2} \quad (2.21)$$

is the effective density of states at the conduction band edge [3].

### 2.1.2.2 Drift-Diffusion Current

The effects of the spatial variation of the electron density and of the associated occurrence of an internal potential in inhomogeneous semiconductors can be described within an extension of Drude's model, the *drift-diffusion model*. In this model, a generalized,  $x$ -dependent drift current  $j_{dr}(x)$  is supplemented [3, 8–10] by a *diffusion current*  $j_{di}(x)$  proportional to the density gradient along the  $x$ -axis, so that the total (conserved) current  $j$  is given by

$$j = j_{dr}(x) + j_{di}(x). \quad (2.22)$$

The generalized drift current is obtained from expression (2.7) by replacing (i) the conductivity  $\sigma$  with the *local conductivity*  $\sigma(x)$  given by Eq. (2.6), with  $n(x)$  in lieu of  $n$ , and (ii) the constant external electric field  $\mathbf{E}$  with the field  $[dE_c(x)/dx]/e$  associated with the potential energy profile  $E_c(x)$ , so that one obtains

$$j_{dr}(x) = \frac{1}{e} \sigma(x) \frac{dE_c(x)}{dx}. \quad (2.23)$$

The diffusion current is written as

$$j_{di}(x) = eD \frac{dn(x)}{dx}, \quad (2.24)$$

where  $D$  is the diffusion coefficient, which is related to the electron mobility  $\nu$  via the Einstein relation [3, 4],

$$D = \frac{\nu}{\beta e} = \frac{\tau}{m^* \beta}, \quad (2.25)$$

and  $\nu$  is now assumed to have the form corresponding to one-dimensional transport,

$$\nu = e \left( \frac{2\beta}{\pi m^*} \right)^{1/2} l \quad (2.26)$$

[see Eq. (2.4) for the three-dimensional form of  $\nu$ ]. Then, generalizing Eq. (2.6), one has

$$\sigma(x) \equiv e\nu n(x) = \beta e^2 D n(x). \quad (2.27)$$

For the total current  $j$ , one now finds from Eqs. (2.22)–(2.24), using Eq. (2.27),

$$j = \frac{1}{e} \sigma(x) \left[ \frac{dE_c(x)}{dx} + \frac{1}{\beta n(x)} \frac{dn(x)}{dx} \right], \quad (2.28)$$

which is the standard drift-diffusion expression (“drift-diffusion equation”) for the total charge current. For the derivation of this expression from Boltzmann’s transport equation and for its application in device simulation, see, e.g., Ref. [11]. In Ref. [12], the expression is derived within a time-dependent, tutorial treatment of diffusion in the presence of an external electric field (“biased-random-walk model”).

### 2.1.3 Current-Voltage Characteristic and Chemical Potential

Substituting expression (2.20) for the equilibrium density  $n(x)$  in Eq. (2.28), we obtain the current  $j$  in the form

$$j = \frac{1}{e} \sigma(x) \frac{d\mu(x)}{dx}, \quad (2.29)$$

which shows that, in the drift-diffusion model, it is the local chemical potential which provides the driving force for electron transport. Using Eqs. (2.20) and (2.27), we can rewrite Eq. (2.29) as

$$\frac{\beta j}{\nu N_c} e^{\beta E_c(x)} = \frac{d}{dx} e^{\beta \mu(x)}. \quad (2.30)$$

Considering a sample extending from  $x_1$  to  $x_2$ , so that

$$S = x_2 - x_1 \quad (2.31)$$

is the sample length, and integrating Eq. (2.30) over the interval  $[x_1, x]$ , we can express the local chemical potential  $\mu(x)$  in the form

$$e^{\beta \mu(x)} = e^{\beta \mu(x_1)} + \frac{\beta j}{\nu N_c} \int_{x_1}^x dx' e^{\beta E_c(x')}. \quad (2.32)$$

An equivalent representation of  $\mu(x)$  is obtained by integrating Eq. (2.30) over the interval  $[x, x_2]$ .

### 2.1.3.1 Current-Voltage Characteristic

Now, setting  $x = x_2$  in Eq. (2.32), identifying the chemical potentials at the end-points  $x_{1,2}$  with the potentials  $\mu_{1,2}$  in the contacts connected to the semiconducting sample,

$$\mu(x_{1,2}) = \mu_{1,2}, \quad (2.33)$$

and solving the resulting equation for the current  $j$ , we then obtain, using Eq. (2.20), the current-voltage characteristic of the drift-diffusion model in the form

$$j = -n(x_1) e^{-\beta E_b^l(x_1, x_2)} \frac{\nu}{\beta \tilde{S}} (1 - e^{-\beta eV}). \quad (2.34)$$

Here,

$$V = \frac{\mu_1 - \mu_2}{e} \quad (2.35)$$

is the voltage applied between the points  $x_1$  and  $x_2$ , and

$$E_b^l(x_1, x_2) \equiv E_c^m(x_1, x_2) - E_c(x_1) \geq 0 \quad (2.36)$$

is the maximum barrier height of the potential energy profile relative to its value  $E_c(x_1)$  at the left end of the sample, where  $E_c^m(x_1, x_2)$  is the overall maximum of  $E_c(x)$  in the interval  $[x_1, x_2]$ . Finally, the quantity

$$\tilde{S} \equiv \int_{x_1}^{x_2} dx e^{-\beta[E_c^m(x_1, x_2) - E_c(x)]} \quad (2.37)$$

is the “effective sample length”. It has the appealing property of becoming equal to the sample length  $S$  when the profile is flat, i.e., when  $E_c(x) = \text{const.}$ , and otherwise satisfies  $\tilde{S} < S$ . Writing the current-voltage characteristic in the particular form (2.34) facilitates comparison with analogous expressions given below.

Expression (2.34) shows that the current-voltage characteristic of the drift-diffusion model is controlled (i) by the “barrier factor”  $e^{-\beta E_b^l(x_1, x_2)}$ , which involves the overall maximum of the profile  $E_c(x)$ , and (ii) by the ratio  $\nu/\tilde{S}$  or, owing to Eq. (2.26), by the ratio  $l/\tilde{S}$ , in which the effective sample length reflects, in an integral way, the shape of  $E_c(x)$ . [In the ballistic description of transport, the barrier factor  $e^{-\beta E_b^l(x_1, x_2)}$  re-appears as the thermally averaged probability for electron transmission from  $x_1$  to  $x_2$ ; see Eq. (2.68) below.]

### 2.1.3.2 Chemical Potential

Now, inserting expression (2.34) in Eq. (2.32), using Eqs. (2.20) and (2.33), and defining

$$I_c(x', x'') = \int_{x'}^{x''} dz e^{\beta E_c(z)}, \quad (2.38)$$

we can express the chemical potential  $\mu(x)$  in the explicit form

$$e^{\beta[\mu(x) - \mu_1]} = 1 - \frac{I_c(x_1, x)}{I_c(x_1, x_2)} (1 - e^{-\beta eV}), \quad (2.39)$$

i.e., solely in terms of the potential energy profile  $E_c(x)$  and the voltage  $V$ . Equivalently, we can write

$$e^{\beta[\mu(x) - \mu_2]} = 1 + \frac{I_c(x, x_2)}{I_c(x_1, x_2)} (1 - e^{-\beta eV}) \quad (2.40)$$

by using for  $\mu(x)$  the representation obtained by integrating Eq. (2.30) over the interval  $[x, x_2]$ . It is easily seen that the two expressions (2.39) and (2.40) indeed represent a unique chemical potential  $\mu(x)$ .



### 2.1.3.3 Field-Driven Transport

As a special case, we consider electron transport in a homogeneous semiconductor (i.e., in a homogeneously doped, monocrystalline semiconducting sample), driven by a static external electric field of arbitrary magnitude (“field-driven transport”). When the effect of Schottky barriers is disregarded, the field is spatially constant, with magnitude  $\mathcal{E} = V/S$ . Assuming the field to be directed antiparallel to the  $x$ -axis, we write the corresponding potential energy profile in the form

$$E_c(x) = E_c(x_1) - \frac{\epsilon}{\beta}(x - x_1), \quad (2.41)$$

where the field parameter  $\epsilon$  is given by

$$\epsilon = \beta e \mathcal{E}. \quad (2.42)$$

For the effective sample length  $\tilde{S}$ , we then have

$$\tilde{S} = \frac{1}{\epsilon}(1 - e^{-\epsilon S}), \quad (2.43)$$

so that, using the relation

$$\epsilon S = \beta e V, \quad (2.44)$$

we obtain for the current  $j$  from Eq. (2.34)

$$j = -n(x_1) \frac{\nu}{\beta} \epsilon = -\sigma \frac{V}{S}, \quad (2.45)$$

where the conductivity  $\sigma$  is given by Eq. (2.6). For the chemical potential  $\mu(x)$ , we find from Eqs. (2.39) and (2.40), using relation (2.44),

$$\begin{aligned} \mu(x) &= E_c(x) + [\mu_1 - E_c(x_1)] = E_c(x) + [\mu_2 - E_c(x_2)] \\ &\equiv \frac{1}{2}(\mu_1 + \mu_2) - eV \frac{x - (x_1 + x_2)/2}{S}. \end{aligned} \quad (2.46)$$

The current  $j$  given by Eq. (2.45) is a pure drift current, i.e., in a homogeneous system, there is no field-induced carrier diffusion in the drift-diffusion regime. Hence, the equilibrium density  $n(x)$  given by Eq. (2.20) must be constant across the sample. As the chemical potential  $\mu(x)$  given by Eq. (2.46) runs parallel to potential energy profile  $E_c(x)$  given by Eq. (2.41), this requirement is indeed fulfilled here.

### 2.1.4 Range of Validity

The drift-diffusion model is based on the assumption of a continuously varying equilibrium chemical potential  $\mu(x)$ , which implies that the sample length is covered by points of local thermodynamic equilibrium that lie arbitrarily dense. Then, strictly speaking, the mean free path  $l$  must be confined to arbitrarily small values. On the other hand,  $l$  (or the mobility  $\nu$ ) must be finite and large enough to give rise to a non-vanishing conductivity of a magnitude in the range of typical experimental values, which calls for a relaxation of the former condition.

To obtain a practical criterion for the range of validity of the drift-diffusion model, one may require  $l$  to be so small that the effective number of points of local thermodynamic equilibrium along the length of the sample is so large that the spatial variations in the potential energy profile  $E_c(x)$ , and hence in the electron density  $n(x)$ , are “resolved” with sufficient accuracy. In terms of a local,  $x$ -dependent mean free path  $l(x)$ , this requirement may be expressed as

$$l(x) \ll \Delta x, \quad (2.47)$$

where  $\Delta x$  is the length of an interval, centered at the point  $x$ , over which the relative variation of  $E_c(x)$  is very small compared to unity, i.e.,

$$\frac{1}{E_c(x)} \left| \frac{dE_c(x)}{dx} \right| \Delta x \ll 1. \quad (2.48)$$

For constant mean free path  $l$ , one may fulfill the above requirement in an overall way by adopting the condition

$$\frac{l}{\tilde{S}} \ll 1. \quad (2.49)$$

The effective sample length  $\tilde{S}$  defined by the integral (2.37) tends to decrease exponentially when rapid variations in  $E_c(x)$  are “switched on”. Condition (2.49) tightens condition (2.14) so as to permit the “resolution” of the details of the profile  $E_c(x)$ .

## 2.2 Ballistic (Thermionic) Transport

In contrast to the drift-diffusion model, in which the points of local thermodynamic equilibrium are assumed to lie arbitrarily dense, the ballistic (thermionic) transport model presupposes the complete absence of such points inside the sample. Then, the electrons in the sample perform a collision-free *ballistic motion* in the field associated with the potential energy profile  $E_c(x)$ . Without thermal equilibration, it is meaningless to speak of a local chemical potential. Only at the sample ends at  $x_{1,2}$ , the electrons are forced into equilibrium, with densities

$$n(x_{1,2}) = N_c e^{-\beta[E_c(x_{1,2}) - \mu_{1,2}]} \quad (2.50)$$

determined by the boundary values of the potential energy profile,  $E_c(x_{1,2})$ , and by the chemical potentials  $\mu_{1,2}$  in the contacts. Here, the mean free path  $l$ , which has been of central importance in Drude's model and in the drift-diffusion model, is effectively of infinite length and does not appear in the formalism of the ballistic model. Hence, roughly speaking, one may use the condition

$$\frac{l}{S} \gg 1 \quad (2.51)$$

to delimit the range of validity of the ballistic model.

### 2.2.1 Nondegenerate Case

In the ballistic model, the end-points  $x_{1,2}$  of the sample are fixed points of local thermodynamic equilibrium with chemical potentials  $\mu(x_{1,2}) = \mu_{1,2}$ , out of which thermal electron currents are symmetrically emitted towards the left and right, so that only *one half* of each of these currents are emitted towards the inner region of the sample.

#### 2.2.1.1 Emitted Currents

For a nondegenerate system, the classical *electron current*  $J^l(x_1)$  emitted at the left end-point  $x_1$  towards the right, say, is expressed, in extension of Eq. (2.15) for the electron density  $n(x)$ , in the form

$$\begin{aligned} J^l(x_1) &= 4\pi \left(\frac{m^*}{h}\right)^3 \int_0^\infty dv_x v_x \int_0^\infty dw w f^{MB}(E(v; x_1) - \mu_1) \\ &= \frac{4\pi m^{*2}}{\beta h^3} \int_0^\infty dv_x v_x f^{MB}(E(v_x; x_1) - \mu_1) \end{aligned} \quad (2.52)$$

[here and in the following, we use the symbol  $J$  to denote any electron current density (current, for short), as opposed to  $j$  used for the charge current density]. Using Eq. (2.50), we then find

$$J^l(x_1) = v_e N_c e^{-\beta[E_c(x_1) - \mu_1]} = v_e n(x_1), \quad (2.53)$$

where

$$v_e = \left( \frac{m^* \beta}{2\pi} \right)^{1/2} \int_0^\infty dv_x v_x f^{MB}(m^* v_x^2/2) = \left( \frac{1}{2\pi m^* \beta} \right)^{1/2} \quad (2.54)$$

is the *emission velocity*, which is actually equal to one half of the one-dimensional mean electron speed

$$u = \left( \frac{2}{\pi m^* \beta} \right)^{1/2}, \quad (2.55)$$

the three-dimensional analogue of which is given by Eq. (2.1).

### 2.2.1.2 Transmitted Currents

The electrons emitted at  $x_1$  with velocity component  $v_x^{(1)}$  move along ballistic trajectories, thereby conserving their total energy,

$$E(v_x; x) = E(v_x^{(1)}; x_1), \quad (2.56)$$

where  $x$  is any point *inside* the interval  $[x_1, x_2]$ . Therefore, although  $x$  is not a point of local thermodynamic equilibrium, we can associate with it an equilibrium energy distribution which is equal to that at  $x_1$ . Now, since only electrons with total energy larger than the overall maximum  $E_c^m(x_1, x_2)$  of  $E_c(x)$  [see Eq. (2.36)] are classically able to reach the right end-point of  $[x_1, x_2]$  at  $x_2$ , part of the current  $J^l(x_1)$  emitted at  $x_1$  will be reflected, and the electrons forming it are absorbed when they return to their origin at  $x_1$ . The other, transmitted part  $J^l(x_1, x_2; x)$ , called the (left) “ballistic current”, is absorbed into the contact connected to the sample at  $x_2$ . Modifying expression (2.52), we have for this part

$$J^l(x_1, x_2; x) = \frac{4\pi m^{*2}}{\beta h^3} \int_0^\infty dv_x v_x f^{MB}(E(v_x; x) - \mu_1) \times \Theta(E(v_x; x) - E_c^m(x_1, x_2)). \quad (2.57)$$

In the integration, the potential energy profile  $E_c(x)$  contained in the function  $E(v_x; x)$  drops out, and we obtain for the (left) ballistic current the expression

$$J^l(x_1, x_2) = v_e N_c e^{-\beta[E_c^m(x_1, x_2) - \mu_1]}, \quad (2.58)$$

which is independent of  $x$ , i.e., the ballistic current is conserved, as expected. The (right) ballistic current  $J^r(x_1, x_2)$  transmitted from the *right* end-point  $x_2$  of the interval  $[x_1, x_2]$  is given by

$$J^r(x_1, x_2) = -v_e N_c e^{-\beta[E_c^m(x_1, x_2) - \mu_2]}, \quad (2.59)$$

in analogy to Eq. (2.58).

The ballistic currents (2.58) and (2.59) bear a close analogy to the “thermionic emission current” associated with the evaporation of electrons from a heated metal (“Richardson effect”) [13–16]. In semiconductor physics, “thermionic emission” was introduced as a mechanism of carrier transport by Bethe [17, 18] in his treatment of electron transport across a Schottky barrier.

### 2.2.1.3 Ballistic Densities

Associated with the ballistic currents  $J^{l,r}(x_1, x_2)$  are the “ballistic densities”  $n^{l,r}(x_1, x_2; x)$  of the electrons making up the currents inside the ballistic interval  $[x_1, x_2]$ . These densities will turn out to be instrumental in establishing the spin-dependent thermoballistic scheme (see Sect. 4.2).

The density  $n^l(x_1, x_2; x)$  associated with the current  $J^l(x_1, x_2; x)$  of Eq. (2.57) is given by

$$\begin{aligned} n^l(x_1, x_2; x) &= \frac{4\pi m^{*2}}{\beta h^3} \int_0^\infty dv_x f^{MB}(E(v_x; x) - \mu_1) \\ &\quad \times \Theta(E(v_x; x) - E_c^m(x_1, x_2)), \end{aligned} \quad (2.60)$$

which is evaluated to yield

$$n^l(x_1, x_2; x) = \frac{N_c}{2} C^m(x_1, x_2; x) e^{-\beta[E_c^m(x_1, x_2) - \mu_1]}. \quad (2.61)$$

Here,

$$C^m(x_1, x_2; x) = e^{\beta[E_c^m(x_1, x_2) - E_c(x)]} \operatorname{erfc}(\{\beta[E_c^m(x_1, x_2) - E_c(x)]\}^{1/2}), \quad (2.62)$$

where the function

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty dz e^{-z^2} \quad (2.63)$$

is the complementary error function [19]. The ballistic density is position-dependent via the  $x$ -dependence of the function  $C^m(x_1, x_2; x)$ , i.e., of the potential energy profile  $E_c(x)$ . The ballistic density  $n^r(x_1, x_2; x)$  associated with the current  $J^r(x_1, x_2)$  is obtained by replacing  $\mu_1$  with  $\mu_2$  in expression (2.61).

The function  $C^m(x_1, x_2; x)$  determines the “ballistic velocities”

$$v^{l,r}(x_1, x_2; x) \equiv \frac{J^{l,r}(x_1, x_2)}{n^{l,r}(x_1, x_2; x)} = \pm \frac{2v_e}{C^m(x_1, x_2; x)}, \quad (2.64)$$

which have the same magnitude for the currents transmitted from the left and right. For constant potential energy profile, one has  $C^m(x_1, x_2; x) = 1$ , and the electrons move with speed  $2v_e$ , i.e., with the mean electron speed  $u$  given by Eq. (2.55). For position-dependent profiles, when  $C^m(x_1, x_2; x) < 1$ , the magnitude of the ballistic velocities is larger than  $u$ .

### 2.2.1.4 Net Currents and Joint Densities

The *net ballistic current*  $J(x_1, x_2)$  in the interval  $[x_1, x_2]$ ,

$$J(x_1, x_2) = J^l(x_1, x_2) + J^r(x_1, x_2) \equiv J \quad (2.65)$$

equals the (conserved) total current  $J$ , which we can express, using Eqs. (2.58) and (2.59), as

$$J = v_e N_c e^{-\beta E_c^m(x_1, x_2)} (e^{\beta \mu_1} - e^{\beta \mu_2}). \quad (2.66)$$

This can be rewritten, using Eqs. (2.35) and (2.50), in the form

$$J = v_e n(x_1) \bar{T}^l(x_1, x_2) (1 - e^{-\beta eV}). \quad (2.67)$$

Here,

$$\bar{T}^l(x_1, x_2) \equiv \beta \int_0^\infty d\epsilon e^{-\beta \epsilon} T(x_1, x_2; \epsilon + E_c(x_1)) = e^{-\beta E_b^l(x_1, x_2)}, \quad (2.68)$$

with  $E_b^l(x_1, x_2)$  given by Eq. (2.36), is the thermal average of the classical transmission probability

$$T(x_1, x_2; E) = \Theta(E - E_c^m(x_1, x_2)) \quad (2.69)$$

for electrons emitted at  $x_1$  with total energy  $E = \epsilon + E_c(x_1)$  to be transmitted to the point  $x_2$ . If, in particular, the potential energy profile is constant across the interval  $[x_1, x_2]$ , or if its maximum lies at the emission point  $x_1$  itself, then  $E_c^m(x_1, x_2) = E_c(x_1)$  in Eq. (2.36), and hence  $\bar{T}^l(x_1, x_2) = 1$ .

Relation (2.67) is the current-voltage characteristic of the (classical) ballistic transport model. In contrast to the characteristic (2.34) of the drift-diffusion model, which involves the mean free path  $l$  and the potential energy profile  $E_c(x)$  [via the effective sample length  $\tilde{S}$ ], the characteristic (2.67) is controlled by one “material parameter” only, *viz.*, the thermally averaged transmission probability  $\bar{T}^l(x_1, x_2)$ .

For the *joint ballistic density*  $n(x_1, x_2; x)$ ,

$$n(x_1, x_2; x) = n^l(x_1, x_2; x) + n^r(x_1, x_2; x), \quad (2.70)$$

we have

$$n(x_1, x_2; x) = \frac{N_c}{2} C^m(x_1, x_2; x) e^{-\beta E_c^m(x_1, x_2)} (e^{\beta \mu_1} + e^{\beta \mu_2}), \quad (2.71)$$

in analogy to expression (2.66) for the net ballistic current.

### 2.2.2 Electron Tunneling

The ballistic transport model is straightforwardly extended so as to include *electron tunneling* by replacing the classical transmission probability  $T(x_1, x_2; E)$  of Eq. (2.69) with the corresponding *quantal* probability  $\mathcal{T}(x_1, x_2; E)$ . The thermally averaged quantal transmission probability is then, in generalization of expression (2.68), given by

$$\bar{\mathcal{T}}(x_1, x_2) = \beta \int_0^\infty d\epsilon e^{-\beta \epsilon} \mathcal{T}(x_1, x_2; \epsilon + E_c^>(x_1, x_2)), \quad (2.72)$$

where

$$E_c^>(x_1, x_2) \equiv \max\{E_c(x_1), E_c(x_2)\}. \quad (2.73)$$

The probability  $\mathcal{T}(x_1, x_2; E)$  is obtained by solving the stationary Schrödinger equation with the potential energy function  $E_c(x)$ . [Owing to time reversal invariance, the probability for transmission from the left equals that for transmission from the right.] The integration in Eq. (2.72) starts at the total energy  $E_c^>(x_1, x_2)$ , so that scattering boundary conditions can be imposed on the wave function both in the ranges  $x \leq x_1$  and  $x \geq x_2$ .

In WKB approximation [20, 21], the transmission probability  $\mathcal{T}(x_1, x_2; E)$  to be used in Eq. (2.72) is composed of the classical (“over-barrier”) part  $T(x_1, x_2; E)$  given by Eq. (2.69) and the remaining quantal (“sub-barrier”) part  $\mathcal{T}_{sb}(x_1, x_2; E)$ ,

$$\mathcal{T}(x_1, x_2; E) = T(x_1, x_2; E) + \mathcal{T}_{sb}(x_1, x_2; E). \quad (2.74)$$

The sub-barrier contribution has the form

$$\mathcal{T}_{sb}(x_1, x_2; E) = \Theta(E_c^m(x_1, x_2) - E) P_c(x_1, x_2; E), \quad (2.75)$$

where

$$P_c(x_1, x_2; E) = \exp \left( -2 \int_{x_1}^{x_2} dx \kappa_c(x) \right), \quad (2.76)$$

with

$$\kappa_c(x) = \frac{1}{\hbar} \{2m^*[E_c(x) - E]\}^{1/2} \Theta(E_c(x) - E), \quad (2.77)$$

is the barrier penetration factor.

In writing  $\mathcal{T}_{sb}(x_1, x_2; E)$  in the form (2.75), we disregard resonance effects that may occur when  $E_c(x)$  exhibits two or more local maxima in the interval  $[x_1, x_2]$ , with a corresponding number of one or more minima in between. Then, when the energy  $E$  is located below the second-highest maximum and above the lowest minimum, there is at least one “valley” in  $E_c(x)$ , across which the electron motion is classically allowed, so that resonance formation due to quantum coherence becomes possible. In semiconductor physics, a concrete realization of this situation occurs in resonant tunneling in multiple-barrier quantum-well structures (see, e.g., Ref. [22]). For this case, the full WKB tunneling probability for double-barrier and triple-barrier structures, respectively, has been presented in Ref. [23].

From Eq. (2.74), we now find for the WKB form of the thermally averaged transmission probability  $\bar{\mathcal{T}}(x_1, x_2)$  of Eq. (2.72)

$$\bar{\mathcal{T}}(x_1, x_2) = \bar{\mathcal{T}}(x_1, x_2) + \bar{\mathcal{T}}_{sb}(x_1, x_2). \quad (2.78)$$

Here, we have

$$\bar{\mathcal{T}}(x_1, x_2) = e^{-\beta E_b(x_1, x_2)}, \quad (2.79)$$

with

$$E_b(x_1, x_2) = E_c^m(x_1, x_2) - E_c^>(x_1, x_2), \quad (2.80)$$

for the over-barrier contribution, and

$$\bar{\mathcal{T}}_{sb}(x_1, x_2) = \beta \int_0^\infty d\epsilon e^{-\beta\epsilon} P_c(x_1, x_2; \epsilon + E_c^>(x_1, x_2)) \Theta(E_b(x_1, x_2) - \epsilon) \quad (2.81)$$

for the sub-barrier contribution.

The thermally averaged quantal probability  $\bar{\mathcal{T}}^l(x_1, x_2)$  for transmission from the left end-point at  $x_1$  can be expressed in terms of  $\bar{\mathcal{T}}(x_1, x_2)$ , using Eqs. (2.36) and (2.80), as



$$\tilde{T}^l(x_1, x_2) = \tilde{T}(x_1, x_2)e^{-\beta[E_c^>(x_1, x_2) - E_c(x_1)]}. \quad (2.82)$$

In analogy to Eq. (2.67) for the classical case, we have

$$J = v_e n(x_1) \tilde{T}^l(x_1, x_2) (1 - e^{-\beta eV}) \quad (2.83)$$

for the current-voltage characteristic of tunneling-enhanced ballistic transport.

### 2.2.3 Degenerate Case

In the degenerate case, when the electron system obeys Fermi-Dirac statistics, we write the ballistic current  $J^l(x_1, x_2)$  in the form [see Eqs. (2.52) and (2.57) for the nondegenerate case]

$$\begin{aligned} J^l(x_1, x_2; x) &= 4\pi \left(\frac{m^*}{h}\right)^3 \int_0^\infty dv_x v_x \int_0^\infty dw w \\ &\times f^{FD}(E(v; x) - \mu_1) \Theta(E(v; x) - E_c^m(x_1, x_2)), \end{aligned} \quad (2.84)$$

where  $f^{FD}(E)$  is the Fermi-Dirac energy distribution function,

$$f^{FD}(E) = \frac{1}{1 + e^{\beta E}}. \quad (2.85)$$

Expression (2.84) for the current  $J^l(x_1, x_2; x)$  formally agrees with the expression for the current of evaporated electrons encountered in the degenerate treatment of the Richardson effect [15, 16]. Following the procedure of Ref. [15], we can reduce the threefold integration in Eq. (2.84) to a single integration over the kinetic energy  $\epsilon = m^* w^2/2$ , obtaining

$$J^l(x_1, x_2) = \frac{4\pi m^*}{\beta h^3} \int_0^\infty d\epsilon \ln(1 + e^{-\beta(\epsilon - \mu_1)}) \Theta(\epsilon - E_c^m(x_1, x_2)). \quad (2.86)$$

The ballistic current  $J^r(x_1, x_2)$  transmitted from the right end-point of the sample at  $x_2$  is the negative of expression (2.86), with  $\mu_2$  substituted for  $\mu_1$ . The total current  $J$  [see Eq. (2.65)] is thus obtained as

$$J = v_e N_c \beta \int_0^\infty d\epsilon [\ln(1 + e^{-\beta(\epsilon - \mu_1)}) - \ln(1 + e^{-\beta(\epsilon - \mu_2)})] \Theta(\epsilon - E_c^m(x_1, x_2)). \quad (2.87)$$

Here, we have expressed the factor preceding the integral in Eq. (2.86) in terms of the emission velocity,  $v_e$ , and the effective density of states,  $N_c$ , which are nondegenerate quantities given by Eqs. (2.21) and (2.54), respectively. Expression (2.87) for the total current  $J$  is the degenerate analogue to the nondegenerate current-voltage characteristic (2.66).

For low external electric fields (“low-field transport”) characterized by the condition

$$\epsilon S = \beta e V \ll 1 \quad (2.88)$$

[see Eq. (2.44)], we find, expanding the right-hand side of Eq. (2.87) to first order in  $\beta e V$ ,

$$\begin{aligned} J &= v_e N_c \beta e V \left[ \frac{\partial}{\partial \mu} \int_0^\infty d\epsilon \ln(1 + e^{-\beta(\epsilon - \mu)}) \Theta(\epsilon - E_c^m(x_1, x_2)) \right]_{\mu=\mu_1} \\ &= v_e N_c \beta e V \ln(1 + e^{-\beta[E_c^m(x_1, x_2) - \mu_1]}), \end{aligned} \quad (2.89)$$

where we have used Eq. (2.35). For the conductance per unit area in the ballistic transport model, we now have

$$g \equiv \frac{eJ}{V} \bigg|_{V \rightarrow 0} = \beta e^2 v_e N_c \ln(1 + e^{-\beta[E_c^m(x_1, x_2) - \mu_1]}). \quad (2.90)$$

In highly doped, degenerate semiconductors, we may have

$$E_c^m(x_1, x_2) - \mu_1 < 0 \quad (2.91)$$

(see, e.g., Ref. [24], where grain-boundary-limited transport in polycrystalline materials is considered). Then, if

$$\beta[\mu_1 - E_c^m(x_1, x_2)] \gg 1, \quad (2.92)$$

we find from Eq. (2.90)

$$g = \beta^2 e^2 v_e N_c [\mu_1 - E_c^m(x_1, x_2)], \quad (2.93)$$

which equals the conductance of a ballistic point contact [25, 26].

### 2.2.4 Interface Resistances and Chemical Potential

In closing this section, we note that the ballistic transport model does not provide information on where the resistance causing the voltage drop is located along the sample. Evidently, it cannot be inside the collision-free sample. In the quantal

description of ballistic electron transport in mesoscopic systems as formulated by Landauer [27–31], the resistance is made up solely of the *interface resistances* arising from the abrupt change in the density of states (“transverse modes”) that the electrons encounter when they move across the interfaces separating the contacts (with infinitely many modes) from the sample (with a few modes only). The voltage drop is located, therefore, in the immediate vicinity of the interfaces, so that, when a chemical potential is introduced *ad hoc*, this must be constant inside the sample and discontinuous at the interfaces. Prior to the work of Landauer, the importance of interface resistances in ballistic transport had been emphasized by Sharvin [25].

Anticipating the later development, we remark at this juncture that in the thermoballistic approach, i.e., for arbitrary, *finite* magnitude of the mean free path, the (local) chemical potential is a constitutive element of the transport mechanism; it is defined, and can be explicitly calculated, all along a semiconducting sample. This potential has discontinuities at the contact-sample interfaces, whose magnitude increases from near-zero in the small- $l$ , drift-diffusion regime to the Sharvin value in the large- $l$ , ballistic regime. For more details, see Sect. 5.2.4.

## References

1. P. Drude, Ann. Phys. (Leipzig) **306**, 566 (1900) [reprinted in *Ostwalds Klassiker der Exakten Wissenschaften*, vol. 298, ed. by H.T. Grahn and D. Hoffmann (Verlag Harri Deutsch, Frankfurt/M., 2006)]
2. P. Drude, Ann. Phys. (Leipzig) **308**, 369 (1900)
3. N.W. Ashcroft, N.D. Mermin, *Solid State Physics* (Harcourt Brace College Publishers, Fort Worth, 1976)
4. B. Sapoval, C. Hermann, *Physics of Semiconductors* (Springer, Berlin, 1995)
5. H.A. Lorentz, *The Theory of Electrons and its Applications to the Phenomena of Light and Radiant Heat* (Columbia University Press, New York, 1909)
6. K.W. Böer, *Survey of Semiconductor Physics: Electrons and Other Particles in Bulk Semiconductors* (Van Nostrand Reinhold, New York, 1990)
7. K.W. Böer, *Introduction to Space Charge Effects in Semiconductors*. Springer Series in Solid-State Sciences, vol. 160 (Springer, Berlin, 2010)
8. C. Wagner, Z. Phys. Chem. B **21**, 25 (1933)
9. J. Frenkel, Phys. Z. Sowjetunion **8**, 185 (1935)
10. J. Bardeen, in *Handbook of Physics*, 2nd edn., ed. by E.U. Condon, H. Odishaw (McGraw-Hill, New York, 1967), Part 8, Chap. 4
11. C. Jacoboni, *Theory of Electron Transport in Semiconductors*. Springer Series in Solid-State Sciences, vol. 165 (Springer, Berlin, 2010)
12. J. Fabian, A. Matos-Abiague, C. Ertler, P. Stano, I. Žutić, Acta Phys. Slovaca **57**, 565 (2007)
13. O.W. Richardson, Phil. Trans. R. Soc. (Lond.) **201**, 497 (1903)
14. O.W. Richardson, *Thermionic Phenomena and the Laws which Govern Them*, Nobel Lecture, 12 Dec 1929 (The Nobel Foundation, Stockholm, 1929)
15. A. Sommerfeld, Z. Phys. **47**, 1 (1928)
16. A. Sommerfeld, H. Bethe, *Elektronentheorie der Metalle*, in *Handbuch der Physik*, vol. 24/2, 2nd edn., ed. by H. Geiger, K. Scheel (Springer, Berlin, 1933) [reprinted in *Heidelberger Taschenbücher*, vol. 19 (Springer, Berlin, 1967)]
17. H.A. Bethe, MIT Radiat. Lab. Report **43–12** (1942) [reprinted in *Semiconductor Devices: Pioneering Papers*, ed. by S. M. Sze (World Scientific, Singapore, 1991), p. 387]

18. S.M. Sze, *Physics of Semiconductor Devices* (Wiley, New York, 1981)
19. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York, 1965), Chap. 7
20. L.I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), Chap. 8.34
21. C.B. Duke, *Tunneling in Solids*, in *Solid State Physics Supplements*, ed. by F. Seitz, D. Turnbull, H. Ehrenreich, vol. 10 (Academic Press, New York, 1969)
22. L.L. Chang, E.E. Méndez, C. Tejedor (eds.), *Resonant Tunneling in Semiconductors: Physics and Applications*. NATO ASI Series: Series B, vol. 277 (Plenum Press, New York, 1991)
23. J.M. Xu, V.V. Malov, L.V. Iogansen, *Phys. Rev. B* **47**, 7253 (1993)
24. M.W.J. Prins, K.-O. Grosse-Holz, J.F.M. Cillessen, L.F. Feiner, *J. Appl. Phys.* **83**, 888 (1998)
25. Yu.V. Sharvin, *Zh. Eksp. Teor. Fiz.* **48**, 984 (1965) [*Sov. Phys. JETP* **21**, 655 (1965)]
26. C.W.J. Beenakker, H. van Houten, in *Solid State Physics*, vol. 44, ed. by H. Ehrenreich, D. Turnbull (Academic Press, Boston, 1991), p. 1
27. R. Landauer, *Z. Phys. B: Condens. Matter* **68**, 217 (1987)
28. R. Landauer, *J. Phys.: Condens. Matter* **1**, 8099 (1989)
29. S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995)
30. Y. Imry, R. Landauer, *Rev. Mod. Phys.* **71**, S306 (1999)
31. Yu.V. Nazarov, Ya.M. Blanter, *Quantum Transport: Introduction to Nanoscience* (Cambridge University Press, Cambridge, 2009)

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