The thermoballistic approach to charge carrier transport in semiconductors

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A comprehensive survey is given of the thermoballistic approach to charge carrier transport in semiconductors. This semiclassical approach bridges the gap between the drift-diffusion and ballistic (“thermionic”) models of carrier transport, whose validity is limited to the range of very small and very large values, respectively, of the carrier mean free path. The physical concept underlying the thermoballistic approach, while incorporating basic features of the drift-diffusion and ballistic descriptions, constitutes a novel, unifying scheme. It is based on the introduction of “ballistic configurations” defined by a random partitioning of the length of a semiconducting sample into ballistic transport intervals. The points linking adjacent ballistic intervals are assumed to be points of local thermodynamic equilibrium characterized by a local chemical potential. Carriers thermally emitted at any such point are ballistically transmitted across either interval, while at the same time carriers transmitted from the equilibrium points next to it are “absorbed” at that point, i.e., they are assumed to be instantaneously equilibrated there. During their transmission, the carriers face, in general, potential energy barriers arising from internal and external electrostatic potentials in the sample. The lengths of the ballistic intervals are stochastic variables, with associated probabilities given by the probabilities for carriers to traverse an interval without collisions with the scattering centers randomly distributed over the sample. These probabilities are controlled by the carrier mean free path, whose magnitude is arbitrary. By averaging the ballistic carrier currents over all ballistic configurations, a position-dependent thermoballistic current is derived, which is the key element of the thermoballistic concept and forms the point of departure for the calculation of various transport properties.

The present article starts out with a preparatory account of the standard drift-diffusion and ballistic transport models which form the cornerstones of the thermoballistic concept, and of a prototype model which paves the way for the fully developed form of that concept. In the main body of the article, a coherent exposition of the thermoballistic approach is given within a general formulation that takes into account arbitrarily shaped, spin-split potential energy profiles and spin relaxation during the carrier motion across ballistic intervals. The calculational procedures devised for implementing the thermoballistic concept are described. Specific examples relevant to present-day semiconductor and spintronics research are considered.

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I. INTRODUCTION

The phenomenon of electric conduction in metals and semiconductors has been a prominent research topic ever since the early days of solid-state physics. The idea that electric currents flowing inside solid materials are effected by the transport of “small” charged particles (“charge carriers”) was first conceived by Weber. Following the discovery of the electron by Thomson, Weber’s idea quickly found its concrete expression in attempts to understand electric (as well as thermal) conduction in solids as a manifestation of electron transport.

The basic concept for a theoretical treatment of conduction in terms of the motion of individual carriers was outlined by Riecke. Relying to some extent on this concept, Drude formulated his celebrated transport model, which subsequently was refined by Lorentz. In Drude’s model, the atomistic picture of matter and the kinetic theory of gases are combined to describe conduction in terms of a homogeneous gas of non-interacting, mobile charge carriers in thermodynamic equilibrium, which are assumed to move against a background of spatially fixed, heavy atoms. When an external electric field is applied, the interplay of field-induced acceleration and subsequent thermalizing collisions with the heavy atoms gives rise to a “drift current” of the carriers. The magnitude of this current is determined by the “mean free path”, i.e., the average distance the carriers travel between two collisions. For the drift current to be a valid concept, the mean free path must be very small as compared with typical dimensions of the sample. While originally conceived to describe carrier transport in metals, Drude’s model later on has been frequently used in qualitative, or semi-quantitative, analyses of transport properties of semiconductors as well.

To overcome the shortcomings of Drude’s model in the quantitative description of carrier transport in semiconductors, particularly in inhomogeneously doped systems, the drift current was supplemented with a diffusion current, whereby Drude’s model has been extended to the “drift-diffusion model” of transport. The latter model, while representing a substantial improvement over Drude’s model and serving as a benchmark of semiclassical transport theories even in modern times, is again valid in the range of very small carrier mean free paths only. In the opposite case of very large mean free paths, carrier transport in semiconductors can be described in terms of the ballistic (“thermionic”) model, in which carriers thermally emitted at the ends of a sample are assumed to traverse it without collisions with the background atoms.

Until recently, no systematic attempts had been made to bridge the gap between the limiting cases of the drift-diffusion and ballistic descriptions within a unified approach. In view of this situation, we set out to develop the “thermoballistic approach” to carrier transport in semiconductors. Apart from perceiving the challenge to fill a long-standing gap in the theory of carrier transport in semiconductors, we found that recent progress in device physics, spintronics, and photovoltaics called for an extension of the theoretical framework hitherto available for analyzing experimental data in these fields.

The physical concept underlying the thermoballistic approach rests on a random partitioning of the length of a semiconducting sample into “ballistic transport intervals”. Here, “random” implies (i) an arbitrary number of intervals and (ii) arbitrary positions of the end-points, and thus arbitrary lengths, of the intervals. The drift-diffusion model may be viewed as implying a partitioning of the sample length into infinitesimally short bal-
listic intervals; in the ballistic transport model, on the other hand, the sample length constitutes a single ballistic interval. An individual partition defines what we call a “ballistic configuration”. The points linking adjacent intervals in a ballistic configuration are assumed to be points of local thermodynamic equilibrium characterized by a local chemical potential. Any such point acts both as a source of, and a sink for, carriers. That is, on the one hand, carriers are thermally emitted there, with a velocity distribution determined by the local temperature; subsequent to their emission, the carriers are ballistically transmitted across either interval to the left and right, facing, in general, potential energy barriers arising from the internal and external potentials inside the sample. On the other hand, carriers emitted at the two equilibrium points neighboring the point under consideration on either side and transmitted to it are “absorbed” there, i.e., they return to thermodynamic equilibrium instantaneously. This equilibration is assumed to result from collisions of the carriers with spatially fixed scattering centers (“impurities”) randomly distributed over the sample, a view adopted from Drude’s transport model.

In the manner by which the ballistic intervals have been introduced, the lengths of these intervals are stochastic variables, with associated probabilities given by the probabilities for carriers to traverse an interval without impurity scattering. These probabilities are governed by the carrier mean free path, which is allowed to have arbitrary magnitude. By averaging the (in general, spin-dependent) carrier currents in the individual ballistic intervals over all ballistic configurations, a position-dependent total (i.e., spin-summed) thermoballistic current as well as a thermoballistic spin-polarized current are derived. These currents, in conjunction with the associated ballistic densities, represent the key elements of the thermoballistic approach. They form the point of departure for the calculation of the spin-resolved equilibrium chemical potentials. From the latter functions, in turn, transport quantities, like the current-voltage characteristic, the magnetoresistance, and (position-dependent) current and density spin polarizations, are obtained in terms of the potential energy profile, the mean free path, the ballistic spin relaxation length, and other parameters characterizing the sample.

The present article is devoted to a comprehensive exposition of the physical concept underlying the thermoballistic approach and its detailed implementation. We begin by describing a prototype model of thermoballistic transport (the “prototype model”, for short). This model introduces averaging over ballistic configurations as the constitutive element of the thermoballistic concept. It is based on the simplifying assumption that the carrier current is conserved across the points of local thermodynamic equilibrium linking the ballistic transport intervals. This assumption allows the derivation of an explicit, transparent expression for the current-voltage characteristic, as well as the construction of a local chemical potential in a heuristic form. After describing the prototype model, we present a general formulation of the thermoballistic concept proper, which makes use of a local chemical potential as the essential dynamical quantity, and takes into account arbitrarily shaped, spin-split potential energy profiles as well as spin relaxation during ballistic carrier motion.

Throughout this article, the formulation deviates in many respects from that in our original publications. Apart from correcting flaws and inconsistencies, we introduce modifications and extensions of the formalism that make it more transparent and more comprehensible. Aiming at a self-contained, unified presentation, we will develop the elements of the thermoballistic concept in considerable detail. This includes a recollection of early attempts to describe charge carrier transport in semiconductors and, at one place or another, the coherent recapitulation of background material which otherwise can be found only scattered over textbooks.

While the thermoballistic approach, in its most general form, would allow a consistent treatment of three-dimensional, bipolar carrier transport in semiconducting systems, we confine ourselves here to the case of one-dimensional, unipolar transport throughout. To be specific, we consider electron transport in the conduction band of n-doped systems, with the understanding that all results for hole transport in the valence band of p-doped systems can be obtained by transcribing the results for electron transport in an obvious way. In implementing the thermoballistic approach, we aim at carrying the development to the point where we obtain explicit equations from which the relevant physical quantities can be calculated. We do not enter here into applications requiring numerical calculations. Pertinent results presented in our previous publications will be briefly mentioned at various places in this article.

The organization of this article is as follows. In the next section, we present an account of Drude’s transport model and the standard drift-diffusion and ballistic models. In Sec. III, we begin with an outline of the probabilistic approach to carrier transport, which is prerequisite to the formulation of the thermoballistic model. This is followed by the description of the prototype model. In Sec. IV, the thermoballistic concept proper is developed at length, where particular emphasis is placed on the inclusion of spin degrees of freedom. The spin-resolved ballistic currents and associated densities are introduced in terms of an “average chemical potential” and a “spin accumulation function” connected with the splitting of the spin-resolved chemical potentials. Total and spin-polarized thermoballistic currents and densities are constructed by averaging the corresponding ballistic quantities over the ballistic configurations, and are evaluated in the drift-diffusion regime and in the ballistic limit. Energy dissipation (“heat production”) is analyzed within the thermoballistic approach. In Sec. IV, in particular, a synopsis of the thermoballistic concept is presented, with emphasis on its physical content as well as its merits and weaknesses. The procedures devised for the im-
plementation of the thermoballistic concept, i.e., for the explicit calculation of the average chemical potential and of the spin accumulation function as functions of intrinsic and external physical parameters, are described in Sec. VII. Expressions are derived for the current and density spin polarizations and the magnetoresistance in terms of the values of the spin accumulation function at the boundaries of a semiconducting sample. As specific examples of current interest in semiconductor and spintronics research, we treat spin-polarized transport in heterostructures formed of a nonmagnetic semiconductor and two ferromagnetic contacts, and spin-polarized transport in heterostructures involving diluted magnetic semiconductors in their paramagnetic phase. Finally, in Sec. VII we summarize the contents of this article and give an outlook towards future developments.

II. DRIFT-DIFFUSION AND BALLISTIC TRANSPORT

As the thermoballistic approach is devised to bridge the gap between the drift-diffusion and ballistic descriptions of transport, we survey, in this section, the standard formulations of these two limiting cases.

A. 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 article.

1. Drude’s model

In the transport model of Drude, 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 $E$. 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

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

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 paper \cite{Drude} 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.\cite{Lorentz}]

Defining the mean free path (or momentum relaxation length) $l$ as the average distance (measured along the transport direction) travelled 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 $E$. On average, they acquire a velocity, the drift velocity $v_{dr}$, given by the acceleration $-eE/m^*$ times their average time-of-flight across the ballistic intervals, i.e., times the collision time $\tau$,

$$v_{dr} = -\frac{eE}{m^*} \equiv -\nu E, \quad (2.3)$$

where

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

is the electron mobility.

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

$$j \equiv j_{dr} = -env_{dr} = envE, \quad (2.5)$$

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

$$\sigma = en\nu, \quad (2.6)$$

the current $j$ is expressed as

$$j = \sigma E, \quad (2.7)$$

i.e., in the form of Ohm’s law.

The transport mechanism in Drude’s model can be elucidated\cite{Drude} by noting that Eq. (2.3), when written as

$$-eE - \frac{m^*}{\tau} v_{dr} = 0, \quad (2.8)$$
states that the effect of the external force $-eE$ is balanced, on average, by that of a friction force $-\gamma \mathbf{v}_{dr}$, with the friction coefficient $\gamma$ given by

$$\gamma = \frac{m^*}{\tau} = \frac{e}{\nu}.$$  

(2.9)

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

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 so 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,

$$|\mathbf{v}_{dr}| \ll u.$$  

(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 $E$,

$$|E| \ll \frac{8}{\pi \beta e l}. $$  

(2.11)

For a homogeneous sample of length $S$ subjected to an external voltage bias $V$, when $|E| = |V|/S$, one has

$$|V| \ll \frac{8S}{\pi \beta e l}. $$  

(2.12)

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

$$\frac{l}{S} \ll \frac{8}{\pi \beta e |V|}. $$  

(2.13)

For room temperature, i.e., $1/\beta \approx 0.025$ eV, and values of $|V|$ 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

$$\frac{l}{S} \ll 1 $$  

(2.14)

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

2. Drift-diffusion model

Electron transport in inhomogeneous semiconductors is outside of the scope of Drude’s model. The nonuniformity 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. Throughout this article, 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 Sec. IV D). Further, the temperature $T$ is assumed to be constant across the sample.

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

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

(2.15)

Here, $\hbar$ 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

$$v = (v_x^2 + v_y^2 + v_z^2)^{1/2}, $$  

(2.16)

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

$$f_{MB}(E) = e^{-\beta E} $$  

(2.17)

is the Maxwell-Boltzmann energy distribution function, and

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

(2.18)

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

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

(2.19)

The potential energy profile $E_c(x)$ 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,

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

(2.20)

where

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

(2.21)

is the effective density of states at the conduction band edge. 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 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

\[
j = j_{dr}(x) + j_{di}(x).
\]  
(2.22)

The generalized drift current is obtained from expression (2.27) by replacing (i) the conductivity \(\sigma\) with the local conductivity \(\sigma(x)\) given by Eq. (2.18), with \(n(x)\) in lieu of \(n\), and (ii) the constant external electric field \(E\) with the field \((dE_c(x)/dx)/e\) associated with the potential energy profile \(E_c(x)\), so that one obtains

\[
j_{dr}(x) = \frac{1}{e \sigma(x)} dE_c(x),
\]  
(2.23)

The diffusion current is written as

\[
j_{di}(x) = eD \frac{dn(x)}{dx},
\]  
(2.24)

where \(D\) is the diffusion coefficient, which is related to the electron mobility \(\nu\) via the Einstein relation

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

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

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

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

\[
\sigma(x) = e \nu n(x) = \beta e^2 Dn(x).
\]  
(2.27)

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

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

which is the standard drift-diffusion expression 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. 21 In Ref. 22, the expression is derived within a time-dependent tutorial treatment of diffusion in the presence of an external electric field (“biased-random-walk model”).

Substituting expression (2.23) for the equilibrium density \(n(x)\) in Eq. (2.28), we obtain the current \(j\) in the form

\[
j = \frac{1}{e \sigma(x)} d\mu(x),
\]  
(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

\[
\frac{\beta j}{\nu N_c} e^{\beta \mu(x)} = \frac{d}{dx} e^{\beta \mu(x)}.
\]  
(2.30)

Considering a sample extending from \(x_1\) to \(x_2\) and integrating Eq. (2.30) over the interval \([x_1, x_2]\), we can express the local chemical potential \(\mu(x)\) in the form

\[
e^{\beta \mu(x)} = e^{\beta \mu(x_1)} + \frac{\beta j}{\nu N_c} \int_{x_1}^{x_2} dx' e^{\beta E_c(x')}.
\]  
(2.31)

An equivalent representation of \(\mu(x)\) is obtained by integrating Eq. (2.30) over the interval \([x, x_2]\), Now, setting \(x = x_2\) in Eq. (2.31), 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,

\[
\mu(x_1, 2) = \mu_{1,2},
\]  
(2.32)

and solving the resulting equation for the current \(j\), we then obtain, using Eq. (2.29), the current-voltage characteristic of the drift-diffusion model in the form

\[
j = -n(x_1)e^{-\beta E_c(x_1, 2)} \frac{\nu}{\beta S} (1 - e^{-\beta eV}).
\]  
(2.33)

Here,

\[
V = \frac{\mu_1 - \mu_2}{e}
\]  
(2.34)

is the voltage bias, and

\[
E_c^0(x_1, 2) \equiv E_c^0(x_1, 2) - E_c(x_1) \geq 0
\]  
(2.35)

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 \(E_c^0(x_1, 2)\) is the overall maximum of \(E_c(x)\) in the interval \([x_1, x_2]\). Finally, the quantity

\[
\hat{S} \equiv \int_{x_1}^{x_2} dx e^{-\beta E_c^0(x_1, 2) - E_c(x)}
\]  
(2.36)

is the “effective sample length”. It has the appealing property of becoming equal to the sample length \(S = x_2 - x_1\) for a flat profile, i.e., if \(E_c(x) = \text{const.}\), and otherwise satisfies \(\hat{S} < S\). Writing the current-voltage characteristic in the particular form (2.33) facilitates comparison with analogous expressions given below.

Expression (2.33) shows that the current-voltage characteristic of the drift-diffusion model is controlled (i) by the “barrier factor” \(e^{-\beta E_c^0(x_1, 2)}\), which involves the overall maximum of the profile \(E_c(x)\), and (ii) by the ratio \(\nu/\beta\) or, owing to Eq. (2.26), by the ratio \(\nu/\hat{S}\), 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 \(e^{-\beta E_c^0(x_1, 2)}\) re-appears as the thermally averaged probability for electron transmission from \(x_1\) to \(x_2\); see Eq. (2.57) below.]
The drift-diffusion model is based on the assumption of a continuously varying equilibrium chemical potential \( \mu(x) \), which implies that the points of local thermodynamic equilibrium 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

\[
l(x) \ll \Delta x, \tag{2.37}
\]

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.,

\[
\frac{1}{E_c(x)} \frac{dE_c(x)}{dx} | \Delta x \ll 1. \tag{2.38}
\]

For constant mean free path \( l \), one may fulfil the above requirement in an overall way by adopting the condition

\[
\frac{l}{S} \ll 1. \tag{2.39}
\]

The effective sample length \( S \) defined by the integral \( \frac{1}{S} \) tends to decrease exponentially when strong variations in \( E_c(x) \) are “switched on”. Condition (2.39) tightens condition (2.14) so as to permit the “resolution” of the details of the profile \( E_c(x) \).

B. 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 \( E_c(x) \). 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

\[
n(x_{1,2}) = N_e e^{-\beta[E_c(x_{1,2})-\mu_{1,2}]} \tag{2.40}
\]

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. Roughly speaking, one may use the condition

\[
\frac{l}{S} \gg 1 \tag{2.41}
\]

to delimit the range of validity of the ballistic model.

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.

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 the electron density \( n(x) \) given by Eq. (2.12), in the form

\[
J^l(x_1) = 4 \pi \left( \frac{m^*}{\hbar} \right)^3 \int_0^\infty dv_x v_x \int_0^{\infty} dw \times f^{MB}(E(v_x; x_1) - \mu_1) \tag{2.42}
\]

\[
= \frac{4 \pi m^*}{\beta \hbar^3} \int_0^{\infty} dv_x v_x f^{MB}(E(v_x; x_1) - \mu_1),
\]

from which we find, using Eq. (2.40),

\[
J^l(x_1) = v_e N_e e^{-\beta[E_c(x_1) - \mu_1]} = v_e n(x_1) \tag{2.43}
\]

Here,

\[
v_e = \left( \frac{m^* \beta}{2 \pi} \right)^{1/2} \int_0^{\infty} dv_x v_x f^{MB}(m^* v_x^2/2) = \left( \frac{1}{2 \pi m^* \beta} \right)^{1/2}, \tag{2.44}
\]

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

\[
u = \left( \frac{2}{\pi m^* \beta} \right)^{1/2}, \tag{2.45}
\]

the three-dimensional analogue of which is given by Eq. (2.14).

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

\[
E(v_x; x) = E'(v_x^{(1)}; x_1), \tag{2.46}
\]

where \( x \) is any point inside the interval \( [x_1, x_2] \) (and is not a point of local thermodynamic equilibrium). The
energy distribution at \( x \) is therefore equal to that at \( x_1 \). However, only electrons with total energy larger than the overall maximum \( E^m(x_1, x_2) \) of \( E_c(x) \) [see Eq. (2.43)] are classically able to reach the right end-point of \([x_1, x_2]\) at \( x_2 \). Thus, 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 (2.42), we have for this part

\[
J^l(x_1, x_2; x) = \frac{4\pi m^2}{\beta h^3} \int_0^\infty dv_x v_x f^{MB}(E(v_x; x) - \mu_1) \times \Theta(E(v_x; x) - E^m(x_1, x_2)).
\]  
(2.47)

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 \( x \)-independent expression

\[
J^l(x_1, x_2) = v_c N_e e^{-\beta [E^m(x_1, x_2) - \mu_1]},
\]  
(2.48)

i.e., the ballistic current is conserved (independent of \( x \)), 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

\[
J^r(x_1, x_2) = -v_c N_e e^{-\beta [E^m(x_1, x_2) - \mu_2]},
\]  
(2.49)
in analogy to Eq. (2.48).

The ballistic currents (2.48) and (2.49) bear a close analogy to the “thermionic emission current” associated with the evaporation of electrons from a heated metal (“Richardson effect”). In semiconductor physics, “thermionic emission” was introduced as a mechanism of carrier transport by Bethe in his treatment of electron transport across a Schottky barrier.

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 Sec. IV.B).

The density \( n^l(x_1, x_2; x) \) associated with the current \( J^l(x_1, x_2; x) \) of Eq. (2.47) is given by

\[
n^l(x_1, x_2; x) = \frac{4\pi m^2}{\beta h^3} \int_0^\infty dv_x v_x f^{MB}(E(v_x; x) - \mu_1) \times \Theta(E(v_x; x) - E^m(x_1, x_2)).
\]  
(2.50)

which is evaluated to yield

\[
n^l(x_1, x_2; x) = \frac{N_e}{2} C^m(x_1, x_2; x) e^{-\beta [E^m(x_1, x_2) - \mu_1]}.
\]  
(2.51)

Here,

\[
C^m(x_1, x_2; x) = e^{\beta [E^m(x_1, x_2) - E_c(x)]} \times \text{erfc} \left( \frac{\beta [E^m(x_1, x_2) - E_c(x)]}{\beta} \right)^{1/2},
\]  
(2.52)

where the function \( \text{erfc}(x) \) is the complementary error function. 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 \( n^l(x_1, x_2; x) \) associated with the current \( J^l(x_1, x_2) \) is obtained by replacing \( \mu_1 \) with \( \mu_2 \) in expression (2.51).

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

\[
v^{l,r}(x_1, x_2; x) = \frac{J^{l,r}(x_1, x_2)}{n^{l,r}(x_1, x_2; x)} = \pm \frac{2v_c}{C^m(x_1, x_2; x)},
\]  
(2.53)

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 \( 2v_c \), i.e., with the mean electron speed \( \bar{u} \) given by Eq. (2.45). For position-dependent profiles, when \( C^m(x_1, x_2; x) < 1 \), the magnitude of the ballistic velocities is larger than \( u \).

The \textit{net ballistic current} \( J(x_1, x_2) \) in the interval \([x_1, x_2]\),

\[
J(x_1, x_2) = J^l(x_1, x_2) + J^r(x_1, x_2) = J
\]  
(2.54)
equals the (conserved) total current \( J \), which we can express, using Eqs. (2.48) and (2.49), as

\[
J = v_c N_e e^{-\beta E^m(x_1, x_2)} (e^{\beta \mu_1} - e^{\beta \mu_2}).
\]  
(2.55)

This can be rewritten, using Eqs. (2.34) and (2.30), in the form

\[
J = v_c n(x_1) \tilde{T}^l(x_1, x_2)(1 - e^{-\beta \mathbf{v} \cdot \mathbf{v}}).
\]  
(2.56)

Here,

\[
\tilde{T}^l(x_1, x_2) = \beta \int_0^\infty d\mathbf{e} e^{-\beta \mathbf{e} \cdot \mathbf{v}} T(x_1, x_2; \mathbf{e} + E_c(x_1)) = e^{-\beta E^l_1(x_1, x_2)}.
\]  
(2.57)

with \( E^l_1(x_1, x_2) \) given by Eq. (2.55), is the thermal average of the classical transmission probability

\[
T(x_1, x_2; E) = \Theta(E - E^c_1(x_1, x_2))
\]  
(2.58)

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 \( E^c_1(x_1, x_2) = E_c(x_1) \) in Eq. (2.55), and hence \( \tilde{T}^l(x_1, x_2) = 1 \).
Relation (2.56) is the current-voltage characteristic of the (classical) ballistic transport model. In contrast to the characteristic (2.33) 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 \( S \)], the characteristic (2.58) is controlled by one “material parameter” only, viz., the thermally averaged transmission probability \( \bar{T}(x_1, x_2) \).

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

\[
n(x_1, x_2; x) = n^l(x_1, x_2; x) + n^r(x_1, x_2; x),
\]

(2.59)

we have

\[
n(x_1, x_2; x) = \frac{N e^{N E_c^m(x_1, x_2)}}{2} \times (e^{\beta \mu_1} + e^{\beta \mu_2}),
\]

(2.60)
in analogy to expression (2.56) for the net ballistic current.

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. (2.58) with the corresponding quantal probability \( \bar{T}(x_1, x_2; E) \). The thermally averaged quantal transmission probability is then, in generalization of expression (2.57), given by

\[
\bar{T}(x_1, x_2) = \beta \int_0^\infty dx \tau(x_1, x_2; \epsilon + E_c > (x_1, x_2)),
\]

(2.61)

where

\[
E_c^\tau(x_1, x_2) = \max\{E_c(x_1), E_c(x_2)\}.
\]

(2.62)
The probability \( T(x_1, x_2; E) \) 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. (2.61) starts at the total energy \( E_c^\tau(x_1, x_2) \), so that scattering boundary conditions can be imposed on the wavefunction both in the ranges \( x \leq x_1 \) and \( x \geq x_2 \).

In WKB approximation (2.58), the transmission probability \( T(x_1, x_2; E) \) to be used in Eq. (2.61) is composed of the classical (“over-barrier”) part \( T(x_1, x_2; E) \) given by Eq. (2.58) and the remaining quantal (“sub-barrier”) part \( T_{sb}(x_1, x_2; E) \),

\[
T(x_1, x_2; E) = T(x_1, x_2; E) + T_{sb}(x_1, x_2; E),
\]

(2.63)
The sub-barrier contribution has the form

\[
T_{sb}(x_1, x_2; E) = \Theta(E_c^m(x_1, x_2) - E) P_c(x_1, x_2; E),
\]

(2.64)

where

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

(2.65)

with

\[
\kappa_c(x) = \frac{1}{\hbar} \left\{2m^*|E_c(x)| - E\right\}^{1/2} \Theta(E_c(x) - E),
\]

(2.66)
is the barrier penetration factor.

In writing \( T_{sb}(x_1, x_2; E) \) in the form (2.64), 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. For this case, the full WKB tunneling probability for double-barrier and triple-barrier structures, respectively, has been presented in Ref. 25.

From Eq. (2.61), we now find for the WKB form of the thermally averaged transmission probability \( \bar{T}(x_1, x_2) \) of Eq. (2.61)

\[
\bar{T}(x_1, x_2) = \bar{T}(x_1, x_2) + \bar{T}_{sb}(x_1, x_2).
\]

(2.67)

Here, we have

\[
\bar{T}(x_1, x_2) = e^{-\beta E_b(x_1, x_2)},
\]

(2.68)

with

\[
E_b(x_1, x_2) = E_c^m(x_1, x_2) - E_c^\tau(x_1, x_2),
\]

(2.69)

for the over-barrier contribution, and

\[
\bar{T}_{sb}(x_1, x_2) = \beta \int_0^\infty dx \tau(x_1, x_2; \epsilon + E_c^\tau(x_1, x_2)) \times \Theta(E_b(x_1, x_2) - \epsilon)
\]

(2.70)

for the sub-barrier contribution.

The thermally averaged quantal probability \( \bar{T}(x_1, x_2) \) for transmission from the left end-point at \( x_1 \) can be expressed in terms of \( \bar{T}(x_1, x_2) \), using Eqs. (2.33) and (2.69), as

\[
\bar{T}(x_1, x_2) = \bar{T}(x_1, x_2) e^{-\beta [E_c^\tau(x_1, x_2) - E_c(x_1)]}.
\]

(2.71)

In analogy to Eq. (2.58) for the classical case, we have

\[
J = v_c n(x_1) \bar{T}(x_1, x_2) (1 - e^{-\beta \epsilon V})
\]

(2.72)
for the current-voltage characteristic of tunneling-enhanced ballistic transport.
3. Degenerate case

In the degenerate case, when the electron system obeys Fermi-Dirac statistics, we write the ballistic current \( J'_{(x_1, x_2)} \) in the form [see Eqs. (2.42) and (2.77) for the nondegenerate case]

\[
J'_{(x_1, x_2; x)} = 4\pi \left( \frac{m^*}{\hbar} \right)^3 \int_0^\infty dv_x v_x \int_0^\infty dw w \times f^{FD} \left( E(v; x) - \mu \right) \times \Theta \left( E(v; x) - E_c^m(x_1, x_2) \right),
\]

(2.73)

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

\[
f^{FD} \equiv \frac{1}{1 + e^{\beta E}}.
\]

(2.74)

Expression (2.73) for the current \( J'_{(x_1, x_2; x)} \) formally agrees with the expression for the current of evaporated electrons encountered in the degenerate treatment of the Richardson effect. Then, following the procedure of Ref. [11], we can reduce the threefold integration in Eq. (2.73) to a single integration over the kinetic energy \( \epsilon = m^*v^2 / 2 \), obtaining

\[
J'_{(x_1, x_2)} = \frac{4\pi m^*}{\beta \hbar^3} \int_0^\infty d\epsilon \ln \left( 1 + e^{-\beta (\epsilon - \mu_1)} \right) \times \Theta (\epsilon - E_c^m(x_1, x_2)).
\]

(2.75)

The ballistic current \( J'_{(x_1, x_2)} \) transmitted from the right end-point of the sample at \( x_2 \) is the negative of expression (2.75), with \( \mu_2 \) substituted for \( \mu_1 \). The total current \( J \) [see Eq. (2.54)] is thus obtained as

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

(2.76)

Here, we have expressed the factor preceding the integral in Eq. (2.76) in terms of the emission velocity, \( v_e \), and the effective density of states, \( N_c \), which are nondegenerate quantities given by Eqs. (2.44) and (2.21), respectively. Expression (2.76) for the total current \( J \) is the degeneracy analogue to the nondegenerate current-voltage characteristic (2.55).

For zero bias, the chemical potentials at the sample ends, \( \mu_1 \) and \( \mu_2 \), differ only by an infinitesimal \( \delta \),

\[
\mu_2 = \mu_1 - \delta.
\]

(2.77)

Then, expanding the right-hand side of Eq. (2.76) to first order in \( \delta \), we find

\[
J = v_e N_c \beta \delta \\
\times \left[ \frac{\partial}{\partial \mu} \int_0^\infty d\epsilon \ln \left( 1 + e^{-\beta (\epsilon - \mu)} \right) \Theta (\epsilon - E_c^m(x_1, x_2)) \right]_{\mu=\mu_1} \\
= v_e N_c \beta \delta \ln \left( 1 + e^{-\beta [E_c^m(x_1, x_2) - \mu_1]} \right).
\]

(2.78)

Setting \( \delta \equiv \mu_1 - \mu_2 = eV \), we now have for the zero-bias conductance per unit area in the ballistic transport model

\[
g = \left( eJ \over V \right)_{V \rightarrow 0} \equiv \beta e^2 v_e N_c \ln \left( 1 + e^{-\beta [E_c^m(x_1, x_2) - \mu_1]} \right).
\]

(2.79)

In highly doped, degenerate semiconductors, we may have

\[
E_c^m(x_1, x_2) - \mu_1 < 0
\]

(2.80)

(see, e.g., Ref. [29], where grain-boundary-limited transport in polycrystalline materials is considered). Then, if

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

(2.81)

we find from Eq. (2.79)

\[
g \approx \beta^2 e^2 v_e N_c \left[ \mu_1 - E_c^m(x_1, x_2) \right],
\]

(2.82)

which equals the conductance of a ballistic point contact.

In closing this subsection, 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,[32,33] 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.[30]

Anticipating the later development, we remark at this point that in the thermoballistic approach, i.e., for finite magnitude of the mean free path, the (local) equilibrium 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 Sec. V B 3.

III. PROTOTYPE THERMOBALLISTIC MODEL

In the drift-diffusion and ballistic transport models, the parameter of central importance is the electron mean...
free path \( l \) or, equivalently, the collision time \( \tau \) originally introduced in Drude’s model. The collision time represents the average time-of-flight that elapses between successive electron collisions with the randomly distributed scattering centers in the sample. The drift-diffusion and ballistic transport mechanisms are limiting cases associated with very small and very large (effectively, infinite) collision times, respectively. In the present section, we proceed to the “prototype thermoballistic model” which represents an attempt to unify the drift-diffusion and ballistic models within a stationary (time-independent) description in which the mean free path is not limited in magnitude and enters as a parameter that controls collision probabilities. [In our original paper, we have called this model the “generalized Drude model”; the new name appears to give a better description of its features.] We begin this section by introducing the probabilistic definition of \( l \) (or \( \tau \)).

A. Probabilistic approach to carrier transport

In the time-dependent probabilistic approach, one introduces the probability \( 1/\tau \) that an electron undergoes a collision, i.e., is equilibrated with its surroundings, within unit time. That is, \( dt/\tau \) is the probability for the collision to occur within an infinitesimally short time interval \( dt \). Then, assuming the collision time \( \tau \) to be constant, the probability \( p(t) \) that an electron moves without collision over a finite time interval \( t \) is given
defined by

\[
p(t) = e^{-t/\tau}, \tag{3.1}
\]
and the conditional probability \( P(t)dt \) that an electron undergoes a collision within the time interval \( dt \) after a collision-free flight over a time interval \( t \), by

\[
P(t)dt = p(t) \frac{dt}{\tau}. \tag{3.2}
\]

The mean time-of-flight between successive collisions now becomes

\[
\bar{\tau} \equiv \int_0^\infty dt P(t) = \tau. \tag{3.3}
\]

Identifying \( \bar{\tau} \) with the collision time \( \tau \) of the Drude model, one sees that the inverse of this quantity is just equal to the collision probability per unit time, \( 1/\tau \), of the probabilistic approach.

We recall that the term “collision” used here is that proffered by Drude, meaning a collision leading to instantaneous, complete equilibration of the momentum of an electron with its surroundings. In that picture, \( \tau \) is the average time of collision-free flight between points of equilibration, hence the appellation. However, \( 1/\tau \) is, more generally, the probability for a complete equilibration to occur in unit time; this may happen as a consequence of a “complete collision” (in the Drude sense) after the average time \( \tau \), or by “incomplete collisions” (leading to incomplete equilibration) in a sequence of shorter collision times, which add up, on average, to the time \( \tau \).

Within the time-dependent probabilistic picture, one can set up an expression for the net electron current \( J(x, t) \) at position \( x \) and time \( t \), which embodies features that are relevant for devising the thermoballistic concept (see Sec. IV C 1). Assuming a sample with position-dependent electron density \( n(x) \), one writes

\[
J(x, t) = J^l(x, t) + J^r(x, t). \tag{3.4}
\]

Considering for the moment electrons with arbitrary, constant velocity \( v_x \), the currents \( J^{l,r}(x, t) \) are expressed, using Eqs. (3.1) and (3.2), as

\[
J^{l,r}(x, t) = \pm v_x \int_{-\infty}^t \frac{dt'}{\tau} e^{-(t-t')/\tau} n(x \mp v_x(t-t')). \tag{3.5}
\]

The contributions to these currents for fixed time \( t \) arise from electrons that are transmitted, subsequent to their emission at the points \( x \equiv x \mp v_x(t-t') \) lying to the left (right) of the point \( x \), without collision from \( x_- \) (\( x_+ \)) to the point \( x \). The intervals \( [x_-, x] \) and \( [x, x_+] \) define “ballistic intervals”; the currents transmitted across these intervals contribute to the total current with weight \( e^{-(t-t')/\tau} \). Note that, in contrast to the situation considered above, where ballistic motion occurs before equilibration in the time interval \( dt \) (with probability \( dt/\tau \)), here the ballistic motion occurs after the electrons have been equilibrated in the time interval \( dt' \) (with probability \( dt'/\tau \)).

When the collision time \( \tau \) is sufficiently small, such that \( v_x\tau \) is much smaller than the average length over which the density \( n(x) \) changes appreciably, one has, by expanding in expressions (3.5) \( n(x) \) to first order,

\[
J(x, t) = -2v_x^2 \frac{dn(x)}{dx} \int_{-\infty}^t \frac{dt'}{\tau} e^{-(t-t')/\tau}(t-t') = -2v_x^2 \frac{dn(x)}{dx} \equiv J(x). \tag{3.6}
\]

Taking into account that only electrons with \( v_x \geq 0 \) (\( v_x < 0 \)) contribute to the current arriving at the point \( x \) from the left (right), thermal averaging of \( v_x^2 \) now yields

\[
\langle v_x^2 \rangle = \frac{1}{2m^*\beta}, \tag{3.7}
\]
so that one obtains the local expression

\[
J(x) = -\frac{\tau}{m^*\beta} \frac{dn(x)}{dx} \tag{3.8}
\]

for the thermally averaged electron current. The charge current \( -eJ(x) \) is then found, in view of expression (2.24) for the diffusion coefficient \( D \), to agree with relation (2.24) for the diffusion (charge) current \( j_d(x) \) of the drift-diffusion model. This result may thus be regarded as a proof of the Einstein relation (2.25).
When $\tau \to \infty$, only electrons emitted at the left and right end, respectively, of the sample contribute to the currents $J_{l,r}(x,t)$. Then, the (thermally averaged) net electron current $J(x,t)$ essentially reduces to the ballistic current given by expression (2.55). In the intermediate regime, i.e., for nonzero, finite values of $\tau$, $J(x,t)$ combines elements of both drift-diffusion and ballistic transport.

In analogy to the time-dependent probability $p(t)$ given by Eq. (3.1), one can introduce the probability $p(x)$ for an electron to travel without collision over a finite distance $x$,

$$p(x) = e^{-x/l},$$

with a constant electron mean free path $l$. The conditional probability for an electron to undergo a collision in the infinitesimal collision interval $dx$ after a collision-free flight over the distance $x$ reads

$$P(x)dx = p(x)\frac{dx}{l}.$$  

Then one finds

$$\bar{x} \equiv \int_0^\infty dx xP(x) = l$$

for the mean distance $\bar{x}$ between successive electron collisions.

In the following, the mean free path $l$ will be assumed to take on any finite value, while, as before, the collisions are assumed to lead instantaneously to a complete equilibration of the electron momenta, and are to be interpreted as a simulation of the real situation where the distances between successive collisions are short (of atomic dimensions), while the equilibration during a collision is (usually) far less than complete. The quantity $l$, in parallel to the collision time $\tau$, is simply to be regarded as a parameter which determines the probability (3.9) of collision-free (complete or not) traversal by an electron of the distance $x$.

It is noted here that when treating inhomogeneous systems, one should, strictly speaking, allow for a position dependence of the collision time, $\tau = \tau(x)$, and of the mean free path, $l = l(x)$. In that case, expressions (3.1) and (3.9) for the probabilities $p(t)$ and $p(x)$, respectively, must be replaced with the more general forms

$$p(t) = \exp \left( -\int_0^\infty \frac{dt'}{\tau(x(t'))} \right)$$

and

$$p(x) = \exp \left( -\int_0^\infty \frac{dx'}{l(x')} \right),$$

respectively. Then, of course, the relation $l = u\tau$ [see Eq. (2.2)] ceases to be valid.

---

**B. Prototype thermoballistic model: Concept and implementation**

The unification of the drift-diffusion and ballistic transport models within the prototype thermoballistic model\cite{12} is based on the introduction of configurations of ballistic transport intervals, which cover the length of the sample. The individual ballistic intervals in a configuration are linked by points of local thermodynamic equilibrium, and their lengths are stochastic variables occurring with probabilities determined by the probabilities for collision-free electron motion across the intervals, where the electron mean free path is allowed to have arbitrary magnitude. The electron current is, of course, conserved in each ballistic interval. In addition, it is assumed that the current is conserved also from one interval to the next. Averaging over the ballistic configurations then leads to a transparent and intuitively appealing expression for the current voltage-characteristic in terms of an effective transport length, in which the detailed shape of the potential energy profile is taken into account. Moreover, a local chemical potential can be constructed in a heuristic way.

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### 1. Ballistic configurations

Here, as well as in Sec. III B 2, we confine ourselves to (one-dimensional) classical transport in nondegenerate systems. The effects of tunneling and degeneracy will be considered in Secs. III B 3 and III B 4, respectively.

For given $N$ ($N = 1,\ldots,\infty$), the length $S$ of the sample is randomly partitioned into $N$ “ballistic intervals” labeled $i$ ($i = 1,\ldots,N$), in which the electrons move ballistically across the potential energy profile $E_c(x)$ [see Fig. 1]. These intervals are linked by points of local thermodynamic equilibrium $x_{i-1}^N$ and $x_i^N$ ($x_{i-1}^N < x_i^N$) which, in addition, include the two (true) equilibrium points at the interfaces with the left and right contacts at $x_0^N = 0$.
and \( x_i^N = S \), respectively. [In this section, in order to avoid confusion with the labeling of the equilibrium points inside, we denote the end-point coordinates of the sample by 0 and \( S \), instead of \( x_1 \) and \( x_2 \), as used elsewhere.] At \( x_i^N \), and electrons are thermally emitted towards the right and left, respectively, into the interval \([x_{i-1}^N, x_i^N]\). Any set

\[
\{x_j^N\} \equiv \{x_0^N, x_1^N, \ldots, x_j^N, \ldots, x_N^N\} \tag{3.14}
\]
of \( N + 1 \) equilibrium points linking \( N \) ballistic intervals characterizes a ballistic configuration.

Introducing an equilibrium chemical potential \( \mu(x) \) all across the sample, in terms of which the values \( \mu(x_i^N) \) and \( x_i^N \) are defined, the net ballistic current \( J^N(i) \equiv \int_{x_{i-1}^N}^{x_i^N} J \, dx \) transmitted across the interval \( i \) in a partition with \( N \) intervals is given, in analogy to expression (2.45) for the current in the ballistic transport model, by

\[
J^N(i) = v_e N_e e^{-\beta E^m_c(i)} [e^{\beta \mu(x_{i-1}^N)} - e^{\beta \mu(x_i^N)}], \tag{3.15}
\]

where

\[
E^m_c(i) \equiv E^m_c(x_{i-1}^N, x_i^N) \tag{3.16}
\]
denotes the absolute maximum of the potential energy profile \( E_c(x) \) in the interval \( i \). In terms of the (classical) thermally averaged transmission probability

\[
\bar{T}(i) = e^{-\beta [E^m_c(i) - E^\gamma_c(i)]} \tag{3.17}
\]
defined in analogy to expression (2.45), we can write \( J^N(i) \) in the form

\[
J^N(i) = v_e N_e \bar{T}(i) e^{-\beta E^\gamma_c(i)} [e^{\beta \mu(x_{i-1}^N)} - e^{\beta \mu(x_i^N)}], \tag{3.18}
\]
where

\[
E^\gamma_c(i) \equiv \max\{E_c(x_{i-1}^N), E_c(x_i^N)\}. \tag{3.19}
\]
The current \( J^N(i) \) is, of course, conserved across each interval \( i \).

In its general form, expression (3.18) obviously does not lend itself for the calculation of transport properties in terms of external physical quantities. Therefore, we make the simplifying assumption that the electron current is conserved also across the points of local thermodynamic equilibrium linking one ballistic interval to its adjacent intervals (and hence is constant all along the length of the sample), so that in Eq. (3.18)

\[
J^N(i) = J = \text{const.} \tag{3.20}
\]
for all \( i \) and \( N \), where \( J \) is the physical current. We can then iterate Eq. (3.18) with respect to \( i \) (for fixed \( N \)), with the result

\[
e^{\beta \mu^N(0)} - e^{\beta \mu^N(S)} = \frac{J}{v_e N_e} e^{\beta E^m_c(0,S)} Z^N. \tag{3.21}
\]

Here, \( E^m_c(0,S) \) denotes the overall maximum of the profile \( E_c(x) \) in the interval \([0,S]\), and the function \( Z^N \), defined as

\[
Z^N \equiv Z^N(\{x_j^N\}) = \sum_{i=1}^{N} \frac{1}{T(i)} e^{-\beta [E^m_c(0,S) - E^\gamma_c(i)]} \tag{3.22}
\]
can be formally viewed as the partition function corresponding to the “energy spectrum” \( \{E^m_c(0,S) - E^m_c(i)\} \). It depends on the equilibrium points \( x_j^N \) in the ballistic configuration \( \{x_j^N\} \) via Eq. (3.10).

2. Averaging over ballistic configurations

In order to arrive at results in terms of physical quantities, we must average Eq. (3.21) over the complete set of ballistic configurations \( \{x_j^N\} \) \((j = 0, 1, \ldots, N; N = 1, \ldots, \infty)\). In doing so, we identify the average of the left-hand side of Eq. (3.21) with the “bias term” \( e^{\beta \mu_0} - e^{\beta \mu_S} \), where \( \mu_0 \) and \( \mu_S \) are the values of the chemical potential at the contact side of the left and right semiconductor interface, respectively, and obtain

\[
e^{\beta \mu_0} - e^{\beta \mu_S} = \frac{J}{v_e N_e} e^{\beta E^m_c(0,S)} \bar{R}. \tag{3.23}
\]

Here,

\[
\bar{R} = \langle Z^N(\{x_j^N\}) \rangle \tag{3.24}
\]
denotes the average of the partition functions \( Z^N \) over all ballistic configurations \( \{x_j^N\} \). From Eq. (3.22), the current-voltage characteristic of the prototype thermoballistic model is now obtained in the general form

\[
J = v_e N_e e^{-\beta [E^m_c(0,S) - \mu_0]} \frac{1}{\bar{R}} (1 - e^{-\beta e V}), \tag{3.25}
\]
with the voltage bias \( V \) given by

\[
V = \frac{\mu_0 - \mu_S}{e}. \tag{3.26}
\]

Aside from the barrier factor involving the absolute maximum, \( E^m_c(0,S) \), of the potential energy profile, the current \( J \) is controlled here by the parameter \( \bar{R} \), which alone comprises the detailed dependence of the current-voltage characteristic on the shape of the profile and on the material parameters characterizing the sample. As it appears in Eq. (3.25), \( \bar{R} \) can be viewed as a (dimensionless) reduced resistance.

In the averaging process implied in Eq. (3.24), the contribution of each ballistic interval \( i \) in a partition with \( N \) intervals is to be weighted with the conditional probability \( P_i^N \, dx_i^N \) for an electron to make a collision in the infinitesimal interval \( dx_i^N \) after having traveled freely
across the interval \( i \) of length \( x_i^N - x_{i-1}^N \), into which it was emitted after a collision in the interval \( dx_{i-1}^N \). The collision probability is connected with the two ends of each ballistic interval, and the collision interval \( dx_i^N \) is the **equilibration interval** for the ballistic interval \( i \), but it is simultaneously the **emission interval** for the ballistic interval \( i + 1 \). This “sharing” of collision intervals \( dx_i^N \) between the ballistic intervals \( i \) and \( i + 1 \) implies that effectively the density of points of equilibration is only **half** of that given originally. Therefore, the conditional probability \( P_i^N dx_i^N \) is, in conformance with Eqs. 3.9 and 3.10, expressed as

\[
P_i^N dx_i^N = e^{-(x_i^N - x_{i-1}^N)/\ell} \frac{dx_i^N}{\ell}, \tag{3.27}
\]

with the **effective mean free path** \( \ell \) given by

\[
\ell = 2l. \tag{3.28}
\]

Here, the meaning of the mean free path \( l \) is the original one introduced within the Drake model.

The conditional probability \( dP^N \) for an electron emitted at \( x_0^N = 0 \) to undergo \( N - 1 \) collisions at the equilibrium points \( x_i^N (i = 1, \ldots, N-1) \), and finally be absorbed with unit probability at \( x_N^N = S \), is then found as

\[
dP^N = \prod_{i=1}^{N-1} \frac{dx_i^N}{\ell} e^{-(x_i^N - x_{i-1}^N)/\ell} \Theta(x_i^N - x_{i-1}^N) \times e^{-(S - x_N^N)/\ell} \tag{3.29}
\]

for \( N \geq 2 \), while

\[
dP^1 = e^{-S/\ell}. \tag{3.30}
\]

In the product in Eq. (3.29), the exponentials cancel out except for the factor \( e^{-S/\ell} \), so that

\[
dP^N = e^{-S/\ell} \prod_{i=1}^{N-1} \frac{dx_i^N}{\ell} \Theta(x_i^N - x_{i-1}^N) \tag{3.31}
\]

and

\[
\int_0^S \int_0^S dx_i^N \int_0^S dx_i^N \int_0^S dx_i^N = 1 \tag{3.32}
\]

[the symbol \( \int_0^S \) is meant to imply \( (N - 1) \)-fold integration over \( x_1^N, \ldots, x_{N-1}^N \) from 0 to \( S \)], i.e., the total probability is unity.

The reduced resistance \( \mathcal{R} \) defined by Eq. (3.24) can now be expressed as

\[
\mathcal{R} = \sum_{N=1}^{\infty} \int_0^S dP^N Z^N \equiv e^{-S/\ell} \sum_{N=1}^{\infty} O^N Z^N \{x_j^N\}, \tag{3.33}
\]

where the operators \( O^N \) acting on the partition functions \( Z^N \) are given by \( O^1 = 1 \) and

\[
O^N = \int_0^S \frac{dx_i^N}{\ell} \int_0^S \frac{dx_i^N}{\ell} \cdots \int_0^S \frac{dx_i^N}{\ell} \tag{3.34}
\]

for \( N \geq 2 \). It can be shown that, owing to the separable form of \( Z^N \) [see Eqs. (3.22) and (3.41)], the multi-dimensional integrals in Eq. (3.33) can always be reduced to one-dimensional and two-dimensional integrals. The remaining infinite series can be summed up in terms of exponentials. For the classical partition function \( Z^N \) of Eq. (3.22), the reduced resistance \( \mathcal{R} \) is thus obtained in the form

\[
\mathcal{R} = e^{-S/\ell} \frac{R(0, S)}{[e^{-S/\ell} \tilde{R}(0, x') + e^{-(S-x')/\ell} \tilde{R}(x', S)]}
+ \int_0^S \frac{dx'}{\ell} e^{-(S-x')/\ell} \tilde{R}(x', x'') \tag{3.35}
\]

where the (dimensionless) function \( \tilde{R}(x', x'') \) is given by

\[
\tilde{R}(x', x'') = \frac{1}{T(x', x'')} e^{-\beta[E_c^m(x') - E_c^m(x'')]} = e^{-\beta[E_c^m(x') - E_c^m(x'')]} \tag{3.36}
\]

Here, the thermally averaged classical transmission probability \( \tilde{T}(x', x'') \) is defined in analogy to Eqs. 2.66 and 3.17, \( E_c^m(x', x'') \equiv E_c^m(x', x') \) is the absolute maximum of the potential energy profile \( E_c(x) \) in the interval \( [x', x''] \), and

\[
E_c^m(x', x'') = \max\{E_c(x'), E_c(x'')\}. \tag{3.37}
\]

In general, we have

\[
\tilde{R}(x', x'') \leq 1 \tag{3.38}
\]

and, in particular, \( \tilde{R}(0, S) = 1 \).

For a flat potential energy profile, \( E_c(x) \equiv \text{const.} \), when \( \tilde{R}(x', x'') \equiv 1 \), expression (3.35) can be immediately evaluated with the result

\[
\mathcal{R} \equiv \mathcal{R}_0 = 1 + \frac{S}{\ell}, \tag{3.39}
\]

so that in the general case, owing to Eq. (3.38),

\[
\mathcal{R} \leq \mathcal{R}_0, \tag{3.40}
\]

i.e., \( \mathcal{R} \) decreases when a position-dependent potential energy profile is introduced. In the current-voltage characteristic (3.25), this decrease of \( \mathcal{R} \) is overcompensated by the effect of the barrier factor \( e^{-\beta[E_c^m(0,S)-\mu_0]} \), so that the current \( J \) decreases as well.

By reducing expression (3.35) for \( \mathcal{R} \) to the form (3.35), we have transcribed the prototype thermoballistic model,
which, according to its original concept, relies on a discrete partitioning of the sample length into ballistic intervals, into a pure continuum model. Expression (3.35) is composed of three contributions. The first corresponds to ballistic transport all across the sample length $S$, with associated probability $e^{-S/\ell}$. The second reflects the integrated effect of ballistic transport across intervals $[0, x']$ and $[x', S]$, respectively, with probabilities $e^{-x'/\ell}$ and $e^{-(S-x')/\ell}$. The third, finally, corresponds to the integrated effect of ballistic transport across intervals $[x', x'']$, with probabilities $e^{-(x''-x')/\ell}$.

The central task in implementing the prototype thermodballistic model is to evaluate the reduced resistance $R_{q}$ from Eq. (3.35) [or from the analogous equation derived from the quantal partition function (3.41)] for given potential energy profile $E_{c}(x)$. In general, the computation of $E_{c}(x)$ is accomplished (see, e.g., Ref. [21]) by solving, for given distribution of the space-fixed charges in the sample, a nonlinear Poisson equation.

### 3. Electron tunneling

In the ballistic transport model (see Sec. II B 2), we have taken into account the effect of electron tunneling by introducing quantal probabilities to describe electron transmission across the whole sample length. In the prototype model, we can include tunneling effects by using quantum transmission probabilities in expression (3.18) for the current $J_{N}(i)$ in the individual ballistic intervals $[x_{i-1}^{N}, x_{i}^{N}]$.

Replacing in Eq. (3.18) the probability $\tilde{T}(i)$ with the thermally averaged quantal transmission probability $\overline{T}(i) \equiv \overline{T}(x_{i-1}^{N}, x_{i}^{N})$ defined in analogy to expression (2.61), with $x_{1,2}$ replaced with $x_{i-1}^{N}, x_{i}^{N}$, the partition function $Z_{N}$ in Eq. (3.21) acquires the form

$$Z_{N}^{q} = \sum_{i=1}^{N} \frac{1}{\overline{T}(i)} e^{-\beta[E_{c}^{\mu_{\nu}}(0,S) - E_{c}^{\nu}(i)]},$$

where Eq. (3.17) for $\tilde{T}(i)$ has been used.

In generalization of expression (3.35), the reduced resistance $R_{q}$ including tunneling effects is obtained from the quantal partition function $Z_{N}^{q}$ as

$$R_{q} = e^{-S/\ell} \overline{R}(0, S) + \int_{0}^{S} \frac{dx'}{\ell} [e^{-(S-x')/\ell} \overline{R}(0, x') + e^{-(S-x')/\ell} \overline{R}(x', S)] + \int_{0}^{S} \frac{dx'}{\ell} \int_{x'}^{S} \frac{dx''}{\ell} e^{-(x''-x')/\ell} \overline{R}(x', x''),$$

where

$$\overline{R}(x', x'') = \frac{1}{\overline{T}(x', x'')} e^{-\beta[E_{c}^{\mu_{\nu}}(0,S) - E_{c}^{\nu}(x', x'')]}.$$  

Here, the thermally averaged quantal transmission probability $\overline{T}(x', x'')$ is defined in analogy to expression (2.61), and $\overline{R}(x', x'')$ is given by Eq. (3.30). In view of Eq. (3.38), the inequality (3.41) providing an upper limit on the values of the classical function $R$ holds also for the quantal function $R_{q}$.

We now adopt the WKB approximation, for which we have, using Eq. (2.67),

$$\overline{R}(x', x'') = \overline{R}(x', x'') + R_{sb}(x', x''),$$

with

$$\overline{R}_{sb}(x', x'') = -\frac{\overline{T}_{sb}(x', x'')}{\overline{T}(x', x'')} R(x', x'').$$

Inserting expression (3.44) in Eq. (3.42), we find that $R_{q}$ separates in the form

$$R_{q} = R_{cl} + R_{sb},$$

where the classical contribution $R_{cl}$ is given by Eq. (3.35), and the tunneling (sub-barrier) contribution $R_{sb}$ by Eq. (3.42), with $\overline{T}(x', x'')$ replaced with $\overline{T}_{sb}(x', x'')$. Evidently, $R_{sb} < 0$ and $|R_{sb}| < R_{cl}$.

According to its definition in analogy to Eq. (2.70), the thermally averaged sub-barrier transmission probability $\overline{T}_{sb}(x', x'')$ is nonzero only if the potential energy profile $E_{c}(x)$ exhibits at least one local maximum in the range $x' < x < x''$ such that $E_{b}(x', x'') > 0$. In the evaluation of the sub-barrier function $R_{sb}$, from Eq. (3.42), ballistic intervals for which $E_{c}(x)$ does not meet this requirement can, therefore, be excluded from the outset.

### 4. Degenerate case

Recalling the procedure developed in the nondegenerate case (see Secs. II B 1 and II B 2), in which expression (3.15) for the net ballistic current $J_{N}(i)$ forms the starting point of the derivation of the current-voltage characteristic (3.20), we find that an analogous procedure cannot be set up, in general, in the degenerate case. The reason is that for the argument leading to Eq. (3.25), $J_{N}(i)$ must factorize into a term depending on the potential energy profile $E_{c}(x)$, and terms depending on the chemical potential $\mu(x)$. In the degenerate case, the current analogous to $J_{N}(i)$ is the current $J(x_{1}, x_{2})$ given by Eqs. (2.54) and (2.70), with $x_{1}$ and $x_{2}$, respectively, replaced with $x_{i-1}^{N}$ and $x_{i}^{N}$. This current does not factorize if the bias is nonzero.

In the zero-bias case, however, the chemical potentials at the sample ends, $\mu(0)$ and $\mu(S)$, differ only infinitesimally, and the increment of $\mu(x)$ across a ballistic interval $i$,

$$\delta_{i} = \mu(x_{i-1}^{N}) - \mu(x_{i}^{N}),$$

(3.47)
is infinitesimally small as well. Then, we find in analogy to Eq. (2.78)
\[ J^N(i) = v_e N_c \beta \delta_i \times \left[ \frac{\partial}{\partial \mu} \int_0^\infty \! dc \ln(1 + e^{-\beta(c-\mu)}) \Theta(c - E^m_c(i)) \right]_{\mu = \mu(x^N_{i-1})} = v_e N_c \beta \delta_i \ln(1 + e^{-\beta[E^m_c(i)-\mu(0)]}), \]  
(3.48)
where we have replaced, in the second equation, \( \mu(x^N_{i-1}) \) with \( \mu(0) \).

Expression (3.48) has the factorization property alluded to above, so that, following the procedure leading to Eq. (3.24) in the nondegenerate case, we here find
\[ \beta[\mu(0) - \mu(S)] = \frac{J}{v_e N_c} \ln(1 + e^{-\beta[E^m_c(0,S)-\mu(0)]}) \],  
(3.49)
where the function
\[ Z_d^N = \sum_{i=1}^N \ln(1 + e^{-\beta[E^m_c(0,S)-\mu(0)]}) \]  
(3.50)
generals the partition function \( Z^N \) given by Eq. (3.22) to the degenerate case. Averaging Eq. (3.49) over the ballistic configurations \( \{x^N_i\} \) yields, in analogy to Eq. (3.23),
\[ \beta(\mu_0 - \mu_S) = \frac{J}{v_e N_c} \ln(1 + e^{-\beta[E^m_c(0,S)-\mu_0]}), \]  
(3.51)
where
\[ R_d = \langle Z^N (\{x^N_i\}) \rangle \]  
(3.52)
is the reduced resistance for the degenerate case.

5. Chemical potential

Within the prototype model, we can construct, in a heuristic way, a unique chemical potential \( \mu(x) \) all along the sample length by modifying relation (3.23) that connects the values of the chemical potential at the contact-semiconductor interfaces, \( \mu_0 \) and \( \mu_S \). We proceed as follows.

On the one hand, by replacing the fixed position \( S \) with a variable position \( x \) inside the sample, we turn \( \mu_S \) into a chemical-potential function \( \mu_1(x) \) and, simultaneously, reduce the range of averaging over the ballistic configurations in Eq. (3.24) for the reduced resistance \( R \) from \([0,S]\) to \([0,x]\). We then obtain
\[ e^{\beta \mu_1(x)} = e^{\beta \mu_0} - \frac{J}{v_e N_c} e^{\beta E^m_c(0,x)} R_1(x) \]  
(3.53)
(0 < \( x < S \)), where we have introduced the “resistance function” \( R_1(x) \) as
\[ R_1(x) = \langle Z^N (\{x^N_i\}) \rangle_{[0,x]}, \]  
(3.54)
which, in turn, can be expressed as
\[ R_1(x) = \frac{v_e N_c}{J} e^{-\beta E^m_c(0,x)}[e^{\beta \mu_0} - e^{\beta \mu_1(x)}]. \]  
(3.55)

On the other hand, by replacing in Eq. (3.23) the fixed position \( 0 \) with the variable \( x \), so that \( \mu_0 \) turns into a chemical-potential function \( \mu_2(x) \) and the range of averaging is reduced to \([x,S]\), we have
\[ e^{\beta \mu_2(x)} = e^{\beta \mu_S} + \frac{J}{v_e N_c} e^{\beta E^m_c(x,S)} R_2(x) \]  
(3.56)
(0 < \( x < S \)), with the resistance function \( R_2(x) \) defined by
\[ R_2(x) = \frac{J}{v_e N_c} e^{-\beta E^m_c(x,S)}[e^{\beta \mu_2(x)} - e^{\beta \mu_S}]. \]  
(3.57)
so that
\[ R_1(x) = R_2(0) = R. \]  
(3.59)

The resistance functions \( R_1(x) \) and \( R_2(x) \) are obtained in explicit form from expression (3.35) [or from expression (3.42), which includes tunneling effects] by transcribing it so as to correspond to samples with end-point coordinates \( 0, x \), and \( x, S \), respectively.

From the potentials \( \mu_1(x), \mu_2(x) \), we now construct a unique chemical potential \( \mu(x) \) by setting
\[ e^{\beta \mu(x)} = \frac{1}{2}[e^{\beta \mu_1(x)} + e^{\beta \mu_2(x)}] \]  
(3.60)
for 0 < \( x < S \), while
\[ \mu(0) = \mu_0, \, \mu(S) = \mu_S. \]  
(3.61)

Using Eqs. (3.53) and (3.56), along with Eq. (3.23) in Eq. (3.60), we obtain
\[ e^{\beta \mu(x)} = \frac{1}{2}(e^{\beta \mu_0} + e^{\beta \mu_S}) - \frac{R_-(x)}{2R}(e^{\beta \mu_0} - e^{\beta \mu_S}), \]  
(3.62)
where the function \( R_-(x) \) is defined as
\[ R_-(x) = e^{-\beta E^m_c(0,S)} \times [e^{\beta E^m_c(0,x)} R_1(x) - e^{\beta E^m_c(x,S)} R_2(x)]. \]  
(3.63)

With the resistance functions \( R_1, R_2(x) \) and the reduced resistance \( R \) calculated from Eq. (3.35) [or Eq. (3.42)], the equilibrium chemical potential in the prototype model can now be explicitly evaluated in terms of the potential energy profile \( E_c(x) \) and the momentum relaxation length \( l \).

A noteworthy feature of the chemical potential \( \mu(x) \) is the occurrence of discontinuities at \( x = 0 \) and \( x = S \).
Using Eqs. (3.23), (3.32), (3.36), and (3.59), we find from Eq. (3.62)
\[ e^{\beta[\mu(x)-\mu_0]} - 1 = -\frac{J}{2v_e N_c} e^{\beta[E_c(x)-\mu_0]} \]
for \( x = 0 \), and
\[ e^{\beta[\mu(x)-\mu_0]} - 1 = -\frac{J}{2v_e N_c} e^{\beta[E_c(x)-\mu_0]} \]
for \( x = S \).

In the fully thermoballistic approach (see Sec. V B 2 below), we will derive an expression for the average chemical potential which closely resembles expression (3.62), and which exhibits discontinuities analogous to those expressed by Eqs. (3.64) and (3.65), but relies on different assumptions.

C. Prototype thermoballistic model: Examples

The present subsection is devoted to the application of the prototype thermoballistic model to specific examples. With a view to inhomogeneous semiconductors and heterostructures, in which barriers in the potential energy profile arise, e.g., at heterojunctions, grain boundaries, and metal-semiconductor contacts (“Schottky barriers”), we deal with the evaluation of the reduced resistance \( R \) for profiles \( E_c(x) \) exhibiting an arbitrary number of barriers and interjacent valleys. As a prelude to the general case, we treat the cases of a single barrier and of two barriers enclosing a valley separately. Another example considered here is that of field-driven transport in inhomogeneous semiconductors, for which we evaluate the position dependence of the chemical potential.

1. Single potential energy barrier

Here, we consider the case of a single barrier in the profile \( E_c(x) \), with its maximum located at some position \( X \in [0, S] \) (see Fig. 1). Then, we have \( E_c^m(0, S) = E_c(X) \). If, in particular, \( X = 0 \) or \( X = S \), the profile is monotonic.

In the calculation of the corresponding reduced resistance \( R \) from expression (3.35), one must distinguish three cases. If the ballistic interval \([x', x'']\) contains \( X \), we have \( E''_c(x', x'') = E_c(X) \); if it lies to the left or right of \( X \), we have \( E''_c(x', x'') = E_c(x') \) or \( E''_c(x', x'') = E_c(x'') \), respectively. We then find
\[ R = 1 + \frac{S}{\ell} \]
where \( S \) is the effective sample length,
\[ S = \int_0^S dx e^{-\beta[E_c(X)-E_c(x)]}. \]

This expression is formally equal to the effective sample length \( 2.56 \) introduced in the context of the drift-diffusion model, but it differs in physical origin. While expression \( 3.67 \) results from averaging over ballistic configurations involving intervals of arbitrary, finite length, expression \( 2.56 \) arises from the assumption of arbitrarily short ballistic intervals, on which the drift-diffusion model is implicitly based.

In expression \( 3.69 \) for \( R \), the unit term corresponds to ballistic transmission all across the sample, governed by the barrier maximum at \( X \), while the effective sample length \( S \) represents the effect of the potential energy profile in an integral way. The (classical) current-voltage characteristic \( 3.25 \) for the case of a single potential energy barrier now reads
\[ J = v_e N_c e^{-\beta[E_c(X)-\mu_0]} \frac{\ell}{S} (1 - e^{-\beta eV}). \]

If the effective mean free path is much longer than the effective sample length, \( \ell \gg S \), the characteristic \( 3.69 \) reduces to that of the ballistic transport model, Eq. (2.56). In the opposite case, \( \ell \ll S \), using the relation
\[ \nu = 2\beta eV, l = \beta ev_e\ell \]
for the electron mobility \( \nu \) [see Eqs. (2.20) and (2.44)], the characteristic of the drift-diffusion model, Eq. (2.54), is retrieved. Expression \( 3.69 \) exemplifies the unification of the ballistic and drift-diffusion transport mechanisms in the prototype thermoballistic model.

We note that a heuristic attempt to unify drift-diffusion and ballistic transport has been made, for the special case of transport across a Schottky barrier, by Crowell and Sze38 (see also Ref. 23), who assumed ballistic transport to prevail in the vicinity of the barrier maximum, and drift-diffusion transport elsewhere. They obtained the expression for the current-voltage characteristic equivalent to \( 3.68 \),

\[ J = N_c e^{-\beta[E_c(X)-\mu_0]} \frac{v_e \nu_d}{v_e + \nu_d} (1 - e^{-\beta eV}), \]

where
\[ \nu_d = \frac{\nu}{\beta eS} = \frac{v_e \ell}{S} \]
is an effective diffusion velocity, with the electron mobility \( \nu \) given by Eq. (3.69). A picture similar to that of Ref. 37 has been developed and applied by Evans and Nelson37 in a study of transport across a single grain boundary barrier. Other studies elucidating the transition region between drift-diffusion and ballistic transport were presented by de Jong9 and Prins et al.9

Considering now, for the single barrier, the effect of electron tunneling, we obtain, following Sec. III B 3
\[ R_{sb} = e^{-S/\ell} R_{sb}(0, S) + \int_X^S \frac{dx}{\ell} e^{-x''/\ell} R_{sb}(0, x''). \]
\[
\begin{align*}
&\int_0^X \frac{dx'}{\ell} e^{-(S-x')/\ell} \mathcal{R}_{ab}(x', S) \\
&+ \int_0^X \frac{dx'}{\ell} \int_X^S \frac{dx''}{\ell} e^{-(x''-x')/\ell} \mathcal{R}_{ab}(x', x'')
\end{align*}
\]

(3.72)

for the sub-barrier part \(\mathcal{R}_{ab}\) of the reduced resistance \(\mathcal{R}\), while the classical part \(\mathcal{R}_{cl}\) is given by Eq. (3.66). Since \(|\mathcal{R}_{ab}(x', x'')| < 1\), we have from Eq. (3.72)

\[|\mathcal{R}_{ab}| < 1.\]  

(3.73)

Since \(E_m(x', x'') \equiv E_c(X)\), the transmission probabilities \(T(x', x'')\) and \(T_{ab}(x', x'')\), and consequently the function \(\mathcal{R}_{ab}(x', x'')\), depend on \(x'\) and \(x''\) only via the function \(E_c(x', x'')\) [see Eqs. (2.68) and (2.70)]. Then, \(\mathcal{R}_{ab}(x', x'')\) is a function of one coordinate only, determined by the potential energy profile \(E_c(x)\),

\[\mathcal{R}_{ab}(x', x'') \equiv \left\{ \mathcal{R}_{ab}(x') : E_c(x', x'') = E_c(x'), \right. \]

\[\left. \mathcal{R}_{ab}(x'') : E_c(x', x'') = E_c(x'') \right\}. \]  

(3.74)

As \(x''\) increases from \(X\) to \(S\), for fixed \(x' \in [0, X]\), \(\mathcal{R}_{ab}(x'')\) changes to \(\mathcal{R}_{ab}(x')\) when \(x'' = x'^*\) or, equivalently, \(x' = x''^*\); here, the “mirror point” \(x^*\) is defined as that position to the right (left) of a maximum or minimum of the potential energy profile where it has the same value as at the point \(x\) to the left (right), i.e.,

\[E_c(x^*) = E_c(x) \]  

(3.75)

(see Figs. 1 and 2). The double integral in expression (3.72) then reduces to two single integrals which, together with the single integrals preceding it, combine to just one single integral, so that \(\mathcal{R}_{ab}\) attains the simple form

\[\mathcal{R}_{ab} \equiv \mathcal{R}_{ab}(\ell) \]  

\[= e^{-\omega/\ell} \mathcal{R}_{ab}(0) + \int_0^{x^*} \frac{dx}{\ell} e^{-|x-x^*|/\ell} \mathcal{R}_{ab}(x). \]  

(3.76)

This expression bears a close formal similarity to the shape term appearing in the classical treatment of the double-barrier case [see Eq. (3.78) below].

2. Double barrier

Next, we consider a potential energy profile of the type shown in Fig. 2 exhibiting two barriers with maxima at \(x = X_0\) and \(x = X_1\), respectively (without loss of generality, the maximum at \(X_0\) is assumed to be the higher one), and a valley with minimum at \(x = Y_1\) in between.

In the evaluation of the reduced resistance \(\mathcal{R}\), a number of cases are to be distinguished when calculating the function \(E_m(x', x'')\) in dependence on the location of the ballistic interval \([x', x'']\) with respect to the different ranges delimited by the points \(x = 0, X_0, X_1, Y_1, X_1, \) and \(S\). From expression (3.56), we obtain

\[\mathcal{R} = 1 + \frac{S + \tilde{\Lambda}}{\ell}, \]  

(3.77)

where the effective sample length \(S\) is given by Eq. (3.67) with \(X = X_0\). The “shape term” \(\tilde{\Lambda}\) has the form

\[\tilde{\Lambda} \equiv \tilde{\Lambda}(\ell) = \int_{X_1^*}^{X_2} dx e^{-|x-x^*|/\ell} e^{-\beta E_c(x)} \times [e^{\beta E_c(x_1)} - e^{\beta E_c(x)}]. \]  

(3.78)

In writing \(\tilde{\Lambda}\) in this compact form, we have used the identity

\[1 - e^{-w_1/\ell} \equiv \int_{X_1^*}^{X_2} dx e^{-|x-x^*|/\ell}, \]  

(3.79)

where \(w_1 = X_1 - X_1^*\) is the width of the valley (see Fig. 2). The position of the minimum of the valley, \(Y_1\), enters \(\mathcal{R}\) implicitly via the shape of \(E_c(x)\) in the interval \([X_1^*, X_1]\). Comparing in Eq. (3.78) the magnitude of the integral involving the term \(e^{\beta E_c(x_1)}\) in the brackets to that of the integral involving \(e^{\beta E_c(x)}\), it is seen that for \(b_{01} \ll \ell \ll w_1\), where \(b_{01}\) are the widths of the two barriers centered about \(X_{01}\), the second integral can be neglected. Hence,

\[\mathcal{R} = 1 + \frac{S}{\ell} + e^{-\beta [E_c(x_0) - E_c(x_1)]}, \]  

(3.80)

i.e., the two barriers contribute independently to the reduced resistance (first and third term).

When \(\ell \gg S\) (ballistic limit), we have

\[\tilde{\Lambda} < w_1 e^{-\beta [E_c(x_0) - E_c(x_1)]} < S, \]  

(3.81)

so that both the terms \(S/\ell\) and \(\tilde{\Lambda}/\ell\) in Eq. (3.77) can be neglected. Then, \(\mathcal{R}\) reduces to the unit term, which reflects ballistic transmission across the higher barrier maximum at \(X_0\); this maximum “eclipses” the lower maximum at \(X_1\).
generalizes expression (3.78) to the case of $M$ most barrier of the different valleys. The contribution of valley $X_v$ maximum of the adjoining lower barrier located at $E_c(X_v)$ in $\tilde{S}$ and $\tilde{\Lambda}$ replaced with $E_c(X_m)$, where $X_m$ is the position of the maximum of the heighest barrier plus additional terms arising from the combined effect of barriers and valleys on the electron transport in the ballistic intervals.

Introducing now the effective transport length as

$$L \equiv R \ell,$$  

(3.83)

we have from Eqs. (3.39), (3.40), and (3.77)

$$L = \ell + \tilde{S} + \tilde{\Lambda}(\ell) \leq \ell + S.$$  

(3.84)

From Eqs. (3.29) and (3.38), we then obtain the current-voltage characteristic for a potential energy profile of the type depicted in Fig. 3 in the form

$$J = v_e N_e e^{-\beta[E_c(X_0) - \mu_0]} \frac{\ell}{L} \left(1 - e^{-\beta eV}\right).$$  

(3.85)

This expression is the principal result of the prototype thermoballistic model. It has been derived here in the framework of classical transport in nondegenerate systems, where its interpretation is most transparent.

The properties of the characteristic (3.85) are determined by the barrier factor $e^{-\beta[E_c(X_0) - \mu_0]}$ and by the ratio $\ell/L$. In the effective transport length $L$, the effective mean free path $\ell$ represents the ballistic contribution to the current, which is associated with the maximum $E_c(X_0)$ of the highest barrier in the potential energy profile. The remaining terms give a quantitative measure of the influence of that part of the electron motion which is not purely ballistic. Their contribution amounts to at most the sample length $S$. The effective sample length $\tilde{S}$ given by Eq. (3.67) with $X = X_0$ represents a contribution that characterizes the potential energy profile $E_c(x)$ in an integral way; it does not manifestly depend on $\ell$, only implicitly so via the profile (an indirect relationship between profile and mean free path arises from their common dependence on the donor density). The shape term $\tilde{\Lambda}$ given by Eq. (3.52), on the other hand, depends on the detailed structure of the profile as well as explicitly on the mean free path, and thus represents the interplay of ballistic and drift-diffusion transport. This term is a distinctive feature of expression (3.85), and therefore of the prototype thermoballistic model.

Tunneling effects in the current-voltage characteristic (3.85) can be taken into account by generalizing the effective transport length $L$ of Eq. (3.83) so as to include the sub-barrier contribution $R_{sb}$ to the reduced resistance. Using Eq. (3.40), we have

$$L_q \equiv R_q \ell = (R_{ct} + R_{sb}) \ell$$

$$= (1 - |R_{sb}(\ell)|) \ell + \tilde{S} + \tilde{\Lambda}(\ell).$$  

(3.86)

Here, as exemplified by expression (3.70) for the single-barrier case, $R_{sb}$ depends explicitly on the effective mean
free path $\ell$. From expression (3.86), the inclusion of tunneling is seen to lower the ballistic contribution to the effective transport length [see Eq. (3.89)]. This behavior is in line with the role of $R_\ell$ as a resistance, which ought to decrease when the barriers become “transparent” to ballistic electron transport.

The (classical) reduced resistance in the degenerate case, $R_d$ [see Eqs. (3.50) and (3.52)], is expressed, in analogy to Eqs. (3.83) and (3.84) for the nondegenerate case, in terms of a (classical) effective transport length $L_d$ given by

$$L_d = R_d \ell = \ell + \tilde{S}_d + \tilde{\Lambda}_d(\ell), \quad (3.87)$$

where, in generalization of Eq. (3.67),

$$\tilde{S}_d = \int_0^S dx \frac{\ln(1 + e^{-\beta [E_v(x_0) - \mu_0]})}{\ln(1 + e^{-\beta [E_v(x) - \mu_0]})} \quad (3.88)$$

is the effective sample length for the degenerate case, and

$$\tilde{\Lambda}_d \equiv \tilde{\Lambda}_d(l) = \sum_{v=1}^M \int_{x_v}^{x_{v+1}} dx e^{-[x - x_v]/\ell} \times \left\{ \frac{\ln(1 + e^{-\beta [E_v(x_0) - \mu_0]})}{\ln(1 + e^{-\beta [E_v(x) - \mu_0]})} - \frac{\ln(1 + e^{-\beta [E_v(x) - \mu_0]})}{\ln(1 + e^{-\beta [E_v(x) - \mu_0]})} \right\} \quad (3.89)$$

generalizes the shape term (3.82). The inclusion of tunneling effects is, in the degenerate case, a highly intricate task and will not be considered here.

Setting $\mu_0 - \mu_S = eV$ in Eq. (3.90), we now have for the zero-bias conductance per unit area in the prototype thermoballistic model

$$g \equiv \left< \frac{eJ}{V} \right>_{V \to 0} = \beta e^2 v_e N_c \ln(1 + e^{-\beta [E_v^0 - \mu_0]}) \frac{\ell}{L_d}, \quad (3.90)$$

in generalization of expression (3.79) for the conductance in the ballistic transport model.

Previously, we have applied the prototype model in calculations of transport properties of polycrystalline semiconducting materials, in particular, of materials relevant to photovoltaics. The occurrence of grain boundaries in this kind of materials gives rise to a multi-barrier structure of the band edge profile. Adopting the trapping model to describe the grain boundaries, we have solved the corresponding nonlinear Poisson equation to obtain zero-bias potential energy profiles for chains of grains. Then, taking into account tunneling corrections and using a phenomenological relation to express the momentum relaxation length $\ell$ in terms of the donor density, we have calculated zero-bias conductivities and electron mobilities as a function of $\ell$, and of the number and lengths of the grains. It turns out that neither the ballistic (thermionic) model nor the drift-diffusion model can provide an adequate description of electron transport in poly- and microcrystalline materials. The application of the prototype model in the analysis of experimental data has led to promising results.

4. Chemical potential for field-driven transport

The chemical potential $\mu(x)$ given by Eq. (3.62) can be expressed in closed form for the case of electron transport in a homogeneous semiconductor (no space charges), driven by a constant external electric field of magnitude $E$.

With the field assumed to be directed antiparallel to the $x$-axis, the corresponding potential energy profile reads

$$E_v(x) = E_v(0) - \frac{\epsilon}{\beta} x, \quad (3.91)$$

where $\epsilon = \beta e\xi$. Using this in the properly transcribed expression (3.35) [or, alternatively, in Eq. (3.66), considering the profile (3.91) a particular case of a barrier], we obtain the resistance functions $R_{1,2}(x)$ in the form

$$R_1(x) = 1 + \frac{1}{\epsilon \ell} (1 - e^{-\epsilon x}) \quad (3.92)$$

and

$$R_2(x) = 1 + \frac{1}{\epsilon \ell} (1 - e^{-\epsilon(S - x)}) \equiv R_1(S - x). \quad (3.93)$$

From Eq. (3.59), we then have

$$R = R_1(S) = 1 + \frac{1}{\epsilon \ell} (1 - e^{-\epsilon S}), \quad (3.94)$$

and from Eq. (3.63),

$$R_{-}(x) = R_1(x) - e^{-\epsilon x} R_2(x) = 1 - e^{-\epsilon x} + \frac{1}{\epsilon \ell} (1 - 2e^{-\epsilon x} + e^{-\epsilon S}). \quad (3.95)$$

Inserting expressions (3.94) and (3.95) in Eq. (3.92) gives $\mu(x)$ in closed form.

For zero bias, when $\epsilon x \leq \epsilon S \ll 1$, we have

$$R = 1 + \frac{S}{\ell}, \quad (3.96)$$

and

$$R_{-}(x) = \frac{2x - S}{\ell}, \quad (3.97)$$

i.e., $e^\beta \mu(x)$ varies linearly with position.

IV. THERMOBALLISTIC APPROACH: CONCEPT

The prototype thermoballistic model developed in the preceding section has been based on the random partitioning of the length of a semiconducting sample into
ballistic transport intervals linked by points of local thermodynamic equilibrium, which make up a ballistic configuration. Electrons thermally emitted at either endpoint of a ballistic interval, and subsequently transmitted across the potential energy profile in the sample, form the net ballistic electron current in the interval. This current is conserved across an individual ballistic interval. A distinctive assumption of the prototype model has been that the current is conserved also across the points of local thermodynamic equilibrium linking the ballistic intervals, and equals the physical current. By averaging over all ballistic configurations, the current-voltage characteristic can then be expressed, without requiring knowledge of the equilibrium chemical potential inside the sample, essentially in terms of a reduced resistance that comprises the effect of the sample parameters. The position dependence of the chemical potential has been constructed in a heuristic way only.

While adhering to the idea of introducing ballistic configurations and averaging thereover, the thermoballistic concept proper refines the prototype model in that it abandons the assumption of current conservation across the points of local thermodynamic equilibrium. [A simple example contradicting this assumption is provided by the case of the ballistic currents in a homogeneous semiconductor at zero bias considered in Sec. VII A below.]

Position-dependent total and spin-polarized thermoballistic currents as well as the associated densities are defined in terms of an average chemical potential and a spin splitting \( \mu(x) \) determined by the values \( \tilde{\mu}(x') \) and \( \tilde{\mu}(x'') \) of the average chemical potential \( \tilde{\mu}(x) \) and the values \( A(x') \) and \( A(x'') \) of the spin accumulation function \( A(x) \) according to Eq. (4.14) with the mean spin function \( A(x) \) expressed in terms of \( \tilde{\mu}(x) \) via Eq. (4.11), and the net relaxing ballistic spin-polarized current \( J_{+}(x',x'') \) determined by \( A(x') \) and \( A(x'') \) according to Eq. (4.15). The quantities \( \mu_{1,2} \) and \( A_{1,2} \) are the values of the equilibrium chemical potential and the spin accumulation function, respectively, at the contact side of the contact-semiconductor interfaces [see Eqs. (4.92) and (4.94)].

We have developed the thermoballistic approach to semiclassical carrier transport in a series of papers. In Ref. 55 the concept of a thermoballistic current was introduced and implemented without regard to spin degrees of freedom. The extension of this concept to spin-polarized electron transport across a spin-degenerate potential energy profile was presented in Ref. 54, in which spin injection out of ferromagnetic contacts into a non-magnetic semiconducting sample was treated in detail. In Ref. 55 we have generalized the thermoballistic concept to the case of arbitrary spin splitting of the profile, thereby covering, in particular, spin-polarized transport in diluted magnetic semiconductors in their paramagnetic phase. In the present section, we formulate the thermoballistic concept within the frame set by Ref. 55. Classical transport in nondegenerate systems is considered throughout. Effects of electron tunneling and degeneracy can be included, in principle, by resorting to the corresponding developments in Secs. III B and III C.

For comprehensive surveys of the fundamentals of spin physics in semiconductors and their application in the field of spintronics, we refer the reader to Refs. 22 and 50–58.

![FIG. 4: Schematic diagram showing, in a one-dimensional representation, a paramagnetic semiconducting sample of length \( S \) enclosed between two metal contacts. The spin splitting \( \Delta(x) \) of the electrostatic potential energy profile \( E_c(x) \) gives rise to the spin-dependent potential energy profiles \( E_{\uparrow,\downarrow}(x) \). The coordinates \( x' \) and \( x'' \) denote points of local thermodynamic equilibrium which delimit a ballistic transport interval \([x',x'']\). Electrons thermally emitted at \( x'(x'') \) toward the right (left) move ballistically across the profiles \( E_{\uparrow,\downarrow}(x) \) to reach the end-point \( x''(x') \) of the ballistic interval, where they are absorbed (equilibrated). Two net electron currents are indicated: The (conserved) net total ballistic current \( J_{+}(x',x'') \) determined by the values \( \tilde{\mu}(x') \) and \( \tilde{\mu}(x'') \) of the average chemical potential \( \tilde{\mu}(x) \) and the values \( A(x') \) and \( A(x'') \) of the spin accumulation function \( A(x) \) according to Eq. (4.12) with the mean spin function \( A(x) \) expressed in terms of \( \tilde{\mu}(x) \) via Eq. (4.11), and the net relaxing ballistic spin-polarized current \( J_{+}(x',x'';x) \) determined by \( A(x') \) and \( A(x'') \) according to Eq. (4.15). The quantities \( \mu_{1,2} \) and \( A_{1,2} \) are the values of the equilibrium chemical potential and the spin accumulation function, respectively, at the contact side of the contact-semiconductor interfaces [see Eqs. (4.92) and (4.94)].]
pling by $x_1$ and $x_2$, respectively, so that we have
\begin{equation}
    x_1 < x' < x'' < x_2,
\end{equation}
and the sample length $S$ is given by $S = x_2 - x_1$.

In Fig. 2 a paramagnetic semiconducting sample enclosed between two metal contacts is depicted in a schematic diagram. Various physical quantities appearing in the thermoballistic description are indicated.

1. Spin-resolved densities

We write the spin-dependent potential energy profiles $E_{\uparrow,\downarrow}(x')$ corresponding to spin-up ($\uparrow$) and spin-down ($\downarrow$) conduction band electrons, respectively, in the form
\begin{equation}
    E_{\uparrow,\downarrow}(x') = E_c(x') \pm \frac{1}{2} \Delta(x').
\end{equation}
Here, the spin-independent part $E_c(x')$ is assumed to comprise the conduction band edge potential and the external electrostatic potential, and $\Delta(x')$ is the spin splitting of the conduction band. Having in mind electron transport in diluted magnetic semiconductors in their paramagnetic phase, we identify this splitting with the (giant) Zeeman splitting due to an external magnetic field. [We restrict ourselves to considering a single Landau level whose energy is assumed to be included in $E_c(x')$.] In presenting the general formalism, we assume both $E_c(x')$ and $\Delta(x')$, and hence $E_{\uparrow,\downarrow}(x')$, to be continuous functions of $x'$ in the interval $[x_1, x_2]$. The case of abrupt changes in one or the other of these functions, which occur at the interfaces in heterostructures, may be described, in a simplified picture, in terms of discontinuous functions (see Sec. VI C below).

In terms of the Boltzmann factors $e^{-\beta E_{\uparrow,\downarrow}(x')}$, the (static) local spin polarization of the conduction band electrons, $P(x')$, is given by
\begin{equation}
    P(x') = \frac{B_{-}(x')}{{B_{+}(x')},}
\end{equation}
where
\begin{equation}
    B_{\pm}(x') = e^{-\beta E_{\pm}(x')} \pm e^{-\beta E_{\mp}(x')},
\end{equation}
so that we have
\begin{equation}
    P(x') = -\tanh(\beta \Delta(x')/2).
\end{equation}
The function $Q(x')$ defined by
\begin{equation}
    Q(x') \equiv \left\{1 - [P(x')]^2\right\}^{1/2}
    = \frac{1}{\cosh(\beta \Delta(x')/2)}
\end{equation}
will be frequently used below.

For the spin-resolved equilibrium electron densities $n_{\uparrow,\downarrow}(x')$, we have, in generalization of expression (2.20),
\begin{equation}
    n_{\uparrow,\downarrow}(x') = \frac{N_c}{2} e^{-\beta[E_{\uparrow,\downarrow}(x')-\mu_{\uparrow,\downarrow}(x')]}.
\end{equation}
Here, $\mu_{\uparrow,\downarrow}(x')$ are the spin-resolved chemical potentials associated with the local thermodynamic equilibrium at $x'$, and $N_c/2$, with $N_c$ given by Eq. (2.21), is the effective density of states of either spin at the conduction band edge (for simplicity, the effective electron mass $m^*$ entering $N_c$ is assumed here to be independent of position and of the external magnetic field).

The spin-resolved chemical potentials $\mu_{\uparrow}(x')$ and $\mu_{\downarrow}(x')$ are independent dynamical functions whose position dependence is to be determined within the thermoballistic approach and from which, subsequently, all transport properties are to be derived. However, in implementing the thermoballistic approach, we will work not with $\mu_{\uparrow}(x')$ and $\mu_{\downarrow}(x')$, but with suitably defined combinations of these functions: (i) an “average chemical potential”, and (ii) a “spin accumulation function” related to the splitting of the potentials $\mu_{\uparrow}(x')$ and $\mu_{\downarrow}(x')$.

2. Average chemical potential and spin accumulation function

We define the “spin functions” $A_{\uparrow,\downarrow}(x')$ as
\begin{equation}
    A_{\uparrow,\downarrow}(x') = e^{\beta \mu_{\uparrow,\downarrow}(x')},
\end{equation}
and the “mean spin function” $\tilde{A}(x)$ as
\begin{equation}
    \tilde{A}(x) = \frac{1}{2} A_{\uparrow}(x') + A_{\downarrow}(x'),
\end{equation}
where
\begin{equation}
    A_{\boldsymbol{\pm}}(x') \equiv A_{\uparrow}(x') + A_{\downarrow}(x').
\end{equation}
We can express $\tilde{A}(x')$ in the form
\begin{equation}
    \tilde{A}(x') = e^{\beta \bar{\mu}(x')} \cosh(\beta \mu_{-}(x')/2),
\end{equation}
where
\begin{equation}
    \bar{\mu}(x') = \frac{1}{2} [\mu_{\uparrow}(x') + \mu_{\downarrow}(x')]\] (4.12)
\end{equation}
is the mean value of $\mu_{\uparrow}(x')$ and $\mu_{\downarrow}(x')$ [mean chemical potential], and
\begin{equation}
    \mu_{-}(x') = \mu_{\uparrow}(x') - \mu_{\downarrow}(x')\] (4.13)
\end{equation}
their splitting. [In the following, the “$\pm$” notation introduced in Eqs. (4.10) and (4.13), respectively, will be frequently used mutatis mutandis to denote spin-summed and spin-polarized quantities.] Further, writing
\begin{equation}
    \tilde{A}(x') = e^{\beta \bar{\mu}(x')},
\end{equation}
we introduce the “average chemical potential” $\bar{\mu}(x')$.

The “spin accumulation function” $A_{\pm}(x')$ is defined as
\begin{equation}
    A_{\pm}(x') \equiv A_{\uparrow}(x') - A_{\downarrow}(x')
    = 2 e^{\beta \bar{\mu}(x')} \sinh(\beta \mu_{-}(x')/2).
\end{equation}
A chemical potential in terms of the splitting \( \eta \) so that their use results in a formulation in terms of the “spin accumulation” there.

Using Eq. (4.11), we can rewrite \( A_-(x') \) in the form

\[
A_-(x') = 2\bar{A}(x') \tanh(\beta \mu_-(x'))/2. \tag{4.16}
\]

Introducing the “reduced” spin accumulation function \( \bar{A}(x') \) as

\[
\bar{A}(x') \equiv \frac{A_-(x')}{A(x')} = 2 \tanh(\beta \mu_-(x'))/2, \tag{4.17}
\]

we then obtain, using Eqs. (4.14)–(4.16), the relations

\[
\bar{\mu}(x') = \bar{\mu}(x') + \frac{1}{\beta} \ln(\cosh(\beta \mu_-(x'))/2)) = \bar{\mu}(x') - \frac{1}{2\beta} \ln(1 - \bar{A}^2(x'))/4 \tag{4.18}
\]

expressing the difference between average and mean chemical potential in terms of the splitting \( \mu_-(x') \) and of \( \bar{A}(x') \), respectively.

The spin functions \( A_{\uparrow,\downarrow}(x') \) are proportional to the spin-resolved electron densities \( n_{\uparrow,\downarrow}(x') \) [see Eqs. (4.7)], so that their use results in a formulation in terms of linear equations, instead of the nonlinear description ensuing from using the spin-resolved chemical potentials \( \mu_{\uparrow,\downarrow}(x') \) themselves. [This aspect has been emphasized previously\(^{55,56}\) within a study, based on the standard drift-diffusion approach, of electric-field effects on spin-polarized transport in nondegenerate semiconductors.]

From Eqs. (4.7), the total (i.e., spin-summed) equilibrium density, \( n_{\pm}(x') \), and the spin-polarized equilibrium density, \( n_{\pm}(x') \), are now obtained in terms of the functions \( A_{\pm}(x') \) as

\[
n_{\pm}(x') = \frac{N_e}{4} B_{\pm}(x') [A_{\pm}(x') + P(x') A_{\mp}(x')], \tag{4.19}
\]

where Eqs. (4.4) and (4.5) have been used.

### B. Ballistic spin-polarized transport

In this subsection, the spin-resolved electron currents transmitted across a ballistic transport interval as well as the associated densities (called “ballistic currents” and “ballistic densities”, for short) are constructed by closely following the development in the ballistic (see Sec. III B) and the prototype thermoballistic (see Sec. III B 1) transport models, in which spin degrees of freedom have been disregarded. Introducing spin relaxation during the ballistic electron motion, we obtain the ballistic spin-polarized currents and densities, whose dynamics are determined from a balance equation.

1. **Ballistic currents**

The left end-point, \( x' \), as well as the right end-point, \( x'' \), of the ballistic interval \([x', x'']\) are points of local thermodynamic equilibrium but are, in general, **not** points of spin equilibrium.

We first assume that the electrons thermally emitted at \( x' \) towards the right are **not** affected by spin relaxation during their motion across the interval \([x', x'']\). The spin-resolved densities \( n_{\uparrow,\downarrow}(x') \) [see Eq. (4.7)] then give rise to conserved ballistic spin-resolved currents (i.e., currents independent of the position \( x \in [x', x''] \)) in that interval, which have the form

\[
J^I_{\uparrow,\downarrow}(x', x'') = v_s n_{\uparrow,\downarrow}(x') \tilde{T}^I_{\uparrow,\downarrow}(x', x'') \tag{4.20}
\]

(see Sec. III B 1), where the thermally averaged (classical) transmission probabilities \( \tilde{T}^I_{\uparrow,\downarrow}(x', x'') \) are given [see Eqs. (2.57) and (2.58)] by

\[
\tilde{T}^I_{\uparrow,\downarrow}(x', x'') = e^{-\beta E^m_{\uparrow,\downarrow}(x', x'')} - E_{\uparrow,\downarrow}(x')], \tag{4.21}
\]

with \( E^m_{\uparrow,\downarrow}(x', x'') \) the overall maxima of the potential energy profiles \( E_{\uparrow,\downarrow}(x) \) in \([x', x'']\). In terms of the spin functions \( A_{\uparrow,\downarrow}(x') \) given by Eqs. (4.8), we can rewrite the currents \( J^I_{\uparrow,\downarrow}(x', x'') \) in the form

\[
J^I_{\uparrow,\downarrow}(x', x'') = v_s N_e \frac{1}{2} e^{-\beta E^m_{\uparrow,\downarrow}(x', x'')} A_{\uparrow,\downarrow}(x') \tag{4.22}
\]

We then have for the total (i.e., spin-summed) ballistic current, \( J^I_+(x', x'') \), and the ballistic spin-polarized current, \( J^I_-(x', x'') \),

\[
J^I_{\pm}(x', x'') = \frac{v_s N_e}{4} B^m_\pm(x', x'') \times [A_\pm(x') + P(x') A_\mp(x')], \tag{4.23}
\]

where

\[
B^m_\pm(x', x'') = e^{-\beta E^m_{\uparrow,\downarrow}(x', x'')} \pm e^{-\beta E^m_{\downarrow,\uparrow}(x', x'')} \tag{4.24}
\]

and

\[
P(x') = \frac{B^m_\pm(x', x'')}{B^m_{\pm}(x', x'')}, \tag{4.25}
\]

which are nonlocal extensions of expressions (4.4) and (4.3) for the functions \( B_{\pm}(x') \) and the local polarization \( P(x') \), respectively.

We now consider the effect of spin relaxation on the ballistic currents inside the interval \([x', x'']\). We introduce functions \( A^I_{\pm}(x', x''); x \) that depend on the position \( x \in [x', x''] \) and are required to satisfy the initial conditions

\[
A^I_{\pm}(x', x''); x = x' = A_{\pm}(x'). \tag{4.26}
\]
Using these functions, we generalize the definitions of the currents $J^l_{\pm}(x', x'')$ given by Eqs. (4.23) to

$$J^l_{\pm}(x', x''; x) = \frac{v_e N_e}{4} B^m(x', x'') \times [A^l_{\pm}(x', x''; x) + P^m(x', x'')A^l_{\pm}(x', x''; x)].$$

(4.27)

Now, also in the presence of spin relaxation, the total ballistic current must be conserved,

$$J^l_{\pm}(x', x''; x) = J^l_{\pm}(x', x''; x = x') \equiv J^l_{\pm}(x', x''),$$

(4.28)

where, from Eq. (4.23),

$$J^l_{\pm}(x', x'') = \frac{v_e N_e}{4} B^m(x', x'') \times [A^l_{\pm}(x') + P^m(x', x'')A^l_{\pm}(x')].$$

(4.29)

Equating this to expression (4.27) for $J^l_{\pm}(x', x''; x)$, we obtain the relation

$$A^l_{\pm}(x', x''; x) = A^l_{\mp}(x') + P^m(x', x'') \times [A^l_{\mp}(x') - A^l_{\pm}(x', x''; x)].$$

(4.30)

Therefore, the spin-polarized current can be written as

$$J^l_{\pm}(x', x''; x) = J^l_{\pm}(x', x''; x = x') + \frac{v_e N_e}{4} B^m(x', x'')A^l_{\pm}(x', x''; x),$$

(4.31)

where

$$B^m(x', x'') = B^m_{\pm}(x', x'')[Q^m(x', x'')]^2,$$

(4.32)

and

$$Q^m(x', x'') \equiv \{1 - [P^m(x', x'')]^2\}^{1/2}$$

(4.33)

is the nonlocal extension of expression (1.6) for the function $Q(x')$.

The ballistic spin-polarized current of Eq. (4.31) has the form

$$J^l_{\pm}(x', x''; x) = \tilde{J}^l_{\pm}(x', x'') + J^l_{\pm}(x', x''; x),$$

(4.34)

where the first (x-independent, nonrelaxing) term is the “persistent” ballistic spin-polarized current,

$$\tilde{J}^l_{\pm}(x', x'') \equiv J^l_{\pm}(x', x'')P^m(x', x''),$$

(4.35)

while the second (x-dependent) term is the “relaxing” ballistic spin-polarized current,

$$J^l_{\pm}(x', x''; x) = \frac{v_e N_e}{4} B^m(x', x'')A^l_{\pm}(x', x''; x).$$

(4.36)

The latter describes the spin dynamics in the current $J^l_{\pm}(x', x''; x)$ via the “spin relaxation function” $A^l_{\pm}(x', x''; x)$. The $x$-dependence of $A^l_{\pm}(x', x''; x)$ will be determined explicitly in Sec. [V.B.3] while the procedure for calculating the spin accumulation function

$$A^-_{\pm}(x') \equiv A^-_{\pm}(x', x''; x = x')$$

(4.37)

will be described in Sec. [V.C].

The persistent ballistic spin-polarized current $\tilde{J}^l_{\pm}(x', x'')$ depends, via the total ballistic current $J^l_{\pm}(x', x'')$, on the spin accumulation function $A^-_{\pm}(x')$. When $A^-_{\pm}(x')$ is calculated within the thermoballistic approach, spin relaxation in all ballistic intervals (including the interval $[x', x'']$ under consideration) is taken into account. Therefore, while being not directly affected by spin relaxation inside the interval $[x', x'']$, the persistent current $\tilde{J}^l_{\pm}(x', x'')$ depends, via the dependence of the factor $J^l_{\pm}(x', x'')$ on $A^l_{\pm}(x')$ [see Eqs. (4.29) and (4.35)], in an indirect way on spin relaxation.

2. Ballistic densities

The ballistic densities $n^l_{\pm}(x', x''; x)$ associated with the ballistic currents $J^l_{\pm}(x', x''; x)$ of Eqs. (4.27) are given by

$$n^l_{\pm}(x', x''; x) = \frac{N_e}{8} D^m_{\pm}(x', x''; x) \times [A^l_{\pm}(x', x''; x) + P^m(x', x''; x)A^l_{\pm}(x', x''; x)]$$

(4.38)

[see Eq. (2.51)]. Here, we have taken into account that the ballistic densities correspond to one half of the thermal currents emitted symmetrically at a point of local thermodynamic equilibrium [see, e.g., Eq. (2.42)].

The functions $D^m_{\pm}(x', x''; x)$ and $P^m(x', x''; x)$ are defined as

$$D^m_{\pm}(x', x''; x) = C^m_{\pm}(x', x''; x) e^{-\beta E^m_{\mp}(x', x'')} \pm C^m_{\mp}(x', x''; x) e^{-\beta E^m_{\pm}(x', x'')}$$

(4.39)

where

$$C^m_{\pm}(x', x''; x) = e^{\beta [E^m_{\mp}(x', x'') - E_{\mp}(x) - \frac{1}{4}(\beta E^m_{\pm}(x', x'') - E_{\pm}(x))]} \text{erfc}(\beta [E^m_{\pm}(x', x'') - E_{\pm}(x)])^{1/2}$$

(4.40)

[see Eq. (2.52)], and

$$P^m_{\pm}(x', x''; x) = \frac{D^m_{\pm}(x', x''; x)}{D^m_{\mp}(x', x''; x)}$$

(4.41)

in generalization of expression (4.25) for the function $P^m(x', x'')$.

Now, inserting expression (4.30) for $A^l_{\pm}(x', x''; x)$ in Eqs. (4.38), we find that the total ballistic density,
\( n^\uparrow_+(x', x''; x) \), and the ballistic spin-polarized density, \( n^\downarrow_-(x', x''; x) \), have the form
\[
\dot{n}^\uparrow_+(x', x''; x) = \dot{n}^\downarrow_-(x', x''; x) + \dot{n}^\uparrow_+(x', x''; x) , \quad (4.42)
\]
Here, the first (\( x \)-dependent, but nonrelaxing) term is the persistent part,
\[
\dot{n}^\uparrow_+(x', x''; x) = \frac{N_s}{8} D^\uparrow_+(x', x''; x) \\
\times \left[ A_+(x') + P^\downarrow_+(x', x''; x) A_-(x') \right] , \quad (4.43)
\]
and the second term is the relaxing part,
\[
\dot{n}^\uparrow_+(x', x''; x) = \frac{N_s}{8} D^\uparrow_+(x', x''; x) A^\uparrow_-(x', x''; x), \quad (4.44)
\]
where
\[
D^\downarrow_+(x', x''; x) = D^\uparrow_+(x', x''; x) \\
- P^\downarrow_+(x', x''; x) D^\downarrow_+(x', x''; x). \quad (4.45)
\]

In contrast to the \( x \)-independent currents \( J^\uparrow_+(x', x'') \) and \( J^\downarrow_-(x', x'') \), the persistent parts of the ballistic densities, \( \dot{n}^\uparrow_+(x', x''; x) \), depend on position via the \( x \)-dependence of the potential energy profiles \( E_{1, \downarrow}(x) \). For zero spin splitting of the conduction band, \( \Delta(x) \equiv 0 \), when \( P^\downarrow_+(x', x'') = D^\uparrow_+(x', x''; x) = D^\downarrow_+(x', x''; x) = 0 \), the persistent part of the spin-polarized density as well as the relaxing part of the total density vanish, \( \dot{n}^\uparrow_+(x', x''; x) = 0 \).

3. Spin balance equation

In a time-dependent formulation, spin relaxation in a system described by spin-resolved electron densities \( n_{1, \downarrow}(x, t) \) and currents \( J_{1, \downarrow}(x, t) \) is governed by the local coupled spin balance equation,
\[
\frac{\partial}{\partial t} n^\uparrow_+(x, t) + \frac{\partial}{\partial x} J^\uparrow_+(x, t) = - \frac{n^\uparrow_+(x, t)}{\tau^{\uparrow\uparrow}} + \frac{n^\downarrow_+(x, t)}{\tau^{\downarrow\uparrow}} \quad (4.46)
\]
and
\[
\frac{\partial}{\partial t} n^\downarrow_-(x, t) + \frac{\partial}{\partial x} J^\downarrow_-(x, t) = - \frac{n^\downarrow_-(x, t)}{\tau^{\downarrow\downarrow}} + \frac{n^\uparrow_-(x, t)}{\tau^{\uparrow\downarrow}} , \quad (4.47)
\]
where \( 1/\tau^{\uparrow\uparrow} (1/\tau^{\downarrow\downarrow}) \) is the rate for spin-flip scattering from spin-up (spin-down) to spin-down (spin-up) states. In the stationary case, when \( \partial n^\uparrow_+(x, t)/\partial t \equiv 0 \), this leads to the balance equation
\[
\frac{d}{dx} J^\downarrow_-(x) = - \frac{1}{\tau_s} \dot{n}^\downarrow_-(x) \left( \frac{1}{\tau^{\uparrow\uparrow}} - \frac{1}{\tau^{\downarrow\downarrow}} \right) \dot{n}^\uparrow_+(x) \quad (4.48)
\]
connecting the relaxing part of the spin-polarized current, \( J^\downarrow_-(x) \), to the relaxing parts of the spin-polarized, \( \dot{n}^\downarrow_-(x) \), and of the total density, \( \dot{n}^\uparrow_+(x) \). Here, \( \tau_s \), defined as
\[
\frac{1}{\tau_s} = \frac{1}{\tau^{\uparrow\uparrow}} + \frac{1}{\tau^{\downarrow\downarrow}} \quad (4.49)
\]
is the spin relaxation time.

We apply Eq. (4.48) to spin relaxation during ballistic transport. In doing this, we will disregard the term involving \( \dot{n}^\uparrow_+(x) \) for two reasons: (i) As it is preceded by the difference of the two relaxation rates \( 1/\tau^{\uparrow\uparrow} \) and \( 1/\tau^{\downarrow\downarrow} \), which are estimated to be of comparable magnitude, the term may generally be considered small in comparison with the term involving \( \dot{n}^\downarrow_-(x) \). (ii) Since both \( \dot{n}^\downarrow_-(x) \) and \( \dot{n}^\uparrow_+(x) \) are proportional to the spin relaxation function \( A^\downarrow_+(x', x''; x) \) [see Eq. (4.44)], we can account for \( \dot{n}^\downarrow_-(x) \) by combining its prefactors with those of \( \dot{n}^\downarrow_-(x) \) in an effective spin relaxation time (still denoted by \( \tau_s \)) depending, in general, on the potential energy profiles. [Note that we must not assume \( \dot{n}^\uparrow_+(x) = 0 \) from the outset by adopting the arguments leading to Eq. (2.7) of Ref. 68.] The density \( n^\uparrow_+ + n^\downarrow_- \) appearing in that equation is the deviation of the total density from its spin equilibrium value. By contrast, the relaxing total density \( \dot{n}^\uparrow_+(x) \), when used in the thermoballistic description, gives the deviation of the total density from the persistent total density. In the latter, a spin non-equilibrium part enters via the spin accumulation function \(\dot{A}^\downarrow_-(x) \) [see Eq. (4.43)].

In the thermoballistic approach, it is assumed that the thermally emitted electrons spend only an infinitely short time span at the emission point, and it is only during their motion across the ballistic interval that they can undergo spin relaxation. Spin relaxation in ballistic transport is commonly described in terms of a (ballistic) spin relaxation length \( l_s \) given by
\[
l_s = 2v_l \tau_s . \quad (4.50)
\]
[As in the case of the effective electron mass \( m^* \), we assume \( \tau_s \), and hence \( l_s \), to be independent of position and of the external magnetic field; we consider \( l_s \) here an effective quantity, in line with the interpretation of \( \tau_s \).] In our description of spin-polarized electron transport, spin relaxation is thus completely separated from momentum relaxation at the points of local thermodynamic equilibrium and, in this respect, is similar to the D’Yakonov-Perel’ relaxation mechanism.\( ^{22,56–58,70–72} \)

In terms of the relaxing ballistic spin-polarized current \( J^\downarrow_-(x', x''; x) \) and the corresponding density \( \dot{n}^\downarrow_-(x', x''; x) \), the balance equation governing spin relaxation during ballistic transport now reads
\[
\frac{d}{dx} J^\downarrow_-(x', x''; x) + \frac{2v_l}{l_s} \dot{n}^\downarrow_-(x', x''; x) = 0 , \quad (4.51)
\]
where the spin relaxation length \( l_s \) is given by Eq. (4.50).
Inserting in Eq. (4.51) the expressions for \( \tilde{J}_e(x', x''; x) \) and \( \tilde{n}_e(x', x''; x) \) from Eqs. (4.36) and (4.44), respectively, we obtain a first-order differential equation for the spin relaxation function \( A_-(x', x''; x) \),

\[
\frac{d}{dx} A_-(x', x''; x) + \frac{C^m(x', x''; x)}{l_s} A_-(x', x''; x) = 0,
\]

(4.52)

where

\[
C^m(x', x''; x) = \frac{D^m(x', x''; x)}{B^m(x', x'')}. \tag{4.53}
\]

The solution of Eq. (4.52) obeying the initial condition (4.26) is

\[
A_-(x', x''; x) = A_-(x') e^{-C^m(x', x''; x')/l_s}, \tag{4.54}
\]

where

\[
C^m(x', x''; z_1, z_2) = \int_{z_1}^{z_2} dz C^m(x', x''; z), \tag{4.55}
\]

with \( z_\text{c} = \min(z_1, z_2) \), \( z_\text{r} = \max(z_1, z_2) \).

Now, inserting expression (4.54) in Eqs. (4.36) and (4.44), respectively, we obtain the relaxing ballistic spin-polarized current and density explicitly in terms of the spin accumulation function \( A_-(x') \),

\[
\tilde{J}_e(x', x''; x) = \frac{v_e N_e}{4} B^m(x', x'') A_-(x') \times e^{-C^m(x', x''; x')/l_s}, \tag{4.56}
\]

and

\[
\tilde{n}_e(x', x''; x) = \frac{N_e}{8} D^m(x', x''; x) A_-(x') \times e^{-C^m(x', x''; x')/l_s}. \tag{4.57}
\]

The \( x \)-dependence of the relaxing spin-polarized current and density in the ballistic interval \([x', x'']\) is hence governed by the factor \( e^{-C^m(x', x''; x')/l_s} \). It departs from a purely exponential behavior unless the potential energy profiles \( E_{\uparrow, \downarrow}(x) \) are constant over the interval, in which case \( C^m(x', x''; x', x) = x - x' \).

4. Net ballistic currents and joint ballistic densities

So far, we have only considered thermal emission at the left end-point, \( x' \), of the ballistic interval \([x', x'']\), obtaining a variety of ballistic currents and densities summarized denoted here by \( J_1(x', x''; x) \) and \( n_1(x', x''; x) \), respectively. The analogous ballistic currents and densities \( J_2(x', x''; x) \) and \( n_2(x', x''; x) \) corresponding to emission at the right end-point \( x'' \) can be expressed in terms of those emitted at \( x' \) as

\[
J_2(x', x''; x) = -J_1(x'', x'; x) \tag{4.58}
\]

and

\[
n_2(x', x''; x) = n_1(x'', x'; x). \tag{4.59}
\]

[Note that, owing to the symmetry of the functions \( E_{\uparrow, \downarrow}^m(x', x'') \), the functions \( B_{\uparrow, \downarrow}^m(x', x'') \), \( D_{\uparrow, \downarrow}^m(x', x'') \), \( \frac{1}{2} D^m(x', x'') \) entering the expressions for \( J_1(x', x''; x) \) and \( n_1(x', x''; x) \) are symmetric under the exchange of \( x' \) and \( x'' \).] We then have

\[
J(x', x''; x) = J_1(x', x''; x) + J_2(x', x''; x) = J_1(x', x''; x) - J_1(x'', x'; x) \tag{4.60}
\]

and

\[
n(x', x''; x) = n_1(x', x''; x) + n_2(x', x''; x) = n_1(x', x''; x) + n_1(x'', x'; x) \tag{4.61}
\]

for the net ballistic currents and joint ballistic densities similarly denoted by \( J(x', x''; x) \) and \( n(x', x''; x) \), respectively.

For the (conserved) net total ballistic current \( J_+ (x', x'') \) inside the ballistic interval, we now find, using Eq. (4.29),

\[
J_+(x', x'') = \frac{v_e N_e}{2} \int_{z_\text{c}}^{z_\text{r}} dz^2 C^m(x', x''; z) \left[ \tilde{A}(x') - \tilde{A}(x'') \right] + \frac{1}{2} \int_{z_\text{c}}^{z_\text{r}} dz^2 C^m(x', x''; z) \left[ A(x') - A(x'') \right]. \tag{4.62}
\]

Here, the function \( A_+(x') \) has been replaced with \( 2 \tilde{A}(x') \) [see Eq. (4.9)], and the subscript attached to the spin accumulation function \( A_-(x') \) has been omitted, i.e., we have set

\[
A(x') = A_-(x'). \tag{4.63}
\]

The current \( J_+ (x', x'') \) is seen to be dynamically determined, in general, both by the average chemical potential \( \mu(x') \) [via the mean spin function \( \tilde{A}(x') \)] and the spin accumulation function \( A(x') \). The same then holds for the net persistent ballistic spin-polarized current \( \tilde{J}_- (x', x'') \), for which we have, using Eq. (4.35),

\[
\tilde{J}_-(x', x'') = J_-(x', x'') P^m(x', x''). \tag{4.64}
\]

For zero spin splitting, when \( \Delta(x) = 0 \) and hence \( P^m(x', x'') = 0 \), the dependence of \( J_+(x', x'') \) on \( A(x) \) drops out and, further, \( \tilde{J}_-(x', x'') = 0 \).

For the net relaxing ballistic spin-polarized current, we have, using Eq. (4.50),

\[
\tilde{J}_-(x', x'') = \frac{v_e N_e}{4} B^m(x', x'') \left[ A(x') e^{-C^m(x', x''; x', x)/l_s} - A(x'') e^{-C^m(x', x''; x, x'')/l_s} \right], \tag{4.65}
\]

which is dynamically determined by the spin accumulation function \( A(x) \) alone.
For the joint total ballistic density, \(n_\pm(x', x''; x)\), and the joint ballistic spin-polarized density, \(n_\pm(x', x''; x)\), respectively, we have from Eq. (4.2)

\[
n_\pm(x', x''; x) = n_\pm(x', x''; x) + \tilde{n}_\pm(x', x''; x),
\]

(4.66)

with persistent parts \(\tilde{n}_\pm(x', x''; x)\) and relaxing parts \(\tilde{n}_\pm(x', x''; x)\) given by

\[
\tilde{n}_\pm(x', x''; x) = \frac{N_c}{4} D_\pm^{m_0}(x', x''; x) \left\{ [\dot{A}(x') + \dot{A}(x'')] + \frac{1}{2} P^m(x', x'') [A(x') + A(x'')] \right\}
\]

(4.67)

[see Eq. (4.43)] and

\[
\tilde{n}_\pm(x', x''; x) = \frac{N_c}{8} D_\pm^{m_0}(x', x''; x) \times \left\{ [A(x') e^{-c_m(x', x''; x)/l_e} + A(x'') e^{-c_m(x', x''; x)/l_e}] + \right\}
\]

(4.68)

[see Eqs. (4.44) and (4.57)], in analogy to Eqs. (4.62), (4.63), and (4.65) for the net currents.

From expressions (4.65) and (4.68), we now derive, using Eqs. (4.53) and (4.55), the balance equation

\[
\frac{d}{dx} \tilde{J}_\pm(x', x''; x) + \frac{2v_e}{l_e} \tilde{n}_\pm(x', x''; x) = 0
\]

(4.69)

connecting the net relaxing ballistic spin-polarized current \(\tilde{J}_\pm(x', x''; x)\) and the associated joint density \(\tilde{n}_\pm(x', x''; x)\). This equation can be obtained, of course, simply by adding the balance equation Eq. (4.51) and the corresponding equation for emission at \(x''\).

### C. Thermoballistic spin-polarized transport

In a significant advance over its prototype presented in Sec. III where overall current conservation was introduced via the condition (3.20), the thermoballistic concept proper rests on the introduction of a “reference coordinate” \(x\) that characterizes an arbitrary point inside the semiconducting sample extending from \(x_1\) to \(x_2\), as shown in Fig. 4. Singling out this coordinate, we consider the net ballistic currents and joint ballistic densities within the ensemble of all ballistic intervals \([x', x'']\) enclosing \(x\). These currents and densities form the building blocks for establishing, at \(x\), the corresponding thermoballistic quantities. The point labeled by the reference coordinate \(x\) is not a point of local thermodynamic equilibrium (we may call it a “ballistic point”). However, the “equilibrium points” \(x', x''\) may come infinitesimally close to \(x\).

#### 1. Thermoballistic currents and densities

The thermoballistic currents and densities at the point \(x\) are constructed by performing weighted summations of the corresponding net ballistic currents and joint ballistic densities over all ballistic intervals \([x', x'']\) subject to the condition

\[
x_1 \leq x' < x < x'' \leq x_2.
\]

(4.70)

Just as in the prototype thermoballistic model (see Sec. III B), we adopt here the probabilistic picture outlined in Sec. III A 2) that the electrons traverse the interval without collisions, multiplied by the probability \(dx'/l (dx''/l)\) that they are absorbed or emitted in an interval \(dx' (dx'')\) around the end-point \(x' (x'')\). At the ends of the semiconducting sample at \(x_{1,2}\), absorption and emission occur with unit probability. Like the effective electron mass \(m^*\) and the spin relaxation length \(l_s\), the momentum relaxation length \(l_e\) is assumed here to be independent of position and of the external magnetic field.

Representing the net ballistic currents and joint ballistic densities of Eqs. (4.62)–(4.68) summarily by a function \(F(x', x''; x)\), and the corresponding thermoballistic currents and densities by \(\tilde{F}(x)\), we write \(\tilde{F}(x)\) in the form

\[
\tilde{F}(x) = \tilde{F}(x_1, x_2; x)\]

\[
= e^{-(x_{2} - x_{1})/l} F(x_1, x_2; x)
\]

\[
+ \int_{x_1}^{x_2} \frac{dx'}{l} e^{-(x_{2} - x_{1})/l} F(x, x_2; x)
\]

\[
+ \int_{x_1}^{x_2} \frac{dx''}{l} e^{-(x^{'} - x_{1})/l} F(x_1, x'; x)
\]

\[
+ \int_{x_1}^{x_2} \frac{dx'}{l} \int_{x_1}^{x_2} \frac{dx''}{l} e^{-|x'' - x'|/l} F(x', x''; x),
\]

(4.71)

where \(x^\pm = x \pm \delta\), and the infinitesimal \(\delta\) has been introduced in accordance with condition (4.70). Further, we set

\[
\tilde{F}(x_{1,2}) = \tilde{F}(x_{1,2} \pm \eta)_{\eta \to 0}.
\]

(4.72)

In parallel to Eq. (4.32) for the total probability in the prototype model, we have \(\tilde{F}(x) = 1\) for \(F(x', x''; x) = 1\).

Specifically, the total thermoballistic current \(\tilde{J}_\pm(x)\) is given by expression (4.71) with \(J_\pm(x', x'')\) of Eq. (4.62) substituted for \(F(x', x''; x)\). The persistent thermoballistic spin-polarized current \(\tilde{J}_\pm(x)\) follows by identifying \(F(x', x''; x)\) with \(\tilde{J}_\pm(x', x'')\) of Eq. (4.64). The relaxing thermoballistic spin-polarized current \(\tilde{J}_\pm(x)\) is obtained by replacing \(F(x', x''; x)\) with \(\tilde{J}_\pm(x', x''; x)\) of Eq. (4.65). Further, the thermoballistic densities \(n_\pm(x), \tilde{n}_\pm(x), \) and \(\tilde{n}_\pm(x)\) corresponding to the currents \(\tilde{J}_\pm(x), \tilde{J}_\pm(x), \) and \(\tilde{J}_\pm(x)\) follow by substituting the respective joint ballistic densities [see Eqs. (4.60)–(4.65)] for \(F(x', x''; x)\) in Eq. (4.71).
In expression (4.71), when specialized to the total thermoballistic current \( \mathcal{J}_+ (x) \), the first term on the right-hand side represents the net electron current passing through the point \( x \) while being ballistically transmitted between \( x_1 \) and \( x_2 \) [which occurs with probability \( e^{-(x_2-x_1)/l} \)], the second term refers to ballistic electron motion between any point \( x' \) \((x_1 \leq x' \leq x^-)\) and \( x_2 \) [probability \( e^{-(x_2-x')/l} dx'/l \)], the third term to ballistic electron motion between \( x_1 \) and any point \( x'' \) \((x^+ \leq x'' \leq x_2)\) [probability \( e^{-(x''-x_1)/l} dx''/l \)], etc. The four types of ballistic current appearing in expression (4.71) are illustrated by the double arrows labeled I to IV in Fig. 5.

The derivatives with respect to \( x \) of the various thermoballistic quantities can be written in the general form

\[
\frac{d}{dx} \mathcal{S}(x) = \left. \frac{d}{dx} \mathcal{S}(x) \right|_F + \mathcal{D}(x), \tag{4.73}
\]

where the first term on the right-hand side comprises the contributions arising from differentiating the functions \( F(x', x''; x) \) in the integrands of expression (4.71), and the second, from differentiating the limits of integration:

\[
\mathcal{D}(x) \equiv \mathcal{D}(x_1, x_2; x; l)
= \left( \frac{\partial}{\partial x^+} + \frac{\partial}{\partial x^-} \right) \mathcal{S}(x_1, x_2; x; l)
= -\frac{1}{l} \left\{ \mathcal{F}_1(x; [F]) - \mathcal{F}_2(x; [F]) \right\}. \tag{4.74}
\]

Here, the functionals \( \mathcal{F}_1(x; [F]) \) and \( \mathcal{F}_2(x; [F]) \), defined by

\[
\mathcal{F}_1(x; [F]) = e^{-(x-x_1)/l} F(x_1, x^+; x)
+ \int_{x_1}^{x^-} \frac{dx'}{l} e^{-(x-x')/l} F(x', x^+; x)
\]

\[
\mathcal{F}_2(x; [F]) = e^{-(x_2-x)/l} F(x^-, x_2; x)
+ \int_{x^+}^{x_2} \frac{dx''}{l} e^{-(x''-x)/l} F(x'', x^+; x), \tag{4.75}
\]

respectively, represent the contributions of the function \( F(x', x''; x) \) arising from the ranges to the left and right of the point \( x \).

For the total thermoballistic current \( \mathcal{J}_+ (x) \) constructed from the \( x \)-independent ballistic current \( J_+ (x', x'') \), the first term on the right-hand side of Eq. (4.73) vanishes, and we have

\[
\frac{d}{dx} \tilde{\mathcal{J}}_+(x) = \mathcal{D}_+(x), \tag{4.77}
\]

with \( \mathcal{D}_+(x) \) given by expression (4.74) for \( F(x', x''; x) \equiv J_+(x', x'') \). We note that \( \mathcal{D}_+(x) \) is not, in general, equal to zero, so that the total thermoballistic current \( \mathcal{J}_+(x) \) is not conserved. The quantity \( \mathcal{D}_+(x) dx \) is the increment of \( \mathcal{J}_+(x) \) across the infinitesimal interval \( dx \) at position \( x \) of the sample. The four types of ballistic current appearing in expression (4.72), which contribute to this increment, are depicted by the double arrows labeled I to IV in Fig. 6 with the arrows I and II representing the term \( \mathcal{F}_1(x; [F]) \), and III and IV the term \( \mathcal{F}_2(x; [F]) \).

If we set \( F(x', x''; x) \equiv \tilde{J}_-(x', x''; x) \) in expressions (4.71) and (4.74), we find from Eq. (4.73) for the relaxing thermoballistic spin-polarized current

\[
\frac{d}{dx} \tilde{\mathcal{J}}_-(x) = -\frac{2\hbar v_x}{l} \tilde{n}_-(x) + \mathcal{D}_-(x). \tag{4.78}
\]

In the first term on the right-hand side of this equation, we have introduced the relaxing thermoballistic spin-polarized density \( \tilde{n}_-(x) \) by using the balance equation (4.69) to replace the derivatives \( \partial \tilde{J}_-(x', x''; x)/\partial x \) which we encounter when differentiating the integrals in expression (4.71).
The thermoballistic currents and densities, Eq. (4.71), are expressed, via the corresponding ballistic currents and densities, Eqs. (4.62)–(4.68), in terms of two dynamical functions, viz., the mean spin function $\bar{A}(x)$ and the spin accumulation function $A(x)$, or, equivalently, the average chemical potential $\bar{\mu}(x)$ and the splitting of the spin-resolved chemical potentials, $\mu_-(x)$ [see Eqs. (4.14), (4.19), and (4.63)]. To implement the thermoballistic concept, we must establish algorithms for calculating $\bar{A}(x)$ and $A(x)$ in terms of the intrinsic parameters of the semiconducting system, like momentum and spin relaxation lengths, as well as the external parameters, like applied voltage and spin polarization in the external leads.

Before establishing these algorithms within the thermoballistic approach, i.e., for arbitrary momentum relaxation length $l$ and for the ballistic case ($l \to \infty$). The results will turn out to be equal to the corresponding standard physical expressions summarized in Sec. III, which demonstrates that the thermoballistic description indeed bridges the gap between the drift-diffusion and ballistic descriptions of carrier transport.

2. Drift-diffusion regime

In the drift-diffusion regime, when $l/S \ll 1$ and $l/l_c \ll 1$, nonzero contributions to the thermoballistic currents and densities defined by Eq. (4.71) arise only from very short ballistic intervals $[x', x'']$ enclosing the point $x$, so that $x - x'$ and $x'' - x$ are infinitesimals and only the double integral over $x'$ and $x''$ contributes.

Then, from Eq. (4.71), the persistent part of the total thermoballistic density, $\hat{n}_+(x)$, is seen to reduce to the total equilibrium density $n_+(x)$ [see Eq. (4.19)],

$$\hat{n}_+(x) = n_+(x),$$

(4.79)

with $n_+(x)$ expressed in terms of the functions $\bar{A}(x)$ and $A(x)$,

$$n_+(x) = \frac{N_c}{2}B_+(x)[\bar{A}(x) + \frac{1}{2}P(x)A(x)].$$

(4.80)

Further, since $\mathcal{D}_n(x', x''; x) = 0$ in the drift-diffusion regime, the relaxing part of the joint total ballistic density, $\hat{n}_+(x', x''; x)$ [see Eq. (4.68)], vanishes. Consequently, we have

$$\hat{n}_+(x) = 0$$

(4.81)

for the relaxing part of the total thermoballistic density, $\hat{n}_+(x)$, and hence

$$n_+(x) = \hat{n}_+(x) + \hat{n}_+(x) = n_+(x)$$

(4.82)

for the total thermoballistic density $n_+(x)$ in the drift-diffusion limit.

The persistent part of the thermoballistic spin-polarized density, $\hat{n}_-(x)$, is obtained from Eq. (4.67) as

$$\hat{n}_-(x) = \frac{N_c}{2}B_-(x)[\bar{A}(x) + \frac{1}{2}P(x)A(x)],$$

(4.83)

and the relaxing part of the thermoballistic spin-polarized density, $\hat{n}_-(x)$, from Eq. (4.68) as

$$\hat{n}_-(x) = \frac{N_c}{4}[B_+(x) - P(x)B_-(x)]A(x) = \frac{N_c}{4}B_+(x)Q^2(x)A(x),$$

(4.84)

with $Q(x)$ given by Eq. (4.19). Then, re-expressing the spin-polarized equilibrium density $n_-(x)$ [see Eq. (4.19)] in the form

$$n_-(x) = \frac{N_c}{2}[B_-(x)\bar{A}(x) + \frac{1}{2}P(x)B_+(x)A(x)],$$

(4.85)

we have

$$n_-(x) \equiv \hat{n}_-(x) + \hat{n}_-(x) = n_-(x)$$

(4.86)

for the thermoballistic spin-polarized density $n_-(x)$ in the drift-diffusion limit.

The net total ballistic current $J_+(x', x'')$ is found from Eq. (4.62), by expanding to first order in $x' - x$ and $x'' - x$, in the form

$$J_+(x', x'') = \frac{\nu}{2}N_c B_+(x)\bar{A}(x')(x' - x''),$$

(4.87)

where

$$\bar{A}(x) = \frac{d\bar{A}(x)}{dx} + \frac{1}{2}P(x)\frac{dA(x)}{dx}.$$

(4.88)

Now, evaluating the double integral over $x'$ and $x''$ in Eq. (4.71) for $F(x', x''; x) = x' - x''$ and taking the limit $\delta \to 0$ at fixed $l > 0$, we are left with a factor $-2l$, so that the drift-diffusion limit of the total thermoballistic current $\bar{J}_+(x)$ is given by

$$\bar{J}_+(x) = -\frac{\nu}{2}N_c B_+(x)\bar{A}(x) \equiv J.$$

(4.89)

Here, we have used relation (4.69) to introduce the electron mobility $\nu$, and we have identified the constant, total thermoballistic current in the drift-diffusion regime with the (conserved) total physical current $J$. Then, using Eqs. (4.80) and (4.89), we can express $J$ in terms of the equilibrium densities $n_\pm(x)$ [see Eqs. (4.82) and (4.86)] in the form

$$J = -\frac{\nu}{e} \left[ n_+(x) \left( \frac{dE_c(x)}{dx} + \frac{1}{\beta} \frac{dn_+(x)}{dx} + \frac{1}{2}n_-(x) \frac{d\Delta(x)}{dx} \right) \right].$$

(4.90)

For zero spin splitting, $\Delta(x) = 0$, this expression becomes equivalent to expression (2.28) for the total current in
the standard drift-diffusion model. However, by contrast with the latter model, we have obtained Eq. (4.90) without invoking the Einstein relation \[ (2.22) \]. This feature can be traced back to the probabilistic description underlying the thermoballistic approach (see Sec. III A), which allows the diffusion current to be directly expressed in terms of the collision time (and hence of the momentum relaxation length \( l \)) [see Eq. (4.83)].

To obtain an explicit expression for the mean spin function \( \hat{A}(x) \), and hence for the average chemical potential \( \bar{\mu}(x) \), we observe that in the drift-diffusion regime the total thermoballistic density \( n_+(x) \) is equal to the total equilibrium density \( n_+(x) \) [see Eq. (4.82)], which, in turn, is related to \( \hat{A}(x) \) via Eq. (4.80). Using Eq. (4.88) to solve Eq. (4.89) for \( d\hat{A}(x)/dx \), integrating over the interval \([x_1, x]\), and using Eqs. (4.83) - (4.85) to simplify the integrals, we can express \( \mu(x) \) in the form

\[
e^{\beta\mu(x)} = e^{\beta\bar{\mu}(x_1)} - \frac{e^{\beta J}}{N_c \nu} \int_{x_1}^{x} dx' e^{\beta E_c(x')} Q(x') - \frac{\beta}{4} \int_{x_1}^{x} dx' \frac{dA(x')}{dx'} Q(x') A(x'),
\]

(4.91)

which generalizes expression \[ (2.31) \]. Integration over the interval \([x, x_2]\) leads to another expression for \( \bar{\mu}(x) \), which is different in form, but numerically equal to expression \[ (4.91) \]. The drift-diffusion form of the spin accumulation function \( \hat{A}(x) \) in expression \[ (4.91) \] is determined by a differential equation [see Eq. (4.100) below].

We now set \( x = x_2 \) in Eq. (4.91) and identify the boundary values of \( \bar{\mu}(x) \) at the interface positions \( x_{12} \) with the values, \( \mu_{12} \), of the equilibrium chemical potential at the contact side of the contact-semiconductor interfaces,

\[
\bar{\mu}(x_{12}) = \mu_{12}
\]

(4.92)

[see Eq. (2.32)], so that from Eq. (4.14)

\[
\hat{A}(x_{12}) = e^{\beta \mu_{12}} = \eta_{12}.
\]

(4.93)

Similarly, we identify the boundary values of \( A(x) \) with external values \( A_{12} \),

\[
A(x_{12}) = A_{12}.
\]

(4.94)

We then obtain the drift-diffusion form of the current-voltage characteristic, which, for simplicity, is written down here for the case of constant spin splitting, when \( d\Delta(x)/dx = 0 \), \( P(x) = P \), and \( Q(x) = Q \),

\[
J = \nu \frac{N_c}{\beta e Q S} e^{-\beta [E^{*}_c(x_1, x_2) - \mu_1]} \times [1 - e^{-\beta e V} + \frac{1}{2} e^{-\beta \mu_1} P(A_1 - A_2)].
\]

(4.95)

Here, we have used Eqs. (2.34) and (2.36), respectively, to introduce the voltage bias \( V \) and the effective sample length \( S \).

For zero spin splitting, when \( P(x) = 0 \) and \( Q(x) = 1 \), expressions (4.91) and (4.95) become equivalent to the expressions (2.31) and (2.33), respectively, in the standard drift-diffusion model.

The drift-diffusion limit of the persistent thermoballistic spin-polarized current \( \hat{J}_-(x) \) immediately follows from Eqs. (4.63) and (4.89) as

\[
\hat{J}_-(x) = -\nu \frac{N_c}{2\beta e} B_-(x) \hat{A}(x) = JP(x),
\]

(4.96)

so that \( \hat{J}_-(x) \) is zero for zero spin splitting.

Proceeding in analogy to the derivation of \( \hat{J}_+(x) \), we find the drift-diffusion limit of the relaxing thermoballistic spin-polarized current \( \hat{J}_-(x) \) from Eqs. (4.63) and (4.71) in the form

\[
\hat{J}_-(x) = -\nu \frac{N_c}{2\beta e} B_+(x) Q_2(x) \frac{dA(x)}{dx},
\]

(4.97)

Using Eq. (4.88), we can express \( \hat{J}_-(x) \) in terms of the analogous thermoballistic density \( \eta_-(x) \),

\[
\hat{J}_-(x) = -\frac{\nu}{e} \left[ \hat{B}_+(x) \hat{n}_-(x) + \frac{1}{\beta} \frac{d\hat{n}_-(x)}{dx} \right],
\]

(4.98)

where

\[
\hat{B}_+(x) = -\frac{1}{\beta} \frac{d \ln(B_+(x) Q^2(x))}{dx}.
\]

(4.99)

so that \( \hat{B}_+(x) = dE_c(x)/dx \) for zero spin splitting.

Inserting expressions (4.97) and (4.84) for \( \hat{J}_-(x) \) and \( \eta_-(x) \), respectively, in the general balance equation (5.9), we obtain a homogeneous second-order differential equation for the spin accumulation function \( A(x) \),

\[
\frac{d^2 A(x)}{dx^2} - \beta \hat{B}_+(x) \frac{dA(x)}{dx} - \frac{1}{L_s^2} A(x) = 0,
\]

(4.100)

where

\[
L_s = \sqrt{\beta l_s}
\]

(4.101)

is the spin diffusion length. Equation (4.100) can be converted into an analogous equation for the density \( \eta_-(x) \),

\[
\frac{d^2 \hat{n}_-(x)}{dx^2} + \beta \frac{d}{dx} \left[ \hat{B}_+(x) \hat{n}_-(x) \right] - \frac{1}{L_s^2} \hat{n}_-(x) = 0,
\]

(4.102)

where Eq. (4.84) has been used. For zero spin splitting, this equation generalizes, by including arbitrarily shaped potential energy profiles, the drift-diffusion equation commonly used to describe electric-field effects in spin-polarized transport in semiconductors [see Eq. (2.8) of Ref. 66]; in that equation, the spin diffusion length appears as \( \sqrt{D_{\tau_s}} \) with \( D \) an effective diffusion coefficient and \( \tau_s \) the spin relaxation time]. Note that, in contrast to Eq. (4.100) for \( A(x) \), Eq. (4.102) for \( \eta_-(x) \) contains terms proportional to the first and second derivatives of \( E_c(x) \) [see Eq. (4.99)].
3. Ballistic limit

In the strictly ballistic limit, when \( l \to \infty \), there are no points of local thermodynamic equilibrium in the interval \([x_1, x_2]\), and the average chemical potential \( \tilde{\mu}(x) \) is not defined inside this interval. Expression (4.71) reduces to

\[
\tilde{\mathfrak{J}}(x) = F(x_1, x_2; x),
\]

(4.103)
i.e., the thermoballistic currents and densities are given by the corresponding expressions for the net ballistic currents and joint ballistic densities (see Sec. IV B 3), evaluated at \( x' = x_1 \) and \( x'' = x_2 \). In expressions (4.62), (4.65), (4.67), and (4.68), the boundary values of the mean spin function, \( \tilde{A}(x_1, 2) \), and those of the spin accumulation function, \( A(x_1, 2) \), are to be identified with the corresponding values in the contacts [see Eqs. (4.93) and (4.94), respectively].

From Eq. (4.102), we then obtain the total thermoballistic current \( \tilde{J}_+(x) \) in the form

\[
\tilde{J}_+(x) = J_+(x_1, x_2) = v_cN_e B_+^m(x_1, x_2)[\eta_{12} + \frac{1}{2}P^m(x_1, x_2)A_{12}],
\]

(4.104)
where

\[
\eta_{12} = \eta_1 + \eta_2,
\]
with \( \eta_{1,2} \) defined by Eq. (4.93), and

\[
A_{12}^+ = A_1 + A_2.
\]

(4.105)
For zero spin splitting, expression (4.104) becomes equivalent to expression (2.56) for the total current in the ballistic transport model. The ballistic limit of the persistent thermoballistic spin-polarized current \( \tilde{J}_-(x) \) is obtained from \( \tilde{J}_+(x) \) by replacing in expression (4.104) the quantity \( B_+^m(x_1, x_2) \) with \( B_+^m(x_1, x_2) \) [see Eqs. (4.23) and (4.64)].

For the total thermoballistic density \( n_+(x) \), we have, defining

\[
A_{12}^+(x_1, x_2; x) = A_1 e^{-c_m(x_1, x_2; x, x)/\beta}, \\
\pm A_2 e^{-c_m(x_1, x_2; x, x)/\beta},
\]
and using Eqs. (4.66–4.68),

\[
n_+(x) = n_+(x_1, x_2; x) = \tilde{n}_+(x_1, x_2; x) + \tilde{n}_+(x_1, x_2; x) = \frac{N_e}{4} \left\{ D_+^m(x_1, x_2; x) \eta_{12} + \frac{1}{2}P^m(x_1, x_2)A_{12}^+ \right\} \\
+ \frac{1}{2}P_+^m(x_1, x_2; x)A_{12}^+(x_1, x_2; x).
\]

(4.107)
For zero spin splitting, this becomes equivalent to expression (2.60).

Further, using Eq. (4.65) and (4.68), we express the relaxing thermoballistic spin-polarized current \( \tilde{J}_-(x) \) and the corresponding density \( \tilde{n}_-(x) \) as

\[
\tilde{J}_-(x) = J_-(x_1, x_2; x) = \frac{v_cN_e}{4} B_+^m(x_1, x_2)A_{12}^+(x_1, x_2; x)
\]

(4.100)
and

\[
\tilde{n}_-(x) = \tilde{n}_-(x_1, x_2; x) = \frac{N_e}{8} D_+^m(x_1, x_2; x)A_{12}^+(x_1, x_2; x),
\]

(4.110)
respectively. In view of Eq. (4.109), the current \( \tilde{J}_-(x) \) and density \( \tilde{n}_-(x) \) in the ballistic limit are trivially connected by the general balance equation (5.9).

4. Thermoballistic energy dissipation

The stochastic equilibration of the electrons that occurs during their motion across the sample is associated with the dissipation of energy, i.e., the net transfer of energy out of the ensemble of conduction band electrons into a reservoir (“heat bath”) of electrons in thermodynamic equilibrium.

To describe this transfer within the thermoballistic concept, we introduce the (conserved) ballistic energy currents \( \mathcal{E}^{l,r}(x', x'') \) generated by thermal electron emission at the end-points \( x' \) and \( x'' \), respectively, of the ballistic interval \([x', x'']\). Neglecting spin degrees of freedom, we have for the current \( \mathcal{E}^{l}(x', x'') \), by an obvious modification of expression (2.47), for the electron current \( J^l(x_1, x_2) \), writing \( \epsilon = m_v^2 v^2/2 \),

\[
\mathcal{E}^l(x', x'') = \frac{4\pi m_v^4}{3\hbar^3} \int_0^\infty d\epsilon e^{-\beta[\epsilon + E_c(x') - \tilde{\mu}(x')]} \times \Theta(\epsilon - E^l_b(x', x'')), \quad (4.111)
\]

where, in analogy to Eq. (2.35),

\[
E^l_b(x', x'') = E^m_c(x', x'') - E_c(x')
\]

(4.112)
is the maximum barrier height of the potential energy profile \( E_c(x) \) relative to its value at \( x' \). Evaluating the integral in expression (4.111), we obtain, in extension of Eq. (2.48),

\[
\mathcal{E}^l(x', x'') = v_c N_e \left\{ \frac{1}{\beta} + E^l_b(x', x'') \right\} e^{-\beta[E^m_c(x', x'') - \tilde{\mu}(x')]}.
\]

(4.113)
For the ballistic energy current \( \mathcal{E}^l(x', x'') \), we have

\[
\mathcal{E}^l(x', x'') = -\mathcal{E}^l(x'', x'),
\]

(4.114)
in line with Eq. (4.68) for the corresponding ballistic electron current, and for the net ballistic energy current in the interval \([x', x'']\),

\[
\mathcal{E}(x', x'') = \mathcal{E}^l(x', x'') + \mathcal{E}^r(x', x''),
\]

(4.115)
in line with Eq. (4.60) for the net ballistic electron current.

Now, we again introduce a “reference coordinate” \( x \) inside the sample, whose meaning, however, differs from
that of the coordinate \( x \) in the definition (4.71) of the thermoballistic currents and densities. While in that definition, \( x \) is a coordinate inside ballistic intervals, we here consider \( x \) a coordinate characterizing the position of a point of local thermodynamic equilibrium. More precisely, we consider a collection of such points, with density \( dx/l \), in an interval \( dx \) centered about \( x \), in which ballistic energy currents are absorbed from, and emitted towards, either side. The equilibrium point \( x \), where incoming electron currents are completely equilibrated and the outgoing currents are solely determined by the parameters of the reservoir (i.e., by the chemical potential), dynamically separates the two sample partitions to the left and right of \( x \).

We denote by \( \mathcal{W}_\text{in}(x) \) the (kinetic) energy transferred per unit volume and unit time into the reservoir by absorption of electrons at the point \( x \), and correspondingly by \( \mathcal{W}_\text{out}(x) \) the change in energy of the reservoir due to thermal electron emission out of it. The net energy \( \mathcal{W}(x) \), i.e., the energy dissipated locally at the point \( x \), is then given by

\[
\mathcal{W}(x) = \mathcal{W}_\text{in}(x) + \mathcal{W}_\text{out}(x). \tag{4.116}
\]

The energies \( \mathcal{W}_\text{in}(x) \) and \( \mathcal{W}_\text{out}(x) \) are each composed of two parts (see also Fig. 5). One part of \( \mathcal{W}_\text{in}(x) \) is given by the weighted sum of the energy currents \( E(x',x'') \) over all ballistic intervals \([x',x'']\) lying to the left of \( x \) and having their right end at \( x'' = x \), where the currents are absorbed. The other part is expressed analogously in terms of the currents \( E'(x',x'') \) in ballistic intervals to the right of the absorption point \( x \). For the energy \( \mathcal{W}_\text{in}(x) dx \) dissipated in an interval \( dx \) centered around \( x \), we then have

\[
\mathcal{W}_\text{in}(x) dx = \frac{dx}{l} \{F_1(x; E) + F_2(x; E')\}. \tag{4.117}
\]

Here, the functionals \( F_1(x; E) \) and \( F_2(x; E') \) are given, for an arbitrary ballistic current \( F(x',x';x) \), by Eqs. (4.75) and (4.76), respectively. The energy current \( \mathcal{W}_\text{out}(x) dx \) is obtained from Eq. (4.117) by interchanging the role of \( E'(x',x'') \) and \( E(x',x'') \),

\[
\mathcal{W}_\text{out}(x) dx = \frac{dx}{l} \{F_1(x; E') + F_2(x; E)\}, \tag{4.118}
\]

which comprises all ballistic energy currents emitted at the point \( x \) towards either side. For the dissipated energy \( \mathcal{W}(x) \), we then have

\[
\mathcal{W}(x) = \frac{1}{l} \{F_1(x; E) + F_2(x; E')\}, \tag{4.119}
\]

where the net ballistic energy current \( E(x',x'') \) is given by Eq. (4.115).

We note that in obtaining expression (4.119) for \( \mathcal{W}(x) \) we have not drawn on the thermoballistic energy current \( E(x) \) that results from identifying in Eq. (4.71) the function \( F(x',x'';x) \) with net ballistic energy current \( E(x',x'') \). Naively, one might expect that the dissipated energy \( \mathcal{W}(x) \) can be represented by the derivative \((\partial/\partial x^+ + \partial/\partial x^-)E(x)\) given by Eq. (4.73). However, comparing expressions (4.119) and (4.73), one observes that the contributions of the ballistic energy currents from the two sides of \( x \) add up in the former, and are subtracted from one another in the latter. The result (4.119) can be obtained from the thermoballistic energy current \( E(x) \) in the form

\[
\mathcal{W}(x) = -\left(\frac{\partial}{\partial x^+} - \frac{\partial}{\partial x^-}\right)E(x), \tag{4.120}
\]

at variance with expression (4.73).

We do not write down here the general expression for \( \mathcal{W}(x) \) in terms of the average chemical potential \( \bar{\mu}(x) \) obtained by using expressions (4.113)–(4.115) in Eq. (4.119), and confine ourselves to considering the ballistic limit and the drift-diffusion regime. Owing to the overall factor \( 1/l \) in the right-hand side of Eq. (4.119), \( \mathcal{W}(x) \) vanishes in the ballistic limit \( l \to \infty \), which reflects the complete absence of equilibration in this limit. In the drift-diffusion regime, on the other hand, when \( l \ll S \), only the integral terms contribute. We evaluate these terms for the special case of a homogeneous sample subjected to a constant external electric field of magnitude \( E \) directed antiparallel to the \( x \)-axis, so that the potential energy profile has the form

\[
E_\epsilon(x) = E_\epsilon(x_1) - \frac{e}{\beta}(x - x_1), \tag{4.121}
\]

where

\[
\epsilon = \beta e E. \tag{4.122}
\]

For this profile, the average chemical potential \( \bar{\mu}(x) \) is found from Eqs. (2.31) and (2.33), using the relation \( \epsilon S = \beta e V \), to run parallel to the profile,

\[
\bar{\mu}(x) = [\mu_1 - E_\epsilon(x_1)] + E_\epsilon(x). \tag{4.123}
\]

Therefore, the total equilibrium electron density is constant, \( n(x) = n(x_1) \). The net ballistic energy current \( E(x',x'') \) can now be expressed as

\[
E(x',x'') = \frac{\nu_e}{\beta} n(x_1) \left\{ 1 - e^{-\epsilon (x'' - x')} \right\} \left[ 1 + e(\epsilon(x'' - x')) \right]
\approx \frac{\nu_e}{2\beta} n(x_1) e^2 (x'' - x')^2, \tag{4.124}
\]

where the second, approximate equation holds in the zero-bias limit \( \epsilon S \ll 1 \). Inserting the approximate representation of \( E(x',x'') \) in the integral terms of expression (4.119), we find for the locally dissipated energy \( \mathcal{W}(x) \) in the drift-diffusion regime

\[
\mathcal{W}(x) \equiv \mathcal{W} = \frac{2\nu_e}{\beta} ln(x_1) e^2 = \sigma \left( \frac{V}{S} \right)^2, \tag{4.125}
\]

where we have introduced the conductivity \( \sigma \) via Eqs. (2.16) and (2.19). For the total energy \( W = \mathcal{W}S \) dissipated per unit time (“heat production”) in a sample with cross-sectional area \( A \) and resistance \( R = S/\sigma A \), we then recover the Ohmic expression \( W = V^2/R \).
D. Synopsis of the thermoballistic concept

We conclude this section with a synopsis of the concept underlying the thermoballistic description of charge carrier transport in semiconductors, in which we briefly comment on its basic ingredients and elucidate the physical content of its formal structure. This will be followed by an assessment of its merits as well as its weaknesses.

1. Ingredients and physical content

The basic ingredients of the (semiclassical) thermoballistic concept are the ballistic carrier currents and densities which are constructed within the following framework. (i) Thermal emission of carriers occurs at points of local thermodynamic equilibrium randomly distributed over the sample. (ii) The equilibrium points link “ballistic transport intervals” across which the emitted carriers move ballistically under the influence of potential energy profiles arising from internal and external electrostatic potentials. During their ballistic motion, the carriers undergo spin relaxation controlled by a ballistic spin relaxation length $l_s$. (iii) At the end-points of the ballistic intervals, instantaneous “point-like” thermalization (“absorption”) of the carriers takes place. Here, we invoke the picture of “reflectionless contacts”\(^{32-34}\), according to which the ballistic carriers that enter a contact (representing a “bath” with an effectively infinite number of transverse modes) are completely absorbed there, after having been emitted from a similar contact at the opposite end of the sample. In the thermoballistic concept, the emission and absorption of carriers are treated in this way at all points of local thermodynamic equilibrium inside the sample. At these points, the absorption of carriers into the bath is complete (“reflectionless”), but at the same instant carriers are emitted out of the bath into the ballistic intervals on either side. The opposing collision-free currents emitted at either end into the ballistic interval combine to form a net ballistic current inside the interval, with an associated joint ballistic density.

The random distribution of points of local thermodynamic equilibrium is mirrored in a random partitioning of the length of the sample into ballistic intervals, where each partition defines a “ballistic configuration”, a central notion of the concept. The ballistic carrier currents and densities in these configurations are assembled to form the corresponding thermoballistic currents and densities. These are constructed, at a reference position $x$ located arbitrarily inside the sample, by performing weighted summations, with weights controlled by a momentum relaxation length $l$, over the net ballistic currents and joint ballistic densities in all ballistic intervals containing the point $x$. The thermoballistic currents and densities constitute the key element of the thermoballistic concept.

The physical content of the thermoballistic transport mechanism can be exhibited by analyzing the underlying formalism with regard to the intertwined effects of thermal electron emission and ballistic motion. Let us consider expressions (4.62)–(4.68) for the net ballistic currents and joint ballistic densities, which are essentially composed of two factors each. On the one hand, they contain the nonlocal barrier factors $B^m_\pm(x', x'')$ and $B^{\mu\nu}_\pm(x', x'')$ in the expressions for the total and persistent spin-polarized currents and the relaxing spin-polarized current, respectively, and the factors $D^{m\mu}_\pm(x', x''; x)$ and $D^{\mu\nu}_\pm(x', x''; x)$ in the analogous expressions for the densities. These factors describe the collision-free motion of the electrons across the ballistic interval $[x', x'']$, which is essentially determined by the potential energy profiles $E_{\pm, \pm}(x)$ inside the interval. They represent the ballistic attribute of thermoballistic transport. The factors in brackets, on the other hand, contain terms depending on the average chemical potentials $\bar{\mu}(x')$, $\bar{\mu}(x'')$ and the spin accumulation functions $A(x')$, $A(x'')$, which are directly related to the spin-resolved chemical potentials $\mu_{\pm, \pm}(x')$, $\mu_{\pm, \pm}(x'')$ at the end-points $x'$, $x''$ of the ballistic interval. These factors, which describe the thermal emission (“thermal activation”) of the ballistic currents at the points of local thermodynamic equilibrium at $x'$ and $x''$, respectively, represent the thermal attribute of thermoballistic transport. The term in brackets is the “activation term”. [The joint appearance of ballistic and thermal attributes shows that the term “thermoballistic” indeed provides an appropriate characterization of our approach.]

The contributions of the ballistic currents and densities (4.62)–(4.68), summarily denoted by $F(x', x''; x)$, to the corresponding thermoballistic currents and densities $\tilde{J}(x)$ are to be read from Eq. (4.71): they are given by the current (or density) $F(x', x''; x)$ in the interval $[x', x'']$, multiplied by the probability $e^{-\beta(x''-x')/l}$ that the electrons traverse this interval ballistically.

The momentum relaxation length $l$ controls the magnitude of the ballistic contribution to the entire transport process. At the same time, it determines the average number of collisions, $S/l$, in a sample of length $S$. In the ballistic limit, when $l \to \infty$ and there is no point of local thermodynamic equilibrium inside the sample, the transport is purely ballistic between the end-points $x_1$ and $x_2$, and only the first term on the right-hand side of Eq. (4.71) contributes. In the opposite limit, when $l \to 0$, the points of local thermodynamic equilibrium at which the electrons are equilibrated, lie infinitesimally close to one another. Then only the double integral in Eq. (4.71) survives, and we arrive at

$$\tilde{J}_+(x) = -v_c N_c IB_+(x) \frac{d}{dx} e^{\beta\tilde{\mu}(x)}$$  \hspace{1cm} (4.126)

for the total thermoballistic current $\tilde{J}_+(x) = J$ [see Eq. (4.33)]. This current is essentially given in terms of equilibrium quantities, a property that characterizes the drift-diffusion limit. Expression (4.126) has the form of the current in the standard drift-diffusion approach.
\[ \mathcal{J}_+(x) = -\frac{\nu}{e} n_+(x) \frac{d\tilde{\mu}(x)}{dx}, \quad (4.127) \]

where \( \nu \) is the electron mobility given by Eq. (3.69), and \( n_+(x) \) the equilibrium electron density given by Eq. (4.80). In that approach, the momentum relaxation length \( l \) is nonzero (so that \( \nu \) remains nonzero), but small compared with the length scales over which the other parameters vary appreciably. The activation term reduces to a derivative, and the relation between the total thermoballistic current and the average chemical potential becomes a local one.

2. Merits and weaknesses

The principal merit of the thermoballistic concept is that it allows to establish a consistent and transparent formalism for bridging, within the semiclassical approximation, the gap between the standard drift-diffusion and ballistic descriptions of charge carrier transport in semiconductors. While incorporating basic features of these descriptions, the thermoballistic concept consistently unifies and generalizes them by introducing random partitionings of the sample length into ballistic configurations.

The concept is transparent in a twofold way. First, as shown above, a lucid interpretation of its physical content can be given in terms of ballistic and thermal attributes. Second, owing to its semiclassical character, the concept allows the effects of the different parameters describing a semiconducting system to be clearly distinguished. In the implementation of this concept, explicit equations for various transport quantities can be derived, and simple solutions can be obtained in important special cases. The merit of transparency of the thermoballistic concept carries with it some simplifications and weak points which, however, in many cases can be remedied, albeit at the cost of increased complexity: they are not detrimental to the concept as a whole.

While the formulation of the full thermoballistic concept given here describes semiclassical transport in non-degenerate semiconducting systems, we have demonstrated within the prototype model how effects of electron tunneling and degeneracy can be taken into account. Quantum interference effects in the electron motion are not treated explicitly, but they may be assumed to be implicitly incorporated via an extended interpretation of the mean free path (or momentum relaxation length) \( l \), which from the outset has been taken as a phenomenological parameter. By treating it formally as the average distance that the carriers travel without collision between points of complete thermodynamic equilibrium, as in the relaxation time approximation, it simulates the effects of incomplete equilibration due to elastic or inelastic impurity scattering, of dimensionality, and, in the extreme, of quantal phase correlations.

Indeed, in this work the momentum relaxation length \( l \) is the determining parameter in which a great diversity of detail is subsumed. It is introduced as a constant, so it must include in an average way the effect of spatial variations in the internal and external parameters characterizing the semiconducting system; in particular, this constant is chosen to be independent of the potential energy profile, to which, however, it should be related in a self-consistent way. Moreover, the choice of the momentum relaxation length \( l \), rather than the relaxation time \( \tau \), is also merely one of convenience for the stationary treatment in this work. We may work with position-dependent momentum relaxation lengths, but this would increase the complexity of the formalism and obscure the general line of argument.

The spin relaxation mechanism in terms of the ballistic spin relaxation length \( l_s \) is again a phenomenological one, having certain similarities with the D’yakonov-Perel’ mechanism. We assume spin relaxation to occur only during the ballistic electron motion; however, simultaneous spin and momentum relaxation could be taken into account by introducing additional terms in the spin balance equation.

In principle, the thermoballistic concept allows a fully three-dimensional treatment of bipolar carrier transport to be implemented. However, in the present paper, in order to keep the formalism manageable, we work within a narrowed framework. First, we confine ourselves to unipolar transport, dealing specifically with electron transport in a spin-split conduction band. Second, we consider three-dimensional “plane-parallel” samples whose parameters (in particular, the average density of the scattering centers associated with impurities) do not vary in the directions perpendicular to the transport direction (the \( x \)-direction). Nevertheless, electron transport in this kind of sample depends on the number of dimensions, \( n \), via “no-scattering probabilities” \( p_n(x) \) [see Sec. II of Ref. 54]. Here, in order to be able to write down physically transparent formulae, we use one-dimensional no-scattering probabilities of the form \( p_1(x) = e^{-x/l} \) (see Sec. IIIA).

V. THERMOBALLISTIC APPROACH: IMPLEMENTATION

Having presented, in the preceding section, the concept underlying the thermoballistic approach, we now turn to the implementation of this concept. We begin by establishing the physical conditions from which the algorithms for calculating the dynamical functions, \( \nu(x) \), the average chemical potential \( \tilde{\mu}(x) \) [via the mean spin function \( \tilde{A}(x) \)] and the spin accumulation function \( A(x) \), are developed. Thereafter, these algorithms will be described in detail.
A. Physical conditions determining the dynamical functions

We call physical conditions (i) a relation introduced to connect the total thermoballistic current \( \mathcal{J}_+ (x) \) with the cognate total physical current \( J \), which allows us to calculate the function \( \tilde{A}(x) \), and (ii) an assumption concerning the detailed spin relaxation mechanism, which leads to the determination of the function \( A(x) \).

1. Determination of the mean spin function

The current \( \mathcal{J}_+ (x) \equiv \mathcal{J}_+ (x_1, x_2; x; l) \), owing to its construction in terms of ballistic currents averaged over random ballistic configurations (with weights controlled by the momentum relaxation length \( l \)), is to be interpreted as an “ensemble average” of the electron current at the point \( x \). This average is spatially varying, and, therefore, it is the spatial average of the ensemble average over the length of the sample which is to be identified with the (constant) total physical current \( J \) inside the sample. By current conservation at \( x_1 \) and \( x_2 \), this current is equal to the total current \( J \) in the left and right leads, so that we have

\[
\frac{1}{x_2 - x_1} \int_{x_1}^{x_2} dx \mathcal{J}_+ (x_1, x_2; x; l) = J_+ \equiv J. \tag{5.1}
\]

In this condition, the current \( \mathcal{J}_+ (x_1, x_2; x; l) \) is defined at a ballistic point \( x \) located inside an ensemble of ballistic intervals \([x', x'']\), where \( x' \) and \( x'' \), unlike \( x \), are points of local thermodynamic equilibrium [see Eqs. (4.70) and (4.71)]. The integration over \( x \) starts at the fixed equilibrium point \( x_1 \) and ends at the fixed equilibrium point \( x_2 \). Now, just as we have introduced the ballistic reference point \( x \), we consider here an equilibrium point of reference, i.e., a point of local thermodynamic equilibrium anywhere inside the sample, which, again, is labeled by the coordinate \( x \) for \( x_1 < x < x_2 \). Such a point acts in the same way as the fixed equilibrium points \( x_1 \) and \( x_2 \). The ballistic current entering \( x \), say, from the left, is completely absorbed, whereupon a thermal current is instantaneously emitted to either side of \( x \). The same happens to the current entering the equilibrium point \( x \) from the right. However, in contrast to the “true”, externally controlled equilibrium points \( x_1, x_2 \), which are located at the contact side of the contact-semiconductor interfaces, no Sharvin-type interface resistance (see Sec. B3) appears at \( x \).

Within this scheme, we introduce the thermoballistic current \( \mathcal{J}_+^{(1)} (x_1, x; \xi; l) \), with \( x_1 < \xi < x \leq x_2 \), where \( x \) is an equilibrium point, and \( \xi \) a ballistic point. In conformance with Eq. (5.1), the spatial average of this current over the range \([x_1, x]\) is again, by current conservation at \( x_1 \), equal to the physical current in the left lead, so that

\[
\frac{1}{x - x_1} \int_{x_1}^{x} dx \mathcal{J}_+^{(1)} (x_1, x; \xi; l) = J. \tag{5.2}
\]

Analogously, we have for the thermoballistic current \( \mathcal{J}_+^{(2)} (x, x_2; \xi; l) \) in the range \([x, x_2]\), using similar arguments as above,

\[
\frac{1}{x_2 - x} \int_{x}^{x_2} dx \mathcal{J}_+^{(2)} (x, x_2; \xi; l) = J \tag{5.3}
\]

\((1 \leq x < \xi \leq x_2)\). Equations (5.2) and (5.3), when expressed in terms of the function \( \tilde{A}(x) \) via Eqs. (4.62) and (4.71), lead to two different Volterra-type integral equations with solutions \( \tilde{A}_1 (x) \) and \( \tilde{A}_2 (x) \), respectively. Trivially, by satisfying Eqs. (5.2) and (5.3), these solutions also satisfy condition (5.1). They define, for given spin accumulation function \( \tilde{A}(x) \), two different total equilibrium densities \( n_1^{(1)} (x) \) and \( n_2^{(2)} (x) \), respectively, via Eq. (4.80). The total equilibrium density at \( x \) is obtained as the mean value of these,

\[
n_+ (x) = \frac{1}{2} [n_1^{(1)} (x) + n_2^{(2)} (x)], \tag{5.4}
\]

so that, using Eq. (4.80) again, we have for the unique (thermoballistic) mean spin function

\[
\tilde{A}(x) \equiv e^{\beta \mu(x)} = \frac{1}{2} [\tilde{A}_1 (x) + \tilde{A}_2 (x)]. \tag{5.5}
\]

The physical conditions (5.2) and (5.3), together with Eq. (5.4), determine the procedure for calculating the average chemical potential \( \bar{\mu}(x) \). Using the mean value (5.4) as the point of departure for constructing \( \bar{\mu}(x) \) reflects the fact that this function expresses an intrinsic property of the semiconducting sample, with no preference for one or the other of the sample ends at \( x_1 \) and \( x_2 \). With \( \tilde{A}(x) \) given by Eq. (5.5), it follows from Eqs. (4.62) and (4.71) that the unique thermoballistic current \( \mathcal{J}_+ (x_1, x_2; x; l) \) is given by

\[
\mathcal{J}_+ (x_1, x_2; x; l) = \frac{1}{2} [\mathcal{J}_+^{(1)} (x_1, x_2; x; l) + \mathcal{J}_+^{(2)} (x_1, x_2; x; l)], \tag{5.6}
\]

a symmetric combination as in Eq. (5.5).

We note that in Ref. [54] we have applied a different procedure for constructing the average chemical potential \( \bar{\mu}(x) \). There, the combination of the functions \( \tilde{A}_1 (x) \) and \( \tilde{A}_2 (x) \) was not chosen to be symmetric as in Eq. (5.5), but was determined by the requirement that the values of the unique total thermoballistic current at the two sample ends be equal,

\[
\mathcal{J}_+ (x_1, x_2; x_1^*; l) = \mathcal{J}_+ (x_1, x_2; x_2^*; l). \tag{5.7}
\]

This condition derives from postulating that the position dependence of the total thermoballistic current is compensated by that of a “background current” \( \mathcal{J}_B (x) \) such that these currents add up to the (conserved) total physical current. The background current is assumed to be fed by sources and sinks whose effect averages out to zero when the current is integrated over the length of the sample. In the present work, this hypothesis has been abandoned for being unphysical.
2. Determination of the spin accumulation function

In the thermoballistic transport mechanism, we assume that spin relaxation takes place only inside the ballistic intervals (see Sec. \[V B 3\]), and that an infinitesimal shift of the end-points of the ballistic intervals does not affect the current \(\tilde{J}_-(x)\). Accordingly, we set the term arising from differentiating the limits of integration in expression (4.14) for \(\tilde{J}_-(x)\) equal to zero,

\[
\tilde{J}_-(x) = 0. \quad (5.8)
\]

From Eq. (4.78), the relaxing thermoballistic spin-polarized current and density are then seen to be connected by the balance equation

\[
\frac{d}{dx} \tilde{J}_-(x) + 2v_e \tilde{n}_-(x) = 0, \quad (5.9)
\]

which is of the same form as the balance equation (4.69) connecting the relaxing spin-polarized current and density in the individual ballistic intervals.

The spin accumulation function \(A(x)\), and hence the relaxing thermoballistic spin-polarized current \(\tilde{J}_-(x)\), are determined by condition (5.8). When written in terms of \(A(x)\) by using expression (4.65) in Eq. (4.74), this condition turns into a linear, inhomogeneous Fredholm-type integral equation of the second kind for \(A(x)\). The explicit form of this equation and its conversion, in a specific case of particular importance, into a differential equation will be the subject of Sec. \[V C\].

B. Average chemical potential

The average chemical potential \(\tilde{\mu}(x)\) is determined, via expression (5.5) for the mean spin function \(\tilde{A}(x)\), by the solutions \(A_1, A_2(x)\) of the integral equations (5.2) and (5.3), respectively, which are conveniently solved in terms of "resistance functions".

1. The resistance functions

We begin by considering Eq. (5.2). To solve it for the function \(\tilde{A}_1(x)\), we define functions \(\mathfrak{A}_1(x)\) and \(\mathfrak{A}(x)\) via

\[
\tilde{A}_1(x) = \frac{v_e N_c}{J} B_{A}^{m}(x_1, x_2) - A_1(x) \quad (5.10)
\]

and

\[
\mathfrak{A}(x) = \frac{v_e N_c}{J} B_{A}^{m}(x_1, x_2) A(x) \quad (5.11)
\]

where the spin accumulation function \(A(x)\) is assumed to be given. Furthermore, we introduce the "resistance function" \(\mathfrak{R}_1(x)\) [the choice of this name will be substantiated in Sec. \[V B 4\] below] as

\[
\mathfrak{R}_1(x) = \mathfrak{A}_1(x_1) - \mathfrak{A}_1(x). \quad (5.12)
\]

along with the function

\[
\mathfrak{R}_1(x) = \frac{1}{l}[A(x_1) - A(x)] \quad (5.13)
\]

[for given \(A(x)\), \(\mathfrak{R}_1(x)\) is a given function as well].

Now, expressing the net total ballistic current \(J_{\pm}(x', x'')\) given by Eq. (4.62) in terms of the functions \(\mathfrak{R}_1(x)\) and \(\mathfrak{A}_1(x)\), we obtain from Eq. (4.71) the total thermoballistic current \(\tilde{J}^{(1)}_+(x_1, x; \xi; l)\) to be inserted in Eq. (5.2) in the form

\[
\tilde{J}^{(1)}_+(x_1, x; \xi; l) = \mathfrak{R}^{(1)}_+(x_1, x; \xi; l) + \mathfrak{R}^{(1)}_-(x_1, x; \xi; l). \quad (5.14)
\]

Here,

\[
\tilde{J}^{(1)}_+(x_1, x; \xi; l) = J \left\{ w_+(x_1, x; l) \mathfrak{R}_1(x) + \int_{x_1}^{x^-} \frac{d x'}{l} w_+(x', x; l) \left[ \mathfrak{R}_1(x) - \mathfrak{R}_1(x') \right] + \int_{x^+}^{x} \frac{d x''}{l} w_+(x_1, x''; l) \left[ \mathfrak{R}_1(x'') - \mathfrak{R}_1(x_1) \right] + \int_{x_1}^{x^-} \frac{d x'}{l} \int_{x^+}^{x} \frac{d x''}{l} w_+(x', x''; l) \left[ \mathfrak{R}_1(x'') - \mathfrak{R}_1(x') \right] \right\}, \quad (5.15)
\]

while the term \(\tilde{J}^{(1)}_-(x_1, x; \xi; l)\) is obtained from expression (5.15) by replacing \(\mathfrak{R}_1(x)\) with \(\mathfrak{R}_1(x)\) throughout, and \(w_+(x', x'', l)\) with \(w_-(x', x'', l)\), where

\[
w_\pm(x', x'', l) = e^{-|x'-x''|/l} B_{\pm}^{m}(x', x'')/B_{\pm}^{m}(x_1, x_2) \quad (5.16)
\]

To evaluate condition (5.2), we use the relation

\[
\int_{x_1}^{x} d \xi \int_{x_1}^{\xi} d x' \int_{x_1}^{x} d x'' F(x', x'') = \int_{x_1}^{x} d x' \int_{x_1}^{x} d x'' F(x', x'') - F(x', x''). \quad (5.17)
\]

Carrying out the integration over \(\xi\), so that the condition can be expressed in the explicit form

\[
\mathfrak{R}_+(x_1, x; x; l) \mathfrak{R}_1(x) + \int_{x_1}^{x} \frac{d x'}{l} \mathfrak{R}_+(x_1, x; x'; l) \mathfrak{R}_1(x') = -\Omega^{(1)}_+(x_1, x; l). \quad (5.18)
\]

Here, the inhomogeneity \(\Omega^{(1)}_-(x_1, x; l)\) is given by

\[
\Omega^{(1)}_-(x_1, x; l) = \int_{x_1}^{x} \frac{d x'}{l} \mathfrak{R}_-(x_1, x; x'; l) \mathfrak{R}_1(x'), \quad (5.19)
\]
and the integral kernels $R_\pm(x_1, x; x'; l)$ are defined as
\[
R_\pm(x_1, x; x'; l) = u_\pm(x', x; l) - u_\pm(x_1, x_1; l) + \int_{x_1}^{x} \frac{dx'}{l} u_\pm(x', x''); l,
\]
(5.20)
with
\[
\begin{align*}
    u_\pm(x', x''); l) &= x'' - x' \quad w_\pm(x', x''); l) \\
    &\equiv -u_\pm(x'', x'; l).
\end{align*}
\]
(5.21)
Equation (5.13) is a linear, inhomogeneous, Volterra-type integral equation of the second kind in the range $x_1 < x < x_2$.

The kernels $R_\pm(x_1, x; x'; l)$ depend on the potential energy profiles $E_{\uparrow, \downarrow}(x)$ solely via the quantities $B_{\pm}^{m}(x', x'')$, and are independent of the total physical current $J$. Nonetheless, for nonzero spin splitting, a $J$-dependence of the function $R_1(x)$ can arise, via the function $R_1(x)$, from a nonlinear $J$-dependence of the spin accumulation function $A(x)$ [see Secs. 5C and 6D below].

In the zero-bias limit, when $A(x)$ is proportional to $J$, the function $R_1(x)$, and hence $R_1(x)$, become independent of $J$. For zero spin splitting, when $B_{\pm}^{m}(x', x'') = 0$, we have
\[
\Omega_{\pm}^{(1)}(x_1, x; l) = \frac{x - x_1}{l},
\]
(5.22)
and $R_1(x)$ does not depend on $A(x)$.

The resistance function $R_1(x)$ is discontinuous at $x = x_1$; we have
\[
\tilde{R}_1(x_1) = 0
\]
(5.23)
from Eq. (5.12), whereas we obtain
\[
\tilde{R}_1(x_1^+) = \frac{B_{\pm}^{m}(x_1, x_2)}{B_{\pm}(x_1)} - P(x_1)R_1(x_1^+)
\]
(5.24)
by expanding Eq. (5.18) to first order in $x - x_1$ (we assume the potential energy profiles $E_{\uparrow, \downarrow}(x)$ to be continuous in the interval $[x_1, x_2]$).

For arbitrary functions $E_c(x)$ and $\Delta(x)$, the calculation of the resistance function $\tilde{R}_1(x)$ for a chosen parameter set consists of three, consecutive steps: (i) calculation of the spin accumulation function $A(x)$ as solution of the integral equation (5.78) [see Sec. 5C below], using the boundary conditions (5.19) with given values $A_{1,2}$ at the contact-semiconductor interfaces; (ii) with $A(x)$ as input in expression (5.18), calculation of the inhomogeneity $\Omega_{\pm}^{(1)}(x_1, x; l)$ from Eq. (5.19); (iii) using $\Omega_{\pm}^{(1)}(x_1, x; l)$ in the Volterra equation (5.13), calculation of $\tilde{R}_1(x)$ by, in general, numerical methods.

Turning now to the function $\tilde{R}_2(x)$, we proceed as for $\tilde{R}_1(x)$. In analogy to Eq. (5.18) for the resistance function $R_1(x)$, we introduce a resistance function $\tilde{R}_2(x)$ as
\[
\tilde{R}_2(x) = \tilde{R}_2(x) - \tilde{R}_2(x_2),
\]
(5.25)
for which we obtain from Eq. (5.23) a Volterra-type integral equation in the range $x_1 \leq x < x_2$,
\[
\tilde{R}_2(x, x_2; x_1; x_2; l) = \frac{l}{2} \tilde{R}_2(x) + \frac{l}{2} \tilde{R}_2(x, x_2; x; l) \tilde{R}_2(x)
\]
(5.26)
with the inhomogeneity $\Omega_{\pm}^{(2)}(x, x_2; l)$ expressed in terms of the function
\[
\tilde{R}_2(x) = \frac{1}{4} [A(x) - A(x_2)]
\]
(5.27)
as
\[
\begin{align*}
    \Omega_{\pm}^{(2)}(x, x_2; l) &= \frac{x_2 - x}{l} + \tilde{R}_2(x, x_2; x; l) \tilde{R}_2(x) \\
    &\quad + \int_{x_1}^{x_2} \frac{dx'}{l} \tilde{R}_2(x, x_2; x'; l) \tilde{R}_2(x').
\end{align*}
\]
(5.28)

The kernels $R_\pm(x_1, x; x', l)$ are obtained by replacing in expression (5.20) for $R_\pm(x_1, x; x', l)$ the pair of arguments $x_1, x$ with $x, x_2$.

The resistance function $\tilde{R}_2(x)$ is discontinuous at $x = x_2$,
\[
\tilde{R}_2(x_2) = 0,
\]
(5.29)
in analogy to the discontinuity of the function $\tilde{R}_1(x)$ at $x = x_1$ [see Eqs. (5.28) and (5.24)].

As to the calculation of $\tilde{R}_2(x)$ from Eq. (5.20), the foregoing discussion regarding the calculation of $\tilde{R}_1(x)$ from Eq. (5.18) applies mutatis mutandis. Alternatively, one may calculate $\tilde{R}_2(x)$ by using the relation
\[
\tilde{R}_2(x) = \tilde{R}_2^\pm(x_1 + x_2 - x),
\]
(5.31)
where $\tilde{R}_2^\pm(x)$ is the solution of Eq. (5.18) corresponding to spatially reversed potential energy profiles,

\[
E_{\uparrow, \downarrow}(x) = E_{\uparrow, \downarrow}(x_1 + x_2 - x),
\]
(5.32)
using as input a spin accumulation function $A(x)$ calculated from Eq. (5.78) below with the reversed profiles and with the boundary values $A_1$ and $A_2$ interchanged.

The calculation of the resistance functions $\tilde{R}_1(x)$ and $\tilde{R}_2(x)$ simplifies considerably if the spin splitting is constant over the sample, $\Delta(x) \equiv \Delta$ [while $E_c(x)$ still may be arbitrary]. With
\[
E_{\uparrow, \downarrow}(x) = E_c(x) \pm \frac{1}{2} \Delta,
\]
(5.33)
we have
\[
E_{\uparrow, \downarrow}(x') = E_c(x') \pm \frac{1}{2} \Delta,
\]
(5.34)
and hence for the functions $B^m_+(x',x'')$ from Eqs. (4.21) and (4.25), using Eqs. (4.3)–(4.6),
\[
B^m_+(x',x'') = \frac{1}{Q} B^m_0(x',x'')
\]
and
\[
B^m_-(x',x'') = P B^m_+(x',x'') = \frac{P}{Q} B^m_0(x',x'').
\]
Here, we have defined
\[
B^m_0(x',x'') = 2e^{-\beta E^m_0(x',x'')},
\]
\[
Q \equiv (1 - P^2)^{1/2} = \frac{1}{\cosh(\beta \Delta/2)},
\]
and
\[
P = - \tanh(\beta \Delta/2)
\]
is the static spin polarization.

Considering, for instance, the calculation of $\tilde{R}_1(x)$, we then find from Eqs. (5.20) for the kernels $\mathcal{R}_\pm(x_1, x; x'; l)$, using expressions (5.35) and (5.36) in Eq. (5.16),
\[
\mathcal{R}_+(x_1, x; x'; l) = \frac{1}{Q} R_0(x_1, x; x'; l)
\]
and
\[
\mathcal{R}_-(x_1, x; x'; l) = P \mathcal{R}_+(x_1, x; x'; l) = \frac{P}{Q} R_0(x_1, x; x'; l),
\]
where the reduced kernel $R_0(x_1, x; x'; l)$ corresponds to $\Delta = 0$.

Now, inserting expressions (5.40) and (5.41) in Eqs. (5.18) and (5.19), respectively, we can rewrite the integral equation (5.18) in the form
\[
\tilde{R}_0(x_1, x; x; l) \tilde{R}_1(x) + \int_{x_1}^x \frac{dx'}{l} R_0(x_1, x; x'; l) \tilde{R}_1(x') = - \frac{x - x_1}{l} \quad (5.42)
\]

where
\[
\tilde{R}_1(x) = \frac{1}{Q} \tilde{R}_1(x) + P \tilde{R}_1(x),
\]
and the function $\tilde{R}_1(x)$ is independent of $\Delta$ (see Sec. IV C.1 below). As a solution of Eq. (5.42), the function $\tilde{R}_1(x)$ is a universal function that describes an intrinsic property of the semiconducting sample; it is determined by the potential energy profile $E_c(x)$ and the momentum relaxation length $l$, and does not depend on the spin splitting $\Delta$ and the spin accumulation function $A(x)$.

The resistance function $\tilde{R}_1(x)$ for constant spin splitting can now be expressed as
\[
\tilde{R}_1(x) = Q \tilde{R}_{10}(x) - P \tilde{R}_1(x).
\]

The calculation here separates into two, independent steps: (i) solution of Eq. (5.42) for $\tilde{R}_{10}(x)$; (ii) calculation of $A(x)$ as solution of the integral equation (5.78) and determination of $\tilde{R}_1(x)$ via Eqs. (5.11) and (5.13). In particular, for zero spin splitting, we have $\tilde{R}_1(x) = \tilde{R}_{10}(x)$.

2. Thermoballistic average chemical potential

Introducing the mean value $\tilde{A}(x)$ of the functions $\tilde{A}_{1,2}(x)$, which both satisfy condition (5.1),
\[
\tilde{A}(x) = \frac{1}{2} [\tilde{A}_1(x) + \tilde{A}_2(x)]
\]
[see Eq. (5.5)], we observe that $\tilde{A}(x)$ satisfies condition (5.1) as well. Using Eqs. (5.12) and (5.23), we can express $\tilde{A}(x)$ in the form
\[
\tilde{A}(x) = \frac{1}{2} [\tilde{A}_1(x) + \tilde{A}_2(x)] - \frac{1}{4} [\tilde{R}_1(x) - \tilde{R}_2(x)].
\]

Now, writing down this expression for $x = x_1$ and $x = x_2$, respectively, and using Eqs. (5.10), (5.23), and (5.29) together with the boundary conditions (4.93), we add the resulting two expressions to obtain for the quantity $\eta_{12}$, defined by Eq. (4.100),
\[
\eta_{12} = \frac{J}{v_e N_e} \frac{2}{B^m_+(x_1, x_2)} \times [\tilde{A}_1(x_1) + \tilde{A}_2(x_2) - \frac{1}{2} (\tilde{R}_1(x_2) - \tilde{R}_2(x_1))].
\]

On the other hand, subtracting the two expressions, we have
\[
\eta_{12} = \frac{J}{v_e N_e} \frac{2}{B^m_+(x_1, x_2)} \tilde{R}_1(x_2) - \tilde{R}_2(x_1)
\]
with the parameter $\tilde{R}$ defined as
\[
\tilde{R} = \frac{1}{2} [\tilde{R}_1(x_2) + \tilde{R}_2(x_1)].
\]

Then, using Eqs. (5.47) and (5.48), we can eliminate from expression (5.46) the dependence on the boundary values $\tilde{A}_1(x_1)$ and $\tilde{A}_2(x_2)$ of the functions $\tilde{A}_{1,2}(x)$. Introducing the function
\[
\tilde{R}_-(x) = \tilde{R}_1(x) - \frac{1}{2} \tilde{R}_1(x_2) - [\tilde{A}_2(x) - \frac{1}{2} \tilde{A}_2(x_1)],
\]
so that, in view of Eqs. (5.20) and (5.24),
\[
\tilde{R}_-(x_1, x_2) = - \tilde{R}_0,
\]
we find for the mean spin function $\tilde{A}(x)$, using Eq. (6.10),
\[ \tilde{A}(x) = \frac{\gamma_2}{2} - \frac{R_-(x)}{2R} \tilde{\mu}_2 \] (5.52)
for $x_1 < x < x_2$, and
\[ \tilde{A}(x_1) = \eta_1, \quad \tilde{A}(x_2) = \eta_2. \] (5.53)
Equivalently, we write
\[ e^{\beta \tilde{\mu}(x)} = \frac{1}{2}(e^{\beta \mu_1} + e^{\beta \mu_2}) - \frac{R_-(x)}{2R}(e^{\beta \mu_1} - e^{\beta \mu_2}) \] (5.54)
for $x_1 < x < x_2$, and
\[ \tilde{\mu}(x_1) = \mu_1, \quad \tilde{\mu}(x_2) = \mu_2. \] (5.55)
Expression (5.54) represents the final, general expression for the (local) thermallibcial average chemical potential $\tilde{\mu}(x)$ inside the sample [henceforth, we drop the attribute “thermolllibcial” when referring to $\tilde{\mu}(x)$]. It is seen to be uniquely determined by the values of the external parameters at the contact sides of the contact-semiconductor interfaces, viz., the values $\mu_{1,2}$ of the equilibrium chemical potential and the values $A_{1,2}$ of the spin accumulation function [which enter via the resistance functions $R_1(x)$ and $R_2(x)$]. Comparing expression (5.54) to expression (3.62) for the chemical potential $\mu(x)$ in the prototype thermallibcial model, we observe a formally identical structure, but differences in the explicit forms of the functions $R_-(x)$ and $R_-(x)$ and of the reduced resistances $R$ and $R$.

An explicit expression for $\tilde{\mu}(x)$ can be obtained if $l/S \gg 1$ (“ballistic regime”), in which case the probability for an electron to suffer a collision when traversing the sample of length $S$, $1 - e^{-S/l} \approx S/l$, is vanishingly small. Then, keeping terms of order $S/l$, we have from Eq. (6.13)
\[ R_1(x) = \frac{B_m(x_1, x_2)}{B_m'(x_1, x_2)} - P_m(x_1, x_2)R_1(x), \] (5.56)
and similarly from Eq. (5.26)
\[ R_2(x) = \frac{B_m'(x_1, x_2)}{B_m''(x_1, x_2)} - P_m(x_1, x_2)R_2(x). \] (5.57)
Since from Eqs. (4.94), (5.10), (5.13), and (5.27)
\[ R_1(x_2) = R_2(x_2) = \frac{v_y N_c B_m(x_1, x_2)}{2J} \frac{B_m'(x_1, x_2)}{2} A_{12}, \] (5.58)
we now find from Eq. (5.49)
\[ \tilde{R} = 1 - \frac{v_y N_c B_m(x_1, x_2)}{2J} \frac{B_m'(x_1, x_2)}{2} P_m(x_1, x_2)A_{12}. \] (5.59)
For the function $R_- (x)$, we have from Eq. (5.50), using Eq. (5.58),
\[ \tilde{R}_-(x) = \tilde{R}_1(x) - \tilde{R}_2(x). \] (5.60)
With expressions (5.59) and (5.60) inserted in Eq. (5.54), we obtain the average chemical potential $\tilde{\mu}(x)$ in explicit form. In the particular case of zero spin splitting, when $B_m'(x_1, x_2) = 2e^{-\beta E_m(x_1, x_2)}$, and $P_m(x_1, x_2) = 0$, we have
\[ \frac{R_- (x)}{R} = e^{-\beta E_m(x_1, x_2)} \left[ e^{\beta E_m(x_1, x_2)} - e^{\beta E_m(x_1, x_2)} \right]. \] (5.61)
This result, here obtained in the ballistic regime, $l/S \gg 1$, contrasts with the (strict) ballistic limit, $l \to \infty$, considered in Sec. IV C 3, when there is absolutely no point of local thermodynamic equilibrium inside the sample. In this extreme case, no meaning can be attached to an average chemical potential, and there is nothing a calculation of such a quantity can be based upon.

In Ref. 54, we have presented and discussed numerical results for $\tilde{\mu}(x)$, calculated with the potential energy profile (4.121) for values of the ratio $l/S$ ranging between $10^{-2}$ to $10^2$. If calculated with the procedure adopted in the present work (see the remarks at the end of Sec. V A 1), the results for $\tilde{\mu}(x)$ would differ quantitatively from the former ones, but would agree with those in all qualitative respects.

3. Sharvin interface resistance

The discontinuities in the resistance functions $R_1(x)$ and $R_2(x)$ at the points of local thermodynamic equilibrium $x = x_1$ and $x = x_2$, respectively, give rise to discontinuities in the function $R_- (x)$ both at $x = x_1$ and $x = x_2$. From Eq. (5.50), we find, using Eqs. (6.28) and (5.21),
\[ R_-(x_1^+) - R_-(x_1) = \frac{B_m'(x_1, x_2)}{B_m'(x_1, x_2)} - P(x_1)R_1(x_1^+), \] (5.62)
and similarly, using Eqs. (5.29) and (5.30),
\[ R_-(x_2^-) - R_-(x_2^-) = \frac{B_m'(x_1, x_2)}{B_m'(x_1, x_2)} - P(x_2)R_2(x_2^-). \] (5.63)
Therefore, according to Eq. (5.54), the average chemical potential $\tilde{\mu}(x)$ exhibits discontinuities at these points as well (“Sharvin effect”; see Ref. 30),
\[ e^{\beta[\tilde{\mu}(x_1^+) - \tilde{\mu}_1]} - 1 = -\frac{\tilde{\eta}_2 e^{-\beta \mu_1}}{2} \tilde{R}_1(x_1^+) \] (5.64)
\[ = -\frac{1}{2} e^{\beta e J \tilde{\rho}_1}, \]
\[ e^{\beta[\tilde{\mu}(x_2^-) - \tilde{\mu}_2]} - 1 = -\frac{\tilde{\eta}_2 e^{-\beta \mu_2}}{2} \tilde{R}_2(x_2^-) \] (5.65)
\[ = \frac{1}{2} e^{\beta e J \tilde{\rho}_2}, \]
where we have used Eqs. (5.48) and (5.49) to introduce the total physical current $J$. The quantities $\tilde{\rho}_{1,2}$ are the Sharvin interface resistances, \cite{39,44} and

$$
\tilde{\rho}_1 = \frac{2}{\beta e^2 v_e N_e B^m_+(x_1, x_2) e^{\beta \mu_1}} \tilde{R}_1(x_1^+),
$$

(5.66)

$$
\tilde{\rho}_2 = \frac{2}{\beta e^2 v_e N_e B^m_+(x_1, x_2) e^{\beta \mu_2}} \tilde{R}_2(x_2^-).
$$

(5.67)

For zero spin splitting, when $P(x_1, x_2) = 0$, so that $\tilde{R}_1(x_1^+) = B^m_+(x_1, x_2)/B_+(x_1)$ and $\tilde{R}_2(x_2^-) = B^m_+(x_1, x_2)/B_+(x_2)$, we can express $\tilde{\rho}_{1,2}$ in the form

$$
\tilde{\rho}_{1,2} = \frac{1}{\beta e^2 v_e n_+^{(0)}(x_1, x_2)},
$$

(5.68)

where

$$
n_+^{(0)}(x_1, x_2) = \frac{N_e}{2} B_+(x_1, x_2) e^{\beta \mu_1, 2} = N_e e^{-\beta [E_c(x_1, x_2) - \mu_1, 2]} \tag{5.69}
$$

are the total equilibrium electron densities at the semiconductor side of the contact-semiconductor interfaces \cite{41,48}. Equations (5.68) and (5.69), respectively, are analogous to Eqs. (5.64) and (5.65) for the discontinuities of the chemical potential $\mu(x)$ in the prototype thermoballistic model.

3. Current-voltage characteristic and magnetoresistance

The current-voltage characteristic of the thermoballistic transport model is obtained from Eq. (5.48) in the form

$$
J = \frac{v_e N_e}{2} B^m_+(x_1, x_2) e^{\beta \mu_1} \frac{1}{R} (1 - e^{-\beta e V}),
$$

(5.70)

where

$$
V = \frac{\mu_1 - \mu_2}{e}
$$

(5.71)

is the voltage bias between the metal contacts (we assume the voltage drop across the contacts to be negligible small). In the zero-bias limit, when $\beta e V \ll 1$, we have

$$
R \equiv \left| \frac{V}{eJ} \right|_{J \rightarrow 0} = \frac{2}{\beta e^2 v_e N_e B^m_+(x_1, x_2) e^{\beta \mu_1}} \tilde{R}
$$

(5.72)

for the resistance times cross-sectional area of the sample. Comparing the current-voltage characteristic \cite{41} to that of the (spinless) prototype thermoballistic model, Eq. (5.25), one sees that the (dimensionless) parameter $\tilde{R}$ directly corresponds to the reduced resistance $R$ of the prototype model, Eq. (4.24). Therefore, $\tilde{R}$ is here also called the reduced resistance of the sample, and the functions $\tilde{R}_1(x)$ and $\tilde{R}_2(x)$ from which it is derived, the resistance functions.

The reduced resistance $\tilde{R}$ is a central element of the thermoballistic description of electron transport in semiconductors. It comprises the effect of the detailed shape of the potential energy profiles as well as that of the momentum relaxation length. Moreover, via its dependence on the spin accumulation function $A(x)$, it takes into account the effect of spin relaxation. As exemplified by expression (5.59) for $R$, which holds in the ballistic regime, the reduced resistance depends on the total current $J$ unless $A(x)$ is proportional to $J$. The explicit form of $\tilde{R}$ in the drift-diffusion regime can be obtained by rewriting Eq. (4.91) for $x = x_2$ in the form of a current-voltage characteristic and comparing it to the characteristic (5.71).

Defining now the relative magnetoresistance $R_m$ of the semiconducting sample \cite{41,45} as

$$
R_m \equiv \frac{R - R_0}{R_0},
$$

(5.73)

where $R_0$ is the resistance at zero external magnetic field, i.e., at zero spin splitting, we have from Eq. (5.72)

$$
R_m = \frac{\tilde{R} - \tilde{R}_0}{\tilde{R}_0}.
$$

(5.74)

The reduced resistance at zero spin splitting, $\tilde{R}_0$, is obtained by solving Eq. (5.32) for the function $\tilde{R}_1(x)$ and the analogous equation for $\tilde{R}_2(x)$ and using Eq. (5.49),

$$
\tilde{R}_0 = \frac{1}{2} \tilde{R}_{10}(x_2) + \tilde{R}_{20}(x_1).
$$

(5.75)

For constant splitting, we find from Eq. (5.49), using Eq. (5.31) and the analogous equation for $\tilde{R}_2(x)$ as well as Eq. (5.56),

$$
\tilde{R} = Q \tilde{R}_0 - \frac{v_e N_e}{4J} B^m_+(x_1, x_2) PA_{12},
$$

(5.76)

and hence

$$
R_m = Q - 1 - \frac{v_e N_e}{4J \tilde{R}_0} B^m_+(x_1, x_2) PA_{12}
$$

(5.77)

for the magnetoresistance.

C. Spin accumulation function

The net relaxing ballistic spin-polarized current $\tilde{J}_-(x; x'; x')$ \cite{41} and the joint relaxing ballistic spin-polarized density $\tilde{n}_-(x; x'; x')$ \cite{41}, and thus also the corresponding thermoballistic current $\tilde{J}_-(x)$ and density $\tilde{n}_-(x)$ evaluated from Eq. (4.71), are dynamically determined solely by the spin accumulation function $A(x)$. The calculation of this function is, in general, prerequisite to a complete determination of the average chemical potential $\bar{\mu}(x)$ \cite{31}.5
1. Integral equation

Following Sec. [VC11] we invoke condition (5.8), which is equivalent to the spin balance equation (5.9), and insert expression (4.65) for the quantity \( P(x', x''; x) \) in Eq. (4.74) to obtain for the spin accumulation function \( A(x) \) an integral equation of the form

\[
\tilde{W}(x_1, x_1; l, l_s) A_1 + \tilde{W}(x_1, x_2; l, l_s) A_2 - \tilde{W}(x_1, x_2; l) A(x) + \int_{x_1}^{x_2} \frac{dx'}{l} \tilde{W}(x', x_1; l, l_s) A(x') = 0,
\]

(5.78)

where

\[
\tilde{W}(x', x''; l, l_s) = \tilde{w}(x', x''; l)e^{-C^m(x', x'')/l_s},
\]

(5.79)

and

\[
\tilde{W}(x; x_1, x_2; l) = \tilde{w}(x_1, x; l) + \tilde{w}(x, x_2; l) + \int_{x_1}^{x_2} \frac{dx'}{l} \tilde{w}(x', x; l).
\]

(5.80)

Here, the values \( A(x_1, 2) \) of the spin accumulation function at the interface positions \( x_1, 2 \) have been set equal to the external values, \( A_1, 2 \), at the contact side of the contact-semiconductor interfaces [see Eq. (4.19)]. The function \( C^m(x', x'') \) is defined as

\[
C^m(x', x'') \equiv C^m(x', x''; x', x'')
\]

(5.81)

[see Eq. (4.55)], and

\[
\tilde{w}(x', x''; l) = e^{-|x'-x''|/l} B^m(x', x'') / B^0(x_1, x_2)
\]

\[
\equiv \tilde{w}(x'', x'; l),
\]

(5.82)

with \( B^m(x', x'') \) given by Eq. (4.32).

With the first two terms in Eq. (5.78) acting as an inhomogeneity, this equation is a linear, inhomogeneous, Fredholm-type integral equation of the second kind[13] for the spin accumulation function \( A(x) \). The corresponding homogeneous equation is solved by \( A(x) \equiv 0 \) only, so that the solution \( A(x) \) of Eq. (5.78) for \( x_1 < x < x_2 \) is linear and homogeneous in \( A_1 \) and \( A_2 \). Just like the average chemical potential \( \tilde{\mu}(x) \), the spin accumulation function \( A(x) \) exhibits the Sharvin effect, i.e., it is not, in general, continuous at the interfaces with the contacts, \( A(x_1) - A_1 \neq 0 \), \( A_2 - A(x_2) \neq 0 \). This will be demonstrated in Sec. [VC21] below by way of a specific example. The solution of Eq. (5.78) is found, in general, numerically by applying matrix methods after discretization.

For constant spin splitting, \( \Delta(x) \equiv \Delta \), when the functions \( E_{i,j}^m(x', x'') \) are given by Eq. (5.33), the function \( B^m(x', x'') \) defined by Eq. (4.32) reduces to

\[
B^m(x', x'') = QB^0_m(x', x''),
\]

(5.83)

with \( B^0_m(x', x'') \) given by Eq. (5.37), and \( Q \) by Eq. (5.38). Further, using Eqs. (5.33) and (5.34) in expression (4.40), we see that \( \Delta \) cancels out in the functions \( C^m_{i,j}(x', x''; x)\).

\[
C^m_{i,j}(x', x'', x) \equiv C^m_{0,0}(x', x''; x).
\]

(5.84)

Inserting this in Eq. (4.39), we then find, via Eqs. (4.45), (5.53), and (4.55), the function \( C^m(x', x'') \) defined by Eq. (5.51) to be independent of \( \Delta \).

\[
C^m(x', x'') \equiv C^m_0(x', x'').
\]

(5.85)

With this result, in conjunction with Eqs. (5.82) and (5.83), used in Eqs. (5.79) and (5.80), the spin splitting \( \Delta \) is seen to drop out from the integral equation (5.78), i.e., its solution \( A(x) \) does not depend on \( \Delta \).

2. Differential equation

In homogeneous semiconductors without space charge, the conduction band edge potential is constant. In this case, the integral equation for \( A(x) \) can be converted into a differential equation. Assuming the electrons to be driven by an external electric field of magnitude \( E \) directed antiparallel to the \( x \)-axis, the potential energy profile (4.2) for zero spin splitting, \( \Delta(x) = 0 \), is given by Eq. (4.121). [According to the above discussion, the inclusion of a nonzero, constant spin splitting would not alter the results.] For the profile (4.121), the function \( C^m(x', x'') \) defined by Eq. (4.53) takes the form

\[
C^m(x', x'') \equiv C^m(\epsilon(x - x'))
\]

\[
= e^{(x-x')^2} \text{erfc}((\epsilon(x - x'))^{1/2})
\]

(5.86)

(\( \epsilon = \beta e E \)), as can be shown by using Eqs. (4.39), (4.40), and (4.57).

Using expression (5.86), via Eq. (4.55), in Eq. (5.81), the integral equation (5.8) can now be reduced to

\[
f_1(x - x_1) A_1 + f_2(x - x_2) A_2 - f(x - x_1) A(x) + \int_{x_1}^{x_2} \frac{dx'}{l} f_1(x - x') A(x') + \int_{x_1}^{x_2} \frac{dx'}{l} f_2(x' - x) A(x') = 0,
\]

(5.87)

where

\[
f_1(x) = e^{-|x+1/l+c(x)/|l|} x,
\]

(5.88)

\[
f_2(x) = e^{-|x-1/l+c(x)/|l|} x,
\]

(5.89)

and

\[
f(x) = \frac{1}{1 + d l} [2 + d l (1 + e^{-(c+1/l)x})].
\]

(5.90)
The function \( c(\zeta) \) defined by

\[
c(\zeta) = \frac{1}{\zeta} \int_{0}^{\zeta} d\zeta' C^m(\zeta')
\]

(5.91)
obesys the relations \( 0 < c(\zeta) \leq 1, c(\zeta) \to 1 \) for \( \zeta \to 0 \), and 
\( c(\zeta) \sim 2(\pi \zeta)^{-1/2} \) for \( \zeta \to \infty \).

We can convert the inhomogeneous integral equation (5.87) into a homogeneous integro-differential equation for \( A(x) \) by supplementing Eq. (5.87) with the equations obtained by forming its first and second derivative with respect to \( x \), and subsequently eliminating from this set of three equations the boundary values \( A_1 \) and \( A_2 \). [In principle, a similar procedure could also be applied to the general equation (5.78), but this does not seem to lead to any advantage.] If we replace in the integral equation (5.87) the function \( c(\zeta) \) with a position-independent average value \( \bar{c} \), the functions \( f_1(x) \) and \( f_2(x) \) become pure exponentials, and the corresponding integro-differential equation reduces to a homogeneous second-order differential equation of the form

\[
\frac{d^2 A(x)}{dx^2} + b_1(x) \frac{dA(x)}{dx} + b_2(x) A(x) = 0.
\]

(5.92)

Here,

\[
b_0(x) = 2 + \epsilon l [1 + b(x)],
\]

(5.93)

\[
b_1(x) = \epsilon (2 + \epsilon l) [1 - b(x)],
\]

(5.94)

and

\[
b_2(x) = \frac{l}{l^2} \{ 2 + \epsilon (l + \bar{c} + \epsilon l \bar{c}) [1 + b(x)] \},
\]

(5.95)

where

\[
b(x) = e^{-(\epsilon+1/l)(x-x_1)}
\]

(5.96)

and

\[
\frac{1}{l} = \frac{1}{l} + \frac{\bar{c}}{L_s},
\]

(5.97)

with the ballistic spin relaxation length \( l_s \) given by Eq. (1.50). [Note that expression (5.95) for the function \( b_2(x) \) differs from the corresponding expression (3.48) of Ref. 64, which was derived by introducing the average value \( \bar{c} \) in the integrodifferential equation, rather than in the integral original equation.] Since, owing to the presence of the factor \( e^{-x/l} \) in the functions \( f_1(x) \) and \( f_2(x) \), only the values of \( c(x) \) in the range \( 0 \leq x \leq l \) contribute appreciably, we may choose \( \bar{c} \) as the average of \( c(x) \) over an \( x \)-interval of length equal to the momentum relaxation length \( l \),

\[
\bar{c} = \frac{1}{l} \int_{0}^{l} d\epsilon c(\epsilon x) \equiv \frac{1}{\epsilon l} \int_{0}^{\epsilon l} d\zeta \ln(\epsilon l/\zeta) C^m(\zeta).
\]

(5.98)

In the right-hand integral in this equation, the range of small \( \zeta \), when \( C^m(\zeta) \approx 1 \), is emphasized because of the weight factor \( \ln(\epsilon l/\zeta) \).

For large \( \epsilon l \) (i.e., in the ballistic regime and/or for strong fields), the variation of \( c(x) \) with \( x \) becomes essential. However, for the purpose of demonstrating the principal effects of the transport mechanism, the approximation in terms of a constant average value \( \bar{c} \) of the function \( c(\zeta) \), in conjunction with the choice \( \bar{c} \) for \( \bar{c} \), appears to be sufficiently accurate.

In the drift-diffusion regime, when \( l/S \ll 1, l/l_s \ll 1 \), and \( \epsilon l \ll 1 \), we have \( \bar{c} = 1 \) and hence \( l = l_s \), where

\[
\frac{1}{l} = \frac{1}{l} + \frac{1}{l_s}.
\]

(5.99)

Equation (5.92) then reduces to

\[
\frac{d^2 A(x)}{dx^2} + \frac{dA(x)}{dx} - \frac{1}{L_s^2} A(x) = 0,
\]

(5.100)

where \( L_s \) is the spin diffusion length given by Eq. (6.101). Setting \( \tilde{B}_e(x) = -\epsilon/\beta \) in Eq. (6.100), we find Eq. (6.100) to agree with the former equation, which was obtained by directly evaluating the thermoballistic current \( \tilde{J}_s(x) \) and density \( n_s(x) \) in the drift-diffusion limit, and which leads to the standard form (6.102) of the drift-diffusion equation for spin-dependent transport.

In the zero-bias limit \( \epsilon \to 0 \), the integral equation (5.87) reduces to

\[
e^{-x/(x-x_1)^{1/2}} A_1 + e^{-x/(x-x_1)^{1/2}} A_2 - 2A(x)
\]

(5.101)

\[
+ \int_{x_1}^{x_2} \frac{dx'}{l} e^{-x/(x-x')^{1/2}} A(x') = 0,
\]

from which we obtain the differential equation

\[
\frac{d^2 A(x)}{dx^2} - \frac{1}{L^2} A(x) = 0.
\]

(5.102)

Here,

\[
L = \sqrt{l_s} = \frac{L_s}{\sqrt{1 + l/l_s}}.
\]

(5.103)

is the generalization of the spin diffusion length \( L_s \) given by Eq. (4.101). The length \( L \) becomes equal to the latter length, \( L = L_s \), in the drift-diffusion regime, when \( l/l_s \ll 1 \), and to the ballistic spin relaxation length, \( L = l_s \), in the ballistic case, when \( l/l_s \to \infty \) and hence \( l = l_s \).

For \( x_1 < x < x_2 \), the general solution of Eq. (5.102) reads

\[
A(x) = C_1 e^{-(x-x_1)^{1/2}} + C_2 e^{-(x-x_2)^{1/2}}.
\]

(5.104)

Inserting this expression for \( A(x) \) in Eq. (5.101) and setting \( x = x_1 \) and \( x = x_2 \), we obtain, using Eq. (4.102), two linear equations for the coefficients, with the solution

\[
C_1 = \frac{1}{D} \left( 1 + \gamma \right) e^{S/L} A_1 - (1 - \gamma) A_2,
\]

(5.105)
\[ C_2 = -\frac{1}{D}[(1 - \gamma)A_1 - (1 + \gamma)e^{S/L}A_2]. \]  
(5.106)

Here,
\[ D = 2[(1 + \gamma^2)\sinh(S/L) + 2\gamma\cosh(S/L)], \]  
(5.107)

with
\[ \gamma = \frac{L}{L_s} = \frac{\tilde{I}}{L} = \sqrt{\frac{\tilde{I}}{\tilde{I} + I_s}} \leq 1. \]  
(5.108)

It then follows from Eqs. (5.104)–(5.108) that \( A(x) \) is discontinuous at \( x = x_1 \) and \( x = x_2 \),
\[ \Delta A_1 = A(x_1^+) - A_1 = -\frac{1}{2}(gA_1 - hA_2), \]  
(5.109)
\[ \Delta A_2 = A_2 - A(x_2^-) = -\frac{1}{2}(hA_1 - gA_2), \]  
(5.110)

where
\[ g = \hbar[cosh(S/L) + \gamma \sinh(S/L)] \leq 1, \]  
(5.111)

with
\[ \tilde{h} = \frac{4\gamma}{D} \leq \frac{2}{1 + \gamma}e^{-S/L}. \]  
(5.112)

In the drift-diffusion regime, when \( L = L_s \) and \( \gamma \ll 1 \), we have
\[ A(x) = A_1e^{-(x-x_1)/L_s} + A_2e^{-(x-x_2)/L_s}, \]  
(5.113)

and in the ballistic case, when \( L = L_s \) and \( \gamma = 1 \),
\[ A(x) = \frac{1}{2}[A_1e^{-(x-x_1)/L_s} + A_2e^{-(x-x_2)/L_s}]. \]  
(5.114)

At \( x = x_1 \), for example, the discontinuity of \( A(x) \) is \( \Delta A_1 = A_2\exp(-S/L_s) \) in the drift-diffusion regime, and \( \Delta A_1 = \frac{1}{2}[-A_1 + A_2\exp(-S/L_s)] \) in the ballistic case.

\section*{D. Current and density spin polarizations}

The position dependence of the current and density spin polarizations as well as the magnetoresistance are the physical quantities of principal interest in the study of spin-polarized electron transport in paramagnetic semiconducting systems.

\subsection*{1. Spin polarizations in the semiconductor}

In the thermoballistic approach, we define the persistent current spin polarization in the semiconducting sample, \( \tilde{P}_J(x) \), in terms of the persistent thermoballistic spin-polarized current \( \tilde{J}_-(x) \) and the total physical current \( J \) as
\[ \tilde{P}_J(x) = \frac{\tilde{J}_-(x)}{J}. \]  
(5.115)

\((x_1 \leq x \leq x_2)\). Analogously, the relaxing current spin polarization \( \tilde{P}_J(x) \) is defined in terms of the relaxing thermoballistic spin-polarized current \( \tilde{J}_-(x) \) and the total current \( J \) as
\[ \tilde{P}_J(x) = \frac{\tilde{J}_-(x)}{J}. \]  
(5.116)

For the total current spin polarization \( P_J(x) \), we then have
\[ P_J(x) = \tilde{P}_J(x) + \tilde{P}_J(x) = \frac{\tilde{J}_-(x) + \tilde{J}_-(x)}{J}. \]  
(5.117)

[Note that in Refs. \[54\] and \[55\], we have defined the current spin polarization in terms of the total thermoballistic current \( \tilde{J}_+(x) \), rather than in terms of the total physical current \( J \).]

The persistent density spin polarization \( \tilde{P}_n(x) \) and the relaxing density spin polarization \( \tilde{P}_n(x) \) are introduced by replacing in expressions (5.113) and (5.114) the thermoballistic currents \( \tilde{J}_-(x) \) and \( \tilde{J}_-(x) \) with the respective densities \( \tilde{n}_-(x) \) and \( \tilde{n}_-(x) \), and the current \( J \) in the denominator of those expressions with the total ballistic joint density \( n_+(x) \). Hence, we obtain
\[ P_n(x) = \tilde{P}_n(x) + \tilde{P}_n(x) = \frac{\tilde{n}_-(x) + \tilde{n}_-(x)}{n_+(x)}. \]  
(5.118)

for the total density spin polarization \( P_n(x) \).

In expression (5.117) for the total current spin polarization inside the semiconductor, the current \( \tilde{J}_-(x) \) depends on the reduced spin accumulation function \( \tilde{A}(x) \), and hence linearly on the boundary values \( \tilde{A}_{1,2} \), via the dependence of the total ballistic current \( J_+(x', x'') \) on \( \tilde{A}(x) \),
\[ \tilde{J}_-(x) \equiv \tilde{J}_-(x; \tilde{A}_1, \tilde{A}_2) \]  
(5.119)
[see Eqs. (4.62) and (4.64); here, we have assumed \( J_+(x', x'') \) to be expressed in terms of \( \tilde{A}(x) \), rather than \( A(x) \), using Eq. (4.110)]. The relaxing thermoballistic spin-polarized current \( \tilde{J}_-(x) \) is determined by the ballistic current \( J_-(x', x'') \) given by Eq. (4.65), which is a linear-homogeneous functional of \( \tilde{A}(x) \). Hence, \( \tilde{J}_-(x) \) is linear and homogeneous in the boundary values \( \tilde{A}_{1,2} \), so that we can write
\[ \tilde{J}_-(x) \equiv \tilde{J}_-(x; \tilde{A}_1, \tilde{A}_2) = \frac{v_n}{2} B_+(x)[F_1(x)e^{\beta \mu_1} \tilde{A}_1 + F_2(x)e^{\beta \mu_2} \tilde{A}_2], \]  
(5.120)

with (dimensionless) “formfactors” \( F_1(x) \) and \( F_2(x) \). Then, we can express the values of the total current spin polarization at the semiconductor side of the interfaces at \( x_{1,2} \) as
\[ P_J^{(sc)}(x_{1,2}) = \tilde{P}_J(x_{1,2}; \tilde{A}_1, \tilde{A}_2) + \frac{v_n B_+(x_{1,2})}{2J}, \]  
(5.121)
\[ x [ \mathcal{F}_1(x_{1,2})e^{\beta \mu_1} \tilde{A}_1 + \mathcal{F}_2(x_{1,2})e^{\beta \mu_2} \tilde{A}_2 ] \]. \tag{5.121}

The boundary values \( \tilde{A}_{1,2} \) of the reduced spin accumulation function, which are undetermined as yet, are to be expressed in terms of the current \( J \) and the parameters of the system by matching the current spin polarization in the semiconductor to the corresponding polarization in the contacts (see Sec. [V.D.3] below).

2. Current spin polarization in the contacts

In order to keep the formulation sufficiently general, we assume the semiconducting sample to be connected to (semi-infinite) ferromagnetic metal contacts, which are treated as fully degenerate Fermi systems.

In the left contact located in the range \( x < x_1 \), the spin-resolved chemical potentials \( \mu_{\uparrow,\downarrow}(x) \) have the form

\[ \mu_{\uparrow,\downarrow}(x) = \frac{e^2 J}{\sigma_{\uparrow,\downarrow}^{(l)}} (x_1 - x) \pm \frac{c_l}{\sigma_{\uparrow,\downarrow}^{(l)}} e^{-(x_1-x)/L_s^{(l)}}. \tag{5.122} \]

Here, \( L_s^{(l)} \) is the spin diffusion length, and \( \sigma_{\uparrow,\downarrow}^{(l)} \) are the \( (x \)-independent) spin-up and spin-down bulk conductivities, respectively. Setting \( x = x_1 \) in Eqs. (5.122), we obtain

\[ c_l = \frac{\sigma_{\uparrow}^{(l)} \sigma_{\downarrow}^{(l)}}{\sigma_{\uparrow,\downarrow}^{(l)}} \mu_-(x_1^-). \tag{5.123} \]

With the spin-resolved currents \( J_{\uparrow,\downarrow}(x) \) given by

\[ J_{\uparrow,\downarrow}(x) = -\frac{\sigma_{\uparrow,\downarrow}^{(l)}}{e^2} \frac{d\mu_{\uparrow,\downarrow}(x)}{dx}, \tag{5.124} \]

we then find for the current spin polarization in the left contact, using \( J_+(x) \equiv J \),

\[ P_J(x) = \frac{J_-(x)}{J_+(x)} \]
\[ = P_l - \frac{G_l}{2e^2 J} \mu_-(x_1^-) e^{-(x_1-x)/L_s^{(l)}}. \tag{5.125} \]

Here,

\[ P_l = \frac{\sigma_{\uparrow}^{(l)}}{\sigma_{\uparrow}^{(l)}} \tag{5.126} \]

is the bulk (current or density) spin polarization, and the parameter

\[ G_l = \frac{4\sigma_{\uparrow}^{(l)} \sigma_{\downarrow}^{(l)}}{\sigma_{\uparrow,\downarrow}^{(l)} L_s^{(l)}} = \frac{\sigma_{\uparrow}^{(l)}}{L_s^{(l)}} (1 - P_l^2) \tag{5.127} \]

which has the dimension of interface conductance, characterizes the spin-dependent transport in the ferromagnet.

For the current spin polarization in the right contact located in the range \( x > x_2 \), we have

\[ P_J(x) = P_r + \frac{G_r}{2e^2 J} \mu_-(x_2^-) e^{-(x-x_2)/L_s^{(r)}}, \tag{5.128} \]

which follows by replacing in Eq. (5.122) the coordinate \( x \) with \( x_1 + x_2 - x \), and the labels “\( l \)” attached to the parameters in Eqs. (5.122)–(5.127) with “\( r \)”. When spin-selective interface resistances are absent, the chemical-potential splitting \( \mu_-(x) \) is continuous at the interfaces,

\[ \mu_-(x_1^-) = \mu_-(x_1^+) \tag{5.129} \]
\[ \mu_-(x_2^-) = \mu_-(x_2^+) \tag{5.130} \]

where \( \mu_-(x_{1,2}) \) are their values at the contact side of the interfaces. The latter values are to be identified with the corresponding values \( \mu_+^{(ct)}(x_{1,2}) \) at the semiconductor side of the interface,

\[ \mu_+(x_{1,2}) = \mu_+^{(sc)}(x_{1,2}) \]
\[ = \frac{1}{\beta} \ln \left( \frac{1 + \tilde{A}_{1,2}/2}{1 - \tilde{A}_{1,2}/2} \right) \tag{5.131} \]

where the right-hand equations have been obtained by solving Eq. (4.117) for \( \mu_-(x') \), setting \( x' = x_{1,2} \), and defining

\[ \tilde{A}_{1,2} = \tilde{A}(x_{1,2}) \tag{5.132} \]

for the boundary values of the reduced spin accumulation function \( \tilde{A}(x') \). With Eqs. (5.129)–(5.131) used in Eqs. (5.125) and (5.128), respectively, we now have for the current spin polarizations at the contact side of the interfaces

\[ P_J^{(ct)}(x_1) = P_l - \frac{G_l}{2\beta e^2 J} \ln \left( \frac{1 + \tilde{A}_{1}/2}{1 - \tilde{A}_{1}/2} \right) \tag{5.133} \]
\[ P_J^{(ct)}(x_2) = P_r + \frac{G_r}{2\beta e^2 J} \ln \left( \frac{1 + \tilde{A}_{2}/2}{1 - \tilde{A}_{2}/2} \right) \tag{5.134} \]

which are to be identified with the corresponding polarizations \( P_J^{(sc)}(x_{1,2}) \) at the semiconductor side of the interfaces [see Eq. (5.137) below].

Spin-selective interface resistances \( \rho^{(1,2)}_{\uparrow,\downarrow} \) give rise to discontinuities of the spin-resolved chemical potentials on the contact sides of the interfaces. At \( x = x_1 \), for example, the discontinuity has the form

\[ \mu_{\uparrow,\downarrow}(x_1^-) - \mu_{\uparrow,\downarrow}^{(ct)}(x_1) = e^2 J_{\uparrow,\downarrow}(x_1) \rho_{\uparrow,\downarrow}^{(1)}. \tag{5.135} \]

The interface resistances \( \rho_{\uparrow,\downarrow}^{(1)} \) are located between \( x = x_1^- \) and \( x_1 \) in the ferromagnetic contact, adjacent to the
Sharvin interface resistance $\hat{\rho}_1$ [see Eq. (5.60)] between $x = x_1$ and $x_1^+$ in the semiconductor. The quantity $\mu_-(x_1^-)$ to be substituted in Eq. (5.125) is obtained from Eqs. (5.122), (5.124), and (5.127) as

$$
\mu_-(x_1^-) = \frac{1}{1 + G_0 \rho_0^{(1)}/4} \times \left\{ \mu_0^{(ct)}(x_1) + \frac{e^2}{2} \left[ P_0 \rho_0^+ + \rho_0^{(1)} \right] \right\}.
$$

(5.136)

The same procedure applies mutatis mutandis to the interface at $x = x_2$. The connection of $\mu_0^{(ct)}(x_1, 2)$ with the interface values of the reduced spin accumulation function, $\tilde{A}_{1,2}$, is again given by Eqs. (5.131).

3. Matching the polarizations at the interfaces

To evaluate the current and density spin polarizations all across the contact-semiconductor system, we have to relate the boundary values of the reduced spin accumulation function, $\tilde{A}_{1,2}$, to the total physical current $J$ and the internal parameters characterizing the system. To this end, we exploit the continuity of the total current spin polarization $P_j(x)$ across the contact-semiconductor interfaces at $x_1, 2$,

$$
P_j^{(ct)}(x_1, 2) = P_j^{(sc)}(x_1, 2).
$$

(5.137)

Using expressions (5.133) and (5.134) for $P_j^{(ct)}(x_1, 2)$ and expressions (5.124) for $P_j^{(sc)}(x_1, 2)$, we obtain a pair of coupled nonlinear equations for $\tilde{A}_{1,2}$, which we will not write down here in their general form.

In the zero-bias limit, when $|\beta_\mu_-| \ll 1$, we have $|\tilde{A}_{1,2}| \ll 1$ [see Eq. (4.11)], so that $P_j^{(ct)}(x_1) \approx P_j^{(ct)}(x_2)$ and $P_j^{(sc)}(x_1, 2)$ become linear in $\tilde{A}_1$ and $\tilde{A}_2$, respectively. Further, to first order, the term involving the reduced spin accumulation function $\tilde{A}(x)$ in the persistent ballistic spin-polarized current $\tilde{J}_-(x', x''^-)$ [see Eq. (4.161)] with $J_{x'}(x', x''^-)$ expressed in terms of $\tilde{A}(x)$ via Eqs. (4.17) and (4.163) can be neglected, so that this current becomes independent of $\tilde{A}_{1,2}$. The same then holds for the corresponding thermoballistic current $\tilde{J}_-(x)$, as well as for the persistent current spin polarization $\tilde{P}_j(x)$ derived therefrom. Hence, the polarizations $P_j^{(sc)}(x_1, 2)$ are linear in $\tilde{A}_{1,2}$, and the coupled equations for $\tilde{A}_{1,2}$ become linear. Since $\mu_1 = \mu_2$ in the zero-bias limit, they can be expressed, using Eq. (4.19), in the form

$$
\begin{align*}
\left[ \frac{G_1}{2}\beta e^2 + v_\infty n_+(x_1) \right] \tilde{A}_1 + v_\infty n_+(x_1) F_2(x_1) \tilde{A}_2 = P_j J - \tilde{\jmath}_-(x_1),
\end{align*}
$$

(5.138)

The current $\tilde{\jmath}_-(x)$ is proportional to $J$, so that the quantities $\tilde{A}_{1,2}$ are, as solutions of Eqs. (5.128) and (5.139), proportional to $J$ as well. Hence, the relaxing thermoballistic spin-polarized current $\tilde{\jmath}_-(x)$ is also proportional to $J$, so that the total current spin polarization $P_j(x)$ calculated from Eq. (5.117) is, in the zero-bias limit, independent of the total physical current $J$.

Summing up, we obtain the total current spin polarization along the entire heterostructure, $P_j(x)$, as follows. In the metal contacts, it is given by expressions (5.125) and (5.128), respectively, with $\mu_-(x_1^-)$ and $\mu_+(x_2^+)$ expressed in terms of $\tilde{A}_{1,2}$ via Eqs. (5.129)–(5.131). In the semiconductor, it is given by expression (5.117) in terms of the persistent, $\tilde{\jmath}_-(x)$, and relaxing, $\tilde{\jmath}_-(x)$, thermoballistic spin-polarized currents, where the formfactors $F_2(x_2)$ entering the latter current are determined by the solution of the integral equation (5.78) for the spin accumulation function $A(x)$. The total density spin polarization $P_n(x)$ is obtained in an analogous way.

VI. EXAMPLES

This section deals with the application of the thermoballistic approach to various specific examples. The emphasis is on spin-polarized transport in heterostructures including nonmagnetic and magnetic semiconductors.

A. Homogeneous semiconductor at zero bias

In considering the case of a homogeneous semiconductor at zero bias, we illustrate the thermoballistic formalism for a particularly simple example and, moreover, collect results needed for treating heterostructures involving homogeneous layers of nonmagnetic and magnetic semiconductors (see Secs. VI B and VI C below).

For a homogeneous semiconducting layer at zero bias, the potential energy profiles $E_{\uparrow, \downarrow}(x)$ are given by

$$
E_{\uparrow, \downarrow}(x) = E_c \pm \frac{1}{2} \Delta
$$

(6.1)

$$(x_1 \leq x \leq x_2).$$

Specializing the development presented in Sec. VI B for constant spin splitting to the case $E_c(x) \equiv E_c$, we find from Eq. (5.20) the reduced ($\Delta = 0$) kernel $\tilde{K}_0(x, x'; l)$ in the explicit form

$$
\tilde{K}_0(x, x; x'; l) = Q_l e^{-|x-x'|/l} - e^{-|x-x'|/l}.
$$

(6.2)

From the corresponding solution $\tilde{R}_{10}(x)$ of Eq. (5.42) and the solution of the analogous equation for the function
For the resistance functions $\tilde{R}_{1,2}(x)$ of the homogeneous semiconductor; at $x = x_1$ and $x = x_2$, on the other hand, we have $\tilde{R}_{1}(x_1) = \tilde{R}_{2}(x_2) = 0$; see Eqs. (5.23) and (5.29).

For the reduced resistance $\tilde{R}$, we then find from Eq. (5.19), using Eq. (5.58),

$$\tilde{R} = 1 + \frac{S}{2l} - \frac{v_e N_e}{2J} P e^{-\beta E_x} A_{12},$$

(6.3)

and for the function $\tilde{R}_-(x)$ from Eq. (5.50), using Eqs. (4.106), (5.11), (5.13), and (5.27),

$$\tilde{R}_-(x) = \frac{x - (x_1 + x_2)/2}{l} + \frac{v_e N_e}{2J} P e^{-\beta E_x} \left[ A(x) - \frac{1}{2} A^+_{12} \right],$$

(6.5)

for $x_1 < x < x_2$, whereas from Eq. (5.51), $\tilde{R}_-(x_{1,2}) = \mp \tilde{R}$. The spin accumulation function $A(x)$ to be inserted in this expression is given by Eqs. (4.94) and (5.104).

Inserting expressions (6.4) and (6.5) in Eq. (5.54) and using Eq. (5.48), we find from Eq. (1.62) for the net total ballistic current in a homogeneous semiconductor at zero bias

$$J_+(x_1, x_2) = J \left( 1 + \frac{S}{2l} \right),$$

(6.6)

$$J_+(x', x_2) = J \left( \frac{1}{2} + \frac{x_2 - x'}{2l} \right),$$

(6.7)

for $x' > x_1$,

$$J_+(x_1, x'') = J \left( \frac{1}{2} + \frac{x'' - x_1}{2l} \right),$$

(6.8)

for $x'' < x_2$, and

$$J_+(x', x'') = J \frac{x'' - x'}{2l},$$

(6.9)

for $x_1 < x' < x'' < x_2$, in which the dependence on $A(x)$ present in $\tilde{R}$ and $\tilde{R}_-(x)$ has cancelled out completely. At this point, it is appropriate to note that the dependence of the ballistic current $J_+(x', x'')$ on the end-point coordinates $x', x''$ exhibited here contradicts the basic assumption of the prototype thermoballistic model as expressed by Eq. (3.20).

Now, using expressions (6.6)–(6.9) in Eq. (4.64), we find

$$\tilde{J}_+(x) = \tilde{J}_+ = J,$$

(6.10)

i.e., the total thermoballistic current is equal to the (constant) total physical current. Further, using Eq. (4.64), we have

$$\tilde{J}_-(x) \equiv \tilde{J}_- = P J,$$

(6.11)

for the persistent thermoballistic spin-polarized current, and hence from Eq. (5.115) for the persistent current spin polarization

$$\tilde{P}_J(x) \equiv \tilde{P}_J = \frac{\tilde{J}_-}{J} = P,$$

(6.12)

thereby retrieving the static spin polarization.

Turning now to the determination of the relaxing thermoballistic spin-polarized current $\tilde{J}_-(x)$ in a homogeneous semiconductor at zero bias, we have from Eq. (4.65) for the corresponding ballistic current

$$J_-(x', x''; x) = \frac{v_e N_e}{2} Q e^{-\beta E_x} \frac{N}{2} \left[ A(x') e^{-(x-x')/\nu_s} - A(x'') e^{-(x''-x)/\nu_s} \right]$$

(6.13)

$$(x_1 < x' < x'' < x_2).$$

Inserting this expression in Eq. (4.71) and subsequently using the derivative of Eq. (5.101) with respect to $x$, we obtain $\tilde{J}_-(x)$ in the form

$$\tilde{J}_-(x) = -\frac{v_e N_e Q e^{-\beta E_x}}{2} \frac{dA(x)}{dx},$$

(6.14)

[see Eq. (4.11) of Ref. 54; the factor 2 appearing in the right-hand side of the latter equation again reflects the fact that the normalization of $A(x)$ used there differs from that used in the present article]. From Eqs. (5.117), (6.11), and (6.14), we now have for the total current spin polarization

$$P_J(x) = P - \frac{v_e N_e Q e^{-\beta E_x}}{J} \frac{dA(x)}{dx},$$

(6.15)

[Note that owing to its normalization to the total thermoballistic current, the expression for $P_J(x)$ given by Eq. (136) of Ref. 55 differs from expression (6.15); see the remark following Eq. (5.117) above.]

As to the density spin polarization in a homogeneous semiconductor, we have from Eq. (1.67) for the persistent part, $\tilde{n}_+(x', x''; x) = \tilde{n}_+(x', x'')$, of the joint total ballistic density

$$\tilde{n}_+(x_1, x_2) = \frac{N_e}{2} e^{-\beta E_x} \left( \tilde{n}_+ + \frac{P}{2} \frac{A_{12}}{Q} \right),$$

(6.16)

$$\tilde{n}_+(x', x_2) = \tilde{n}_+(x_1, x_2) - \frac{J}{2v_e} \left( \frac{1}{2} + \frac{x' - x_1}{2l} \right),$$

(6.17)

for $x' > x_1$,

$$\tilde{n}_+(x_1, x'') = \tilde{n}_+(x_1, x_2) + \frac{J}{2v_e} \left( \frac{1}{2} + \frac{x_2 - x''}{2l} \right),$$

(6.18)
for \( x'' < x_2 \), and
\[
\tilde{n}_+(x', x'') = \tilde{n}_+(x_1, x_2) - \frac{J}{2v_e} \left( x' - x_1 - (x_2 - x'') \right)
\]  
(6.19)
for \( x_1 < x' < x'' < x_2 \). For the relaxing part of the joint total ballistic density, \( \tilde{n}_+(x', x'') \equiv \tilde{n}_+(x', x'', x) \), we find from Eq. (4.68)
\[
\tilde{n}_+(x', x'') = 0,
\]  
(6.20)
so that
\[
n_+(x', x'') = \tilde{n}_+(x', x'').
\]  
(6.21)
Observing Eq. (6.21), we now use expressions (6.16)–(6.19) in Eq. (4.71) to obtain for the thermoballistic joint total density
\[
n_+(x) = \tilde{n}_+(x) = \frac{J}{2v_e} \left( x - x_1 + x_2 \right)
\]  
(6.22)
with \( \tilde{n}_+(x_1, x_2) \) given explicitly by Eq. (6.16). Since
\[
\tilde{n}_-(x', x'') = P\tilde{n}_+(x', x'')
\]  
(6.23)
from Eq. (4.67), we have for the persistent part of the joint ballistic spin-polarized density
\[
\tilde{n}_-(x) = P\tilde{n}_+(x) = Pn_+(x),
\]  
(6.24)
and hence for the persistent density spin polarization
\[
P_n(x) = \frac{\tilde{n}_-(x)}{n_+(x)} = P,
\]  
(6.25)
in agreement with the corresponding current spin polarization.

By inserting expression (6.13) for the corresponding current \( \tilde{J}_-(x) \) in the balance equation (5.9) and using Eq. (6.102) for the spin accumulation function \( A(x) \), the relaxing thermoballistic spin-polarized density \( \tilde{n}_-(x) \) for a homogeneous semiconductor is readily obtained in the form
\[
\tilde{n}_-(x) = \frac{N_e}{2} Q e^{-\beta E_v} A(x),
\]  
(6.26)
so that we have for the total density spin polarization
\[
P_n(x) = P + \frac{N_e}{2n_+(x)} Q e^{-\beta E_v} A(x),
\]  
(6.27)
with \( n_+(x) \) given by Eq. (6.22). Now, omitting in expression (6.22) for \( n_+(x) \) the term proportional to \( J \), so that \( n_+(x) = \tilde{n}_+(x_1, x_2) \), we can use expression (6.102) for \( P_n(x) \) in Eq. (6.15) to express the current spin polarization \( P_J(x) \) in terms of \( P_n(x) \) in the form
\[
P_J(x) = P - \frac{2v_e \tilde{n}_+(x_1, x_2)}{J} \int \frac{dP_n(x)}{dx}.
\]  
(6.28)
Differentiating this equation and using Eqs. (5.102) and (6.27), we then obtain
\[
P_n(x) = P - \frac{J}{2v_e \tilde{n}_+(x_1, x_2)} l \frac{dP_J(x)}{dx}
\]  
(6.29)
for the density spin polarization \( P_n(x) \) in terms of \( P_J(x) \).

For the magnetoresistance of a homogeneous semiconductor at zero bias, we find
\[
R_m = Q - 1 - \frac{v_e N_c}{2J} \frac{P}{Q} e^{-\beta E_v} A_{12} \frac{2l}{2l + S}
\]  
(6.30)
by inserting the zero-field limit of expression (6.4),
\[
\tilde{\gamma}_0 = 1 + \frac{S}{2l},
\]  
(6.31)
for \( \tilde{\gamma}_0 \) in Eq. (5.77).

### B. FM/NMS/FM heterostructures

We now consider heterostructures formed of a homogeneous, nonmagnetic semiconducting (NMS) layer and two ferromagnetic metal (FM) contacts. The study of spin-polarized transport in this kind of structure, both experimentally and theoretically, marked the beginning of semiconductor spintronics \(^{20-28}\) (for recent surveys of the physics of semiconductor-based spintronic devices, see Refs. \(^{57-59}\) ). For zero bias, we evaluate the position dependence of the current and density spin polarizations using the results of Secs. V D 2, V D 3, and VI A.

For nonzero bias, we obtain the spin polarizations “injected” from the contacts into the semiconductor, i.e., the polarizations generated inside the semiconductor in the vicinity of either FM/NMS interface regardless of the influence of the opposite interface.

#### 1. Zero-bias spin polarizations

Inside the semiconducting layer, we have from Eq. (6.15) with \( P = 0 \) and \( Q = 1 \), using expression (5.104) for the spin accumulation function \( A(x) \),
\[
P_J(x) = \frac{v_e N_c}{J} e^{-\beta E_v} \gamma [C_1 e^{-(x-x_1)/L} - C_2 e^{-(x-x_2)/L}],
\]  
(6.32)
where \( \gamma \) is given by Eq. (5.108). The coefficients \( C_{1,2} \) can be expressed via Eqs. (6.105) and (6.106), and, using Eq. (4.17), in terms of the values \( \tilde{A}_{1,2} \) of the reduced spin accumulation function \( \tilde{A}(x) \) on the contact sides of the interfaces.

In order to determine the quantities \( \tilde{A}_{1,2} \), we evaluate expression (6.32) on the semiconductor sides of the interfaces, obtaining
\[
P_J^{(sc)}(x_1) \equiv P_J(x_1^+) = \frac{v_e n_+^{(0)}}{2J} (g \tilde{A}_1 - h \tilde{A}_2),
\]  
(6.33)
Here, we have introduced the total equilibrium density for zero spin splitting and zero bias,
\[ n_+^{(0)} = N_ne^{-\beta(E_n - \mu)}, \]  
which is obtained inside the semiconducting layer. The coefficients \( g \) and \( h \) in expressions (6.33) and (6.34) are given by Eqs. (5.111) and (5.112), respectively.

Using the continuity of \( P_j(x) \) at the interfaces, Eq. (5.133), we now equate expressions (6.33) and (6.34), and expressions (5.134) and (6.34). When spin-selective interface resistances are included, expression (6.33) for \( P_j^{(c)}(x_1) \) is to be replaced with the more general expression obtained from using expression (6.136) for \( \mu_-(x_1) \) in Eq. (5.125), and analogously for \( P_j^{(c)}(x_2) \).

For zero bias, when \( |A_{1,2}| \ll 1 \), this results in a system of coupled linear equations for \( A_{1,2} \) [see Eqs. (5.138) and (5.139)],
\[ [g + \tilde{G}_l^{(0)}] A_1 - h A_2 = \frac{2J}{v_cn_+^{(0)}} P_l, \]
\[ h A_1 - [g + \tilde{G}_r^{(0)}] A_2 = \frac{2J}{v_cn_+^{(0)}} P_r, \]
where
\[ \tilde{G}_{l,r}^{(0)} = \frac{G_{l,r}}{\beta e^2 v_c n_+^{(0)}}. \]

The solutions of Eqs. (6.36) and (6.37) are found to be
\[ A_1 = \frac{2J}{v_cn_+^{(0)}} \Gamma \{ [g + \tilde{G}_r^{(0)}] P_l - h P_r \}, \]
\[ A_2 = \frac{2J}{v_cn_+^{(0)}} \Gamma \{ h P_l - [g + \tilde{G}_l^{(0)}] P_r \}, \]
where
\[ \Gamma = [g + \tilde{G}_l^{(0)}] [g + \tilde{G}_r^{(0)}] - h^2. \]
Expressions (6.39) and (6.40) determine the values of the reduced spin accumulation function, \( \check{A}_1 \) and \( \check{A}_2 \) in terms of the current \( J \), of the polarizations \( P_l \) and \( P_r \) in the left and right ferromagnetic contact, respectively, and of material parameters, such as the conductivities \( \sigma_{l,r} \) and the spin diffusion lengths \( L_{d_{l,r}} \) of the contacts [via \( \tilde{G}_{l,r}^{(0)} \)] and the momentum relaxation length \( l \) and the spin relaxation length \( l_s \) in the semiconducting sample as well as the sample length \( S \) (via \( g \) and \( h \)) and the (constant) total equilibrium electron density \( n_+^{(0)} \). Since the quantities \( \check{A}_{1,2} \) are proportional to the total current \( J \), the current spin polarization \( P_j(x) \) is independent of \( J \), while the density spin polarization \( P_n(x) \) is proportional to \( J \).

The spin polarizations along the entire heterostructure are now obtained as follows. Inside the semiconductor, the current spin polarization \( P_j(x) \) is given by expression (6.32), with \( C_{1,2} \) calculated from the solutions \( \check{A}_{1,2} \) of Eqs. (6.39) and (6.40). The corresponding density spin polarization \( P_n(x) \) is then readily obtained from Eq. (6.20). The expressions for \( P_j(x) \) in the ferromagnetic contacts are provided by Eqs. (5.126) and (5.128), respectively, where the quantities \( \mu_-(x_1) \) and \( \mu_-(x_2) \) are calculated from Eq. (5.136) and from its analogue for \( \mu_-(x_3) \), respectively. We do not write down the density spin polarizations in the ferromagnets, but only mention that they do not, in general, match the polarizations \( P_n(x_1^+) \) and \( P_n(x_2^-) \) on the semiconductor sides of the interfaces.

In Refs. [54] and [90], we have presented results of detailed calculations for \( P_j(x) \) at zero bias for typical parameter values of FM/NMS/FM heterostructures, emphasizing the dependence of the polarization on the momentum and spin relaxation lengths, \( l \) and \( l_s \), and on the spin-selective interface resistances \( \rho_{l,r}^{(1,2)} \) [see Sec. V D 2].

2. Injected spin polarizations at nonzero bias

We define the “injected spin polarization” as the polarization inside the semiconductor in the vicinity of the interface, e.g., at \( x = x_1 \), generated by the bulk polarization \( P_l \) of the left ferromagnet regardless of the influence of the right ferromagnet. More explicitly, we define the injected current and density spin polarizations as the polarizations \( P_j(x_1^+) \) and \( P_n(x_1^+) \), respectively, in the limit of infinite sample length, \( S \rightarrow \infty \). The injected spin polarizations at \( x = x_1^+ \) provide the initial values of the left-generated polarizations in the semiconductor, which propagate into the region \( x > x_1 \) while being degraded by the effect of spin relaxation.

We now consider the injected spin polarizations for electron transport in a homogeneous semiconductor, driven by an external electric field, i.e., for a (spin-degenerate) potential energy profile of the form (4.121), with the parameter \( \epsilon \) defined by Eq. (4.122). In order to obtain the spin accumulation function \( A(x) \) for this case, one has to solve Eq. (5.92) [in general, numerically] under the asymptotic condition
\[ A(x) \propto e^{-x/\lambda} \quad \text{for} \quad x \rightarrow \infty. \]

To determine the decay length \( \lambda \), we solve Eq. (5.92) in the range \( x - x_1 \gg 1/(\epsilon + 1/l) \) in which the \( x \)-dependence of the coefficient functions \( b_0(x) \), \( b_1(x) \), and \( b_2(x) \) arising from the function \( b(x) \) can be disregarded. This yields
\[ \frac{1}{\lambda} = \frac{\epsilon}{2} + \left[ \frac{\epsilon^2}{4} + \frac{l - l}{l_l^2} \left( 1 + \frac{\epsilon^2 + 1 + \epsilon l}{2 + \epsilon l} \right) \right]^{1/2}. \]
Since \( l > \bar{L} \), \( \lambda \) is a real number.

The injected current spin polarization is obtained from Eq. (5.117) with \( \tilde{J}_\gamma(x) = 0 \). We calculate the relaxing thermoballistic spin-polarized current at the interface, \( \tilde{J}_\gamma(x^+_1) \), from the relation

\[
\tilde{J}_\gamma(x^+_1) = \frac{v_e N}{2} \tilde{W}(x_1; x_1, x_2; l)[A_1 - A(x^+_1)],
\]

(6.44)

where the function \( \tilde{W}(x; x_1, x_2; l) \) is given by Eq. (5.80). This relation can be shown to hold, for arbitrary sample length \( S \) and potential energy profiles \( E_{x_1}(x) \), by (i) evaluating \( \tilde{J}_\gamma(x^+_1) \) from Eq. (4.71) with \( F(x', x''; x) \equiv \tilde{J}_\gamma(x^+_1, x''; x) \) [see Eq. (4.65)] and (ii) eliminating from the resulting expression the boundary value \( A_2 \) by using the integral equation (5.73) for \( x = x_1 \).

For the case considered here, we write down the integral equation (5.87) [with \( \zeta(x') = \tilde{\zeta} \)] for \( x = x_1 \) and take the limit \( x_2 \to \infty \) to obtain the relation

\[
2A(x^+_1) - \bar{A}_1 = A_1, \quad (6.45)
\]

where

\[
\bar{A}_1 = \int_{x_1}^{\infty} dx \frac{e^{-(x-x_1)/l}}{A(x)}. \quad (6.46)
\]

Relation (6.45) fixes the normalization of the spin accumulation function \( A(x) \) in terms of the boundary value \( A_1 \). Then, using this relation in Eq. (6.44) with \( \tilde{W}(x_1; x_1, x_2; l) = 2e^{-\beta E_{x_1}(x_1)} \), we can express the current \( \tilde{J}_\gamma(x^+_1) \) in the form

\[
\tilde{J}_\gamma(x^+_1) = \frac{v_e n^{(0)}(x_1)}{2} A_{1,1}^{(1)} \bar{A}_1, \quad (6.47)
\]

where the quantity

\[
A_{1,1}^{(1)} = \frac{A(x^+_1) - \bar{A}_1}{A(x^+_1) - \bar{A}_1/2} \quad (6.48)
\]

is independent of the normalization of \( A(x) \), and

\[
n^{(0)}(x_1) = N e^{-\beta[E(x_1) - \mu_1]}. \quad (6.49)
\]

In obtaining Eq. (6.47), we have used Eq. (4.80), with \( P(x) = 0 \), as well as Eq. (4.114).

For the injected current spin polarization, we now have from Eq. (6.117)

\[
P_J(x^+_1) = \frac{\tilde{J}_\gamma(x^+_1)}{J} = \frac{v_e n^{(0)}(x_1)}{2J} A_{1,1}^{(1)} \bar{A}_1, \quad (6.50)
\]

which, by continuity, is equal to the polarization \( P_J(x_1) \) at the contact side of the interface. Then, equating the right-hand sides of Eqs. (5.133) and (6.50), we obtain

\[
P_J = \frac{G_l}{2 \beta e^2 J} \ln \left( \frac{1 + \bar{A}_1/2}{1 - \bar{A}_1/2} \right) = \frac{v_e n^{(0)}(x_1)}{2J} A_{1,1}^{(1)} \bar{A}_1. \quad (6.51)
\]

This nonlinear equation for \( \bar{A}_1 \) is to be solved for given values of the parameters \( \epsilon, P_1, G_l, n^{(0)}_+(x_1), l, \) and \( L_s \).

We now turn to the calculation of the injected density spin polarization from Eq. (5.118), where \( \tilde{n}_-(x) = 0 \) and \( n_+(x) = \tilde{n}_+(x) \) in the present case. Proceeding similarly as for the current \( \tilde{J}_\gamma(x^+_1) \), we obtain the relaxing thermoballistic spin-polarized density at the interface, \( \tilde{n}_-(x^+_1) \), in the form

\[
\tilde{n}_-(x^+_1) = \frac{n^{(0)}(x_1)}{4} A_1^{(1)} \bar{A}_1, \quad (6.52)
\]

where

\[
A_1^{(1)} = \frac{A(x^+_1)}{A(x^+_1) - \bar{A}_1/2}. \quad (6.53)
\]

For the persistent total thermoballistic density at the interface, \( \tilde{n}_+(x^+_1) \), we find by evaluating Eq. (4.71) with \( F(x', x''; x) \equiv \tilde{n}_+(x', x''; x) \) [see Eq. (4.67)] and taking the limit \( S \to \infty \)

\[
\tilde{n}_+(x^+_1) = \frac{n^{(0)}(x_1)}{2} (1 + \bar{A}_1), \quad (6.54)
\]

where the quantity

\[
\bar{A}_1 = \int_{x_1}^{\infty} dx \frac{e^{-(x-x_1)/l}}{e^\beta[\tilde{\mu}(x) - \mu_1]}. \quad (6.55)
\]

has been expressed in terms of the average chemical potential \( \tilde{\mu}(x) \) using Eq. (4.14). The injected density spin polarization now follows as

\[
P_n(x^+_1) = \frac{\tilde{n}_+(x^+_1)}{\tilde{n}_+(x^+_1)} = \frac{A_1^{(1)} \bar{A}_1}{2(1 + \bar{A}_1)}, \quad (6.56)
\]

where the boundary value \( \bar{A}_1 \) of the reduced spin accumulation function is again to be determined by solving Eq. (6.51).

The dependence of the injected current spin polarization, \( P_J(x^+_1) \), on the electric-field parameter \( \epsilon \), for \( l \)-values ranging from the drift-diffusion to the ballistic regime and for zero as well as nonzero interface resistances \( \rho_{1,1}^{(1)} \), has been studied numerically in Ref. [54].

In the drift-diffusion regime, when \( l/\bar{L}_s \ll 1 \) and \( \epsilon l \ll 1 \), the spin accumulation function \( A(x) \) is given by the exponentially decreasing solution of Eq. (5.100),

\[
A(x) \propto e^{-(x-x_1)/L_s} \quad (6.57)
\]

(\( x \geq x_1 \)), with the field-dependent spin diffusion length \( L_s \) given by

\[
\frac{1}{L_s} = \frac{\epsilon}{2} + \left( \frac{\epsilon^2}{4} + \frac{1}{L_s} \right)^{1/2}, \quad (6.58)
\]

where \( L_s \) is the spin diffusion length defined by Eq. (4.101). From Eqs. (6.48) and (6.53), respectively, we then have

\[
A_1^{(1)} = \frac{2l}{L_s}. \quad (6.59)
\]
and
\[ A_n^{(1)} = 2, \]  
(6.60)

and hence from Eqs. (6.59) and (6.60), respectively,
\[ P_J(x_1^+) = \frac{v_e n_+^{(0)}(x_1)}{J} \frac{l}{L_s} A_1 = \frac{1}{2eL_s} \tilde{A}_1 \]  
(6.61)

and
\[ P_n(x_1^+) = \frac{\tilde{A}_1}{1 + \tilde{A}_1} = \frac{\tilde{A}_1}{2} \]  
(6.62)

for the injected current and density spin polarizations in the drift-diffusion regime. In deriving the right-hand equation (6.61), we have used Eq. (4.95), with \( P = 0 \), \( Q = 1 \), and \( \beta eV = \epsilon S \), as well as Eq. (6.49), to express the total current \( J \) in the form
\[ J = 2v_e n_+^{(0)}(x_1) \epsilon l = \frac{1}{\beta e^2} \sigma_+^{(0)} \epsilon, \]  
(6.63)

where
\[ \sigma_+^{(0)} = 2\beta e^2 v_e n_+^{(0)}(x_1) \epsilon \]  
(6.64)

is the (spin-summed) conductivity of the semiconductor [see Eq. (2.27)]. The right-hand equation (6.62) has been obtained by using Eq. (4.91) in Eq. (6.59). The boundary value \( \tilde{A}_1 \) is determined by the equation
\[ P_l - \frac{G_1}{2\sigma_+^{(0)} \epsilon} \ln \left( \frac{1 + \tilde{A}_1/2}{1 - \tilde{A}_1/2} \right) = \frac{1}{2eL_s} \tilde{A}_1, \]  
(6.65)

which follows from Eq. (6.51) by replacing its right-hand side with the right-hand side of Eq. (6.61) and inserting expression (6.63) for \( J \).

The effect of external electric fields on the current spin polarization injected at FM/NMS interfaces has been studied within the standard drift-diffusion approach by Yu and Flatté. Comparing our description to that of these authors, we find that the field-dependent spin diffusion length \( L_s^* \) given by Eq. (6.58) agrees with the “upstream” spin diffusion length \( L_s \), given by Eq. (2.23b) of Ref. 66, provided the “intrinsic” spin diffusion length \( L \) of that reference is identified with the spin diffusion length \( L_s = \sqrt{l/s} \) of the present work. Then, identifying in Eq. (3.5) of Ref. 66 (with the interface resistances set equal to zero) the spin-summed conductivity of the semiconductor, \( \sigma_s \), with \( \sigma_+^{(0)} \), and the spin injection efficiency at the interface, \( \alpha_0 \), with \( P_l(x_1^+) = \tilde{A}_1/2eL_s^* \), and using Eq. (5.127), we observe the equivalence of the former equation with Eq. (6.65). Consequently, the injected current and density spin polarizations of either work are actually identical.

For arbitrary \( l \), we now consider the injected current spin polarization in the zero-bias limit, when \( |\tilde{A}_1| \ll 1 \).

Here, the spin accumulation function \( A(x) \) is given by the exponentially decreasing solution of Eq. (5.102),
\[ A(x) \propto e^{-(x-x_1)/L} \]  
(6.66)
\((x \geq x_1)\), where the generalized spin diffusion length \( L \) is given by Eq. (5.103). From Eq. (6.48), we then have
\[ A_n^{(1)} = \frac{2\gamma}{1 + \gamma} \equiv \gamma^*, \]  
(6.67)

with \( \gamma \) given by Eq. (5.105), and hence from the zero-bias limit of Eq. (6.51)
\[ \tilde{A}_1 = \frac{2J}{v_e n_+^{(0)}(x_1) \Gamma_l/\tilde{G}_1 + \gamma^*}, \]  
(6.68)

where
\[ \tilde{G}_1 = \frac{1}{\rho_1} = \beta e^2 v_e n_+^{(0)}(x_1) \]  
(6.69)

is the Sharvin interface conductance [see Eq. (5.68)]. Inserting this in Eq. (6.68), we find
\[ P_J(x_1^+) = \frac{P_l}{1 + \Gamma_l/\gamma^* \tilde{G}_1}, \]  
(6.70)

i.e., for zero bias, the injected current spin polarization is independent of the total current \( J \).

In the drift-diffusion regime, when \( l/l_s \ll 1 \), we have
\[ \gamma^* = 2 \sqrt{\frac{l}{l_s}}, \]  
(6.71)

so that \( P_J(x_1^+) \) reduces to
\[ P_J(x_1^+) = \frac{P_l}{1 + \Gamma_l/\gamma^* \tilde{G}_1}, \]  
(6.72)

where
\[ \tilde{G}_1 = 2\tilde{G}_1 \sqrt{\frac{l}{l_s}} = \frac{\sigma_+^{(0)}}{L_s}, \]  
(6.73)

with \( \sigma_+^{(0)} \) defined by Eq. (6.64), and \( L_s \) by Eq. (4.101). The quantity \( \tilde{G}_1 \) is seen to be the semiconductor analogue of the “interface conductance” \( G_1 \) characterizing the ferromagnet [see Eq. (5.127)]. For typical values of the parameters of the FM/NMS/FM system (see, e.g., Ref. 54), the values of \( G_1 \) exceed those of \( \tilde{G}_1 \) by several orders of magnitude. This indicates a “conductance mismatch” between ferromagnet and semiconductor, which gives rise to very low values of the injected spin polarizations at FM/NMS interfaces. To remedy this mismatch, one may introduce spin-selective interface resistances, for example, in the form of tunneling barriers. In the ballistic regime, when \( l/l_s \gg 1 \), we have
\[ \gamma^* = \gamma = 1, \]  
(6.74)
so that

\[ P_J(x^+) = \frac{P_1}{1 + G_1/G_1}. \]  

(6.75)

Here, the Sharvin interface conductance \( G_1 \) takes the place of the quantity \( G_1 \) in Eq. (6.72). As \( G_1 \) is proportional to the density \( n_0(x, 1) \), Eq. (6.75) yields values for \( P_J(x^+) \) close to the bulk spin polarization of the ferromagnet, \( P_1 \), if \( n_0(0) \) is sufficiently high. For typical parameter values, however, the high donor densities needed to obtain the required high electron densities implies very small values of the momentum relaxation length \( l \), such that ballistic transport is excluded as the dominating transport mechanism. On the other hand, for densities so low that ballistic transport prevails, the injected spin polarization is confined to very small values. This result corroborates previous estimates\(^{50} \) according to which spin injection is suppressed even in the ballistic regime unless spin-selective interface resistances are introduced.

C. DMS/NMS/DMS heterostructures

As an example of particular interest from the point of view of applications, we now consider spin-polarized electron transport in heterostructures involving diluted magnetic semiconductors (DMS) in their paramagnetic phase (see, e.g., Refs. 86 and 91-104). In structures of this kind, a nonmagnetic semiconducting (NMS) layer is sandwiched between two DMS layers which, in turn, are enclosed between nonmagnetic metal contacts (see Fig. 7).

In a complete thermoballistic description, the semiconductor part of a DMS/NMS/DMS structure should be treated as a single sample. Then, the ballistic intervals \([x', x'']\) covering the sample may contain one or both of the DMS/NMS interfaces, at which the potential energy profiles must be expected to change abruptly. The same holds for the material parameters, in particular the momentum and spin relaxation lengths, so that a description in terms of position-dependent parameters would become necessary. Here, we adopt a simplified treatment by assuming the different layers in a DMS/NMS/DMS heterostructure to be homogeneous and requiring the interfaces to act as fixed points of local thermodynamic equilibrium. This allows us to apply the thermoballistic description separately to the different layers (the potential energy profiles are then, in general, discontinuous at the interfaces). For each layer, we evaluate the spin accumulation function and the zero-bias current spin polarization for a homogeneous semiconductor (see Sec. VIA), and subsequently match the current spin polarization at the interfaces to obtain its full position dependence as well as the magnetoresistance.

![FIG. 7: Schematic zero-bias potential energy profiles for a DMS/NMS/DMS heterostructure composed of three homogeneous semiconducting layers enclosed between nonmagnetic metal contacts.](image)

1. Zero-bias current spin polarization

Heterostructures of the kind depicted schematically in Fig. 7 are parametrized here by attaching labels \( j = 1, 2, 3 \) to quantities referring to the left DMS layer, the NMS layer, and the right DMS layer, respectively. The positions of the interfaces (including the interfaces between the DMS layers and the contacts) are denoted by \( x_k \) \((k = 1, 2, 3, 4)\); this notation deviates from the one used in the preceding sections.

Inside the left and right metal contacts, the position dependence of the current spin polarization is given by Eqs. (5.12a) and (5.12b), respectively [with \( x_j \) in the latter equation replaced with \( x_4 \)], with \( \mu_\bot(x, 1, 4) = A_1,4/\beta \) [see Eq. (4.17) for \( |\beta\mu_\bot(x)| \ll 1 \)] and \( P_1 = P_r = 0 \),

\[ P_J(x) = \mp \frac{G_{1,r}}{2\hbar e^2 J} A_{1,4} e^{-|x-x_{1,4}|/L_s^{(\beta, r)}} \]  

(6.76)

for \( x < x_1 \) and \( x > x_4 \).

Inside the semiconducting part of the heterostructure, \( P_J(x) \) is found in terms of the static spin polarizations \( P_j \) of the three layers, and of the boundary values of the spin accumulation function \( A(x) \) at the interface positions \( x_k \), \( A(x_k) = A_k \), which are all points of local thermodynamic equilibrium. [The interface positions \( x_{2,3} \) are points of local thermodynamic equilibrium in the same sense as are the interface positions \( x_{1,4} \), except that there the interface is between metal contact and DMS, while here it is between DMS and NMS.] In each layer \( j \), the function \( A(x) \) has the Sharvin discontinuities \( A(x_j^+) - A_j \) and \( A_{j+1} - A(x_{j+1}^-) \) at the interface positions \( x_j \) and \( x_{j+1} \), respectively [see Eqs. (5.109) and (5.110)]. Using now, for zero bias, Eq. (6.15) together with Eq. (5.104) separately in each layer, we have

\[ P_J(x) = P_1 + \frac{\hbar e N_c}{\beta J} Q J e^{-\beta E_{\nu,1}^{(j)}(x_j)} \gamma_j \]

\[ \times \left[ C_1^{(j)} e^{-(x-x_j)/L_j} - C_2^{(j)} e^{-(x_{j+1}-x)/L_j} \right] \]  

(6.77)
for \( x_j \leq x \leq x_{j+1} \) (\( j = 1, 2, 3 \)). Here,
\[
\gamma_j = \frac{\bar{t}_j}{L_j} = \frac{L_j}{l^{(j)}_s}, 
\tag{6.78}
\]
with \( \bar{t}_j \) and \( L_j \) defined by Eqs. (5.99) and (5.103) in terms of the momentum relaxation length, \( l_j \), and spin relaxation length, \( l^{(j)}_s \), of layer \( j \). Further,
\[
C^{(j)}_1 = \frac{1}{D_j}[(1 + \gamma_j)e^{S_j/L_j}A_j - (1 - \gamma_j)A_{j+1}] 
\tag{6.79}
\]
and
\[
C^{(j)}_2 = -\frac{1}{D_j}[(1 - \gamma_j)A_j - (1 + \gamma_j)e^{S_j/L_j}A_{j+1}], 
\tag{6.80}
\]
where
\[
D_j = 2[(1 + \gamma_j^2) \sinh(S_j/L_j) + 2\gamma_j \cosh(S_j/L_j)], 
\tag{6.81}
\]
and
\[
S_j = x_{j+1} - x_j 
\tag{6.82}
\]
is the thickness of layer \( j \). [Owing to a difference in normalization, expression (6.77) for \( P_J(x) \) differs from the corresponding expression given by Eq. (141) of Ref. 55, see the remark following Eq. (6.13) above.]

In order to relate the quantities \( \bar{A}_k \) to the total physical current \( J \) and the parameters of the contact-semiconductor system, we invoke the continuity of the current spin polarization \( P_J(x) \) at all interfaces, setting \( P_2 = 0 \) \((Q_2 = 1)\) in Eq. (6.77). From Eqs. (6.76) and (6.77), we then obtain a set of four coupled linear equations for \( \bar{A}_k \),
\[
(G^{(1)}_t + Q_1g_1)\bar{A}_1 - Q_1h_1\bar{A}_2 = -\frac{2J}{v_e n_+^{(0,1)}}P_1, 
\tag{6.83}
\]
\[
- Q_1h_1\bar{A}_1 + (Q_1g_1 + e^{\beta\delta_2}g_2)\bar{A}_2 
- e^{\beta\delta_2}h_2\bar{A}_3 = \frac{2J}{v_e n_+^{(0,1)}}P_1, 
\tag{6.84}
\]
\[
- e^{\beta\delta_2}h_2\bar{A}_2 + (e^{\beta\delta_2}g_2 + Q_3g_3)\bar{A}_3 
- Q_3h_3\bar{A}_4 = -\frac{2J}{v_e n_+^{(0,3)}}P_3, 
\tag{6.85}
\]
\[
- Q_3h_3\bar{A}_3 + (G^{(3)}_t + Q_3g_3)\bar{A}_4 = \frac{2J}{v_e n_+^{(0,3)}}P_3. 
\tag{6.86}
\]

Here,
\[
\bar{G}^{(1,3)}_{l,r} = \frac{G_{l,r}}{\beta e^2 v_e n_+^{(0,1,3)}}, 
\tag{6.87}
\]

where
\[
n_+^{(0,j)} = N_+ e^{-\beta[V^{(j)}_c - \mu_1]} 
\tag{6.88}
\]
is the (constant) total equilibrium electron density in layer \( j \), and
\[
\delta_{j,j'} = E^{(j)}_c - E^{(j')}_c 
\tag{6.89}
\]
are the band offsets. Further,
\[
g_j = h_j [\cosh(S_j/L_j) + \gamma_j \sinh(S_j/L_j)], 
\tag{6.90}
\]
with
\[
h_j = \frac{4\gamma_j}{D_j}. 
\tag{6.91}
\]

The system of equations (6.83)-(6.86) can be easily solved, so that the complete position dependence of the zero-bias current spin polarization is obtained in explicit form.

We now specialize to the case of a symmetric heterostructure, for which the parameters of the right DMS layer and metal contact are identical to those of the left DMS layer and metal contact. Assuming arbitrarily high conductivities of the contacts, \( \sigma^{(l,r)}_{j} \rightarrow \infty \), so that \( \bar{G}^{(1,3)}_{l,r} \rightarrow \infty \), we have from Eqs. (6.70) and (6.87)
\[
\bar{A}_{1,4} \rightarrow 0, 
\tag{6.92}
\]
such that \( \bar{G}^{(1,3)}_{l,r} \bar{A}_{1,4} \) remains nonzero and finite. Then, from Eqs. (6.84) and (6.85) with \( P_1 = P_3 = P \) and \( Q_1 = Q_3 = Q \),
\[
\bar{A}_2 = -\bar{A}_3 = \frac{2J}{v_e n_+^{(0,D)}} \frac{P}{Q_{DN}}, 
\tag{6.93}
\]
where
\[
Q_{DN} = Qg_D + (g_N + h_N)e^{\beta\delta_{DN}}. 
\tag{6.94}
\]
Hence, from Eqs. (6.83) and (6.86),
\[
\bar{G}^{(1)}_t \bar{A}_1 = -\bar{G}^{(4)}_t \bar{A}_4 = -\frac{2J}{v_e n_+^{(0,D)}}P + Qh_D \bar{A}_2 
\tag{6.95}
\]
\[
= -\frac{2J}{v_e n_+^{(0,D)}} \left(1 - \frac{Qh_D}{Q_{DN}}\right). 
\tag{6.95}
\]
Here, the DMS parameters have been labeled by “D”, and the NMS parameters by “N”.

Thus, in the symmetric case, the zero-bias current spin polarization \( P_J(x) \) is completely determined by the quantity \( \bar{A}_2 \). Explicitly, we obtain, setting \( L^{(l)}_s = L^{(r)}_s = L^{(mc)}_s \) (where the superscript “mc” refers to the metal contacts) in Eq. (6.70) and using Eqs. (6.87) and (6.95),
\[
P_J(x) = P \left(1 - \frac{Qh_D}{Q_{DN}}\right) e^{-|x-x_{1,4}|/L^{(mc)}_s}, 
\tag{6.96}
\]
if \( x < x_1 \) and \( x > x_4 \), respectively. Further, from Eq. (6.77), we have, using Eqs. (6.78)-(6.81) along with
Eqs. (1.17), (6.35), and (6.93),

\[ P_j(x) = P \left\{ 1 - \frac{Q h_D}{Q_{DN}} \cosh([x - x_{1.4}]/L_D) + \gamma_D \sinh([x - x_{1.4}]/L_D) \right\}, \quad (6.97) \]

if \( x_1 \leq x \leq x_2 \) and \( x_3 \leq x \leq x_4 \), respectively, and

\[ P_j(x) = \frac{2e\beta_D x n P}{Q_{DN}} \times \left[ \cosh(S_N/2L_N) + \gamma_N \sinh(S_N/2L_N) \right] \times \cosh([x - (x_2 + x_3)/2]/L_N), \quad (6.98) \]

if \( x_2 \leq x \leq x_3 \).

In Refs. [53] and [105], we have presented numerical results for \( P_j(x) \) for values of the momentum relaxation length \( l \) ranging from the drift-diffusion regime to the ballistic regime.

2. Magnetoresistance

The relative magnetoresistance \( R_m \) of the DMS/NMS/DMS heterostructure follows by inserting in Eq. (5.74) the reduced resistance \( \hat{R} \) and the corresponding zero-field resistance \( \hat{R}_0 \) obtained by summing up the respective contributions \( \hat{R}_j \) and \( \hat{R}_0^{(j)} \) of the (homogeneous) layers \( j \). These contributions are obtained from the (appropriately labeled) expressions (6.4) and (6.31) by multiplication with a factor \( B_m^{(j)}(x_1, x_4)/B_m^{(j)}(x_j, x_{j+1}) \), such that \( \hat{R} \) and \( \hat{R}_0 \) are normalized in conformance with the definition (6.10) for a single sample extending from \( x_1 \) to \( x_4 \).

Specializing immediately to the case of the symmetric structure considered above, we have, defining

\[ S_j = 1 + \frac{S_j}{2l_j} \quad (6.99) \]

(\( j = D, N \)) and using Eqs. (6.92),

\[ \hat{R} = 2Qe\beta_D x_s^{(j)} S_D + e\beta_D x_s^{(N)} S_N + \frac{ve_N e\beta_D x_s^{(j)}}{2J} (\hat{A}_2 - \hat{A}_3) \quad (6.100) \]

(we have omitted here the overall factor \( B_m^{(j)}(x_1, x_4) \) which drops out when \( R_m \) is formed), from which \( \hat{R}_0 \) follows by setting \( P = 0 \) and \( Q = 1 \). Then, using Eq. (6.93), we obtain

\[ R_m = (Q - 1)S_D + \frac{P^2/Q_{DN}}{S_D + e^{-\beta_D x_s^{(j)}} S_N/2} \quad (6.101) \]

Here, we note that in Ref. [53], in contrast to its definition in terms of the zero-field resistance \( \hat{R}_0 \) via Eq. (5.74), the relative magnetoresistance \( R_m \) has been defined with respect to the spin-equilibrium resistance obtained by setting \( A_2 = A_3 = 0 \) in expression (6.100). The latter definition does not seem to correspond to a genuine magnetoresistance, and so one should not attach quantitative significance to the numerical results for \( R_m \) shown in Fig. 4 of Ref. [53].

In the limit of low external magnetic field, when the static spin polarization \( P \) depends linearly on the field strength, we have from Eq. (6.101), keeping terms of order \( P^2 \),

\[ R_m = \frac{1/[g_D + (g_N + h_N)e^{-\beta_D x_s^{(j)}}] - S_D/2} {S_D + e^{-\beta_D x_s^{(j)}} S_N/2} \quad (6.102) \]

While based on assumptions that differ from, and are more general, than those underlying the "two-band model" for the (transverse) magnetoresistance, the expression (6.102) exhibits the quadratic dependence on the field strength characterizing the latter model in the low-field limit.

3. Drift-diffusion and ballistic regimes

Considering first the thermoballistic description of spin-polarized transport in DMS/NMS/DMS heterostructures in the drift-diffusion regime, we can compare our results to those of Ref. [100] obtained within the standard drift-diffusion approach.

In the drift-diffusion regime, when \( l_j \ll S_j \) and \( l_j \ll l_s^{(j)} \), we have

\[ L_j \rightarrow L_s^{(j)} = \sqrt{l_j l_s^{(j)}} \quad (6.103) \]

and

\[ \gamma_j \rightarrow \frac{l_j}{l_s^{(j)}} = \sqrt{\frac{l_j}{l_s^{(j)}}} \ll 1 \quad (6.104) \]

[see Eqs. (4.101), (6.59), (6.103), and (6.78)]. Hence, from Eqs. (6.90) and (6.91),

\[ g_j = h_j \cosh(S_j/L_s^{(j)}) \quad (6.105) \]

and

\[ h_j = \frac{2l_j}{L_s^{(j)} \sinh(S_j/L_s^{(j)})} \quad (6.106) \]

respectively. Then, specializing to the symmetric heterostructure, we find for the quantity \( Q_{DN} \) defined by Eq. (6.94),

\[ Q_{DN} = 2 \left[ Q \frac{l_D}{L_s^{(j)}} \coth(S_D/L_s^{(D)}) + \frac{l_N}{L_s^{(N)}} \coth(S_N/2L_s^{(N)}) e^{-\beta_D x_s^{(j)}} \right] \quad (6.107) \]
Introducing the (spin-summed) conductivity \( \sigma_+^{(j)} \) for layer \( j \) \((j = D, N)\),

\[
\sigma_+^{(j)} = 2\beta e^2 v_e n_+^{(j)} l_j
\]  

(6.108)

[see Eq. (2.27)], with

\[
n_+^{(j)} = \frac{n_+^{(0,j)}}{Q_j}
\]  

(6.109)

\((Q_D = Q, Q_N = 1)\), we can rewrite expression (6.110) in the form

\[
Q_{DN} = \frac{2}{Q} \frac{l_D}{L_s^{(D)}} \left[ Q^2 \coth(S_D/L_s^{(D)}) + \frac{\sigma_+^{(N)}}{L_s^{(N)}} \coth(S_N/2L_s^{(N)}) \right].
\]  

(6.110)

Now, inserting expression (6.110) in Eq. (6.93) and using the resulting expression for \( \tilde{A}_2 \) in Eq. (6.77), we find that the values of the zero-bias current spin polarization \( P_j(x) \) at the positions \( x_{1,4}, x_{2,3}, \) and \( (x_2 + x_3)/2 \), respectively, agree with those given by Eqs. (17), (16), and (18) of Ref. 100 if we identify in the latter equations the spin-flip lengths \( \lambda_D \) and \( \lambda_N \) with \( L_s^{(D)} \) and \( L_s^{(N)} \), respectively, and the layer thicknesses \( d \) and \( 2x_0 \) with \( S_D \) and \( S_N \), respectively.

For the magnetoresistance in the drift-diffusion regime, we obtain from Eq. (6.110), setting \( S_j = S_j/2l_j \) and inserting expression (6.110) for \( Q_{DN} \),

\[
R_m = \frac{S_D[1/\sigma_+^{(D)} - 1/\sigma_+^{(0,D)}] + P^2/Q_{DN}}{S_D/\sigma_+^{(0,D)} + S_N/2\sigma_+^{(0,N)}},
\]  

(6.111)

where \( \sigma_+^{(0,j)} \) is the conductivity for zero spin splitting, which is given by Eq. (6.108) with \( n_+^{(j)} = n_+^{(0,j)} \), and

\[
Q_{DN} = Q^2 \frac{\sigma_+^{(D)}}{L_s^{(D)}} \coth(S_D/L_s^{(D)}) + \frac{\sigma_+^{(0,N)}}{L_s^{(N)}} \coth(S_N/2L_s^{(N)}).
\]  

(6.112)

Then, identifying the parameters as above, we find that \( R_m \) agrees with expression (13) of Ref. 100.

Turning now to the ballistic regime, when \( l_j \gg S_j \) and \( l_s \gg l_s^{(j)} \), we have

\[
L_j \rightarrow l_s^{(j)}
\]  

(6.113)

and

\[
\gamma_j \rightarrow 1
\]  

(6.114)

[see Eqs. (6.101), (5.99), (5.103), and (6.78)], so that

\[
g_j = 1
\]  

(6.115)

and

\[
h_j = e^{-S_j/l_s^{(j)}}.
\]  

(6.116)

For the symmetric heterostructure, we then find from Eq. (6.54)

\[
Q_{DN} = Q + [1 + e^{-S_N/l_s^{(N)}}]e^{\delta S_{DN}}.
\]  

(6.117)

With this used in Eq. (6.93) for \( \tilde{A}_2 \) as well as in Eq. (6.95) for \( G_j^{(1)} \tilde{A}_1 \), we obtain the position dependence of the zero-bias current spin polarization from Eqs. (6.76) and (6.77).

For the magnetoresistance in the ballistic regime, we have from Eqs. (6.111), setting \( S_j = 1 \) and inserting expression (6.117) for \( Q_{DN} \),

\[
R_m = \frac{Q - 1 + P^2/Q + [1 + e^{-S_N/l_s^{(N)}}]e^{\delta S_{DN}}}{1 + e^{-\delta S_{DN}}/2}.
\]  

(6.118)

Depending on the values assigned to the different parameters in this expression, the ballistic (relative) magnetoresistance is positive or negative.

VII. SUMMARY AND OUTLOOK

In this article, we have presented a comprehensive survey of the thermoballistic approach to charge carrier transport in semiconductors. The principal aim has been to develop the basic physical concept underlying this approach in detail, and to give a coherent exposition of the ensuing formalism, which unifies, and partly modifies, generalizes, and corrects, the formal developments presented in our previous publications.

To make the presentation self-contained and easy to follow, we have proceeded step by step, starting with an account of Drude’s model as the origin of all semiclassical transport models. We then reviewed the standard drift-diffusion and ballistic transport models, basic features of which have been adopted to shape the thermoballistic description of carrier transport in terms of averages over random configurations of ballistic transport intervals. The contributions of the individual ballistic intervals to the total carrier current are governed by collision probabilities involving the carrier mean free path, or momentum relaxation length, as the determining parameter of the thermoballistic concept.

This concept finds a first concrete expression in the prototype thermoballistic model, which is based on the simplifying assumption of current conservation across the points of local thermodynamic equilibrium linking ballistic intervals. The implementation of the prototype model results in a current-voltage characteristic containing a reduced resistance, which can be expressed explicitly in terms of the parameters of the semiconducting system.

In the full thermoballistic concept, current conservation across the equilibrium points is abandoned, and
position-dependent, total and spin-polarized thermoballistic currents and densities are introduced in terms of an average chemical-potential function and a spin accumulation function related to the spin splitting of the chemical potential. The algorithms for determining these dynamical functions follow from two physical conditions. First, the average of the total thermoballistic current over the length of the semiconducting sample (as well as over the range between either end and an arbitrary point of local thermodynamic equilibrium) is required to equal the conserved physical current, whereby one is able to set up a scheme for obtaining the average chemical potential. The explicit calculation of this function is implemented in terms of resistance functions, for which Volterra-type integral equations are derived. Second, spin relaxation is assumed to act only inside the ballistic transport intervals. As a result, the thermoballistic spin-polarized current and density are connected by a spin balance equation, from which one obtains an inhomogeneous Fredholm-type integral equation for the spin accumulation function. In the general case of arbitrarily shaped potential energy profiles, considerable numerical effort is needed for solving the integral equations for the resistance functions and the spin accumulation function. In a number of important special cases, however, these equations reduce to a form which greatly facilitates their solution. Examples are the equations for the resistance functions when the spin splitting of the band edge profile is independent of position, or the equation for the spin accumulation function for a homogeneous sample in an external electric field. In the latter case, the integral equation can be converted into an easily tractable second-order differential equation. For homogeneous semiconductors at zero bias, the solutions of the equations for the dynamical functions can be obtained in closed form throughout.

For the purpose of demonstrating the potentialities of the thermoballistic approach in present-day semiconductor and spintronics research, we have summarized in this article the treatment of a number of specific examples. The prototype model is employed to describe electron transport across potential energy profiles exhibiting an arbitrary number of barriers, where effects of tunneling and degeneracy are included. This approach proves to be of particular relevance to the description of grain boundary effects in electron transport in polycrystalline semiconductors and has already been applied with promising results in the analysis of experimental data. The full thermoballistic approach is used in the treatment of spin-polarized transport in heterostructures. For the prototype problem of semiconductor spintronics, viz., the injection of spin polarization from ferromagnetic contacts into a semiconducting sample, the thermoballistic description extends the standard drift-diffusion description so as to allow for arbitrary values of the momentum relaxation length. The same holds for transport in heterostructures composed of layers of diluted magnetic and nonmagnetic semiconductors at zero bias, where the position dependence of the current spin polarization as well as the magnetoresistance are obtained in closed form.

In our previous publications, we have presented results of explicit calculations for a variety of specific cases. These calculations were mostly of exploratory character, with the aim to reveal qualitative trends in the parameter dependence of the relevant transport properties. In future work, emphasis should be placed on the application of the thermoballistic approach in quantitative studies, as demanded for the analysis of specific experimental results. For these studies to become successful, the careful evaluation of the potential energy profiles is prerequisite, and advanced numerical techniques for solving the integral equations for the dynamical functions are to be employed. With these goals achieved, the thermoballistic approach will certainly prove useful as a practical tool, beyond its basic theoretical relevance as the bridge between the drift-diffusion and ballistic descriptions of charge carrier transport in semiconductors.

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Throughout this article, we use the term “chemical potential” as defined in Ref. [16] in which this term is used in quite a different context.

After having introduced the term "thermoballistic" into the theory of carrier transport in semiconductors, we became aware of Ref. [14], in which this term is used in quite a different context.

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