Journal of Statistical Physics, Vol. 59, Nos. 5/6, 1990

A Stochastic Approach to Hopping Transport in Semiconductors

Eckhard Platen[1]

Received April 19, 1989

Generalized charge carrier equations for hopping transport in semiconductors are derived which include also the widely used Van Roosbroeck equations. The approach is based on a microscopic stochastic interacting particle system which models the hopping of electrons on a random set of states.

KEY WORDS: Stochastic charge carrier transport; hopping transport; exclusion process in random media; nonequilibrium dynamics; nonlinear diffusion equation.

1. INTRODUCTION

The use of semiconducting materials such as silicon, amorphous silicon, or selenium plays an increasing role in microelectronics and other fields. A theoretical understanding of the charge transport dynamics in such materials provides a basis for any effective way to design electronic device materials and structures.

Van Roosbroeck[13] developed phenomenological charge transport equations for a homogeneous nondegenerate semiconductor. These equations are widely used to model semiconductor devices.[1]

For high-resistivity semiconductors[2] and degenerate semiconducting materials the Van Roosbroeck transport equations fail in many situations. In particular, for the case of hopping transport there is no general theoretical approach.[9,12]

Starting from a microscopic stochastic hopping model with particle interaction, we derive in this paper charge transport equations which work in several previously unsatisfactorily modeled situations. Theses equations

[1] Karl-Weierstrass-Institut für Mathematik der AdW der DDR, DDR-1086 Berlin, East Germany.

0022-4715/90/0600-1329$06.00/0

include also Van Roosbroeck's equations as a special case which followed originally from a band model. Therefore, the present paper may be considered also as an attempt to unify hopping and band transport phenomenona.

The general plan of the paper is the following: First we describe the semiconductor equations. Then we introduce a microscopic interacting particle system which models the motion of electrons. From a law of large numbers we get a macroscopic equation for the evolution of the density of the electrons. Finally, we derive the equations for the charge transport in semiconductors.

For $i, k \in \{0, 1, \ldots\}$ we denote by $\mathbf{C}^i(G)$ the set of all i-times continuously differentiable functions on a domain $G \subseteq \mathbf{R}^d$. The set $\mathbf{C}^{i,j}([0, t_0], G)$ is the set of all functions on $[0, t_0] \times G$, $t_0 \in (0, \infty)$, which are i-times continuously differentiable with respect to the first coordinate and j-times continuously differentiable with respect to the other coordinates. $\bar{G}$ is the closure of G. We let $W \subset \mathbf{R}^3$ be a bounded 3-dimensional open connected domain with smooth boundary, which will represent the spatial extension of the semiconductor.

2. THE EQUATIONS FOR THE FLOW OF ELECTRONS AND HOLES

In a semiconductor there are charge carriers of two types: electrons in the conduction band

$$\bar{E}_c = [\underline{e}_c, \bar{e}_c]$$

and positive holes in the filled valence band

$$\bar{E}_v = [\underline{e}_v, \bar{e}_v]$$

These two bands are separated by a gap $(\bar{e}_v, \underline{e}_c)$ of length

$$\Delta E = \underline{e}_c - \bar{e}_v$$

The equations for the flow in three dimensions of electrons and holes in a semiconductor contain, as principal dependent variables, the hole and electron concentrations p and n, the flow densities J_p and J_n, and the electrostatic potential V. For simplicity in this paper we consider V as a given function from $\mathbf{C}^{1,2}([0, \infty), \bar{W})$. It will usually be characterized by the Poisson equation, such as in Van Roosbroeck's equations.

The charge carrier transport equations have the form

$$\frac{\partial p}{\partial t} = -r - \operatorname{div} J_p \tag{2.1}$$

$$\frac{\partial n}{\partial t} = -r - \operatorname{div} J_n \tag{2.2}$$

in $\mathbf{R}_+ \times W$. Here

$$J_p = -\sigma_p \operatorname{grad}(eV + \mu_v) \tag{2.3}$$

and

$$J_n = \sigma_n \operatorname{grad}(eV + \mu_c) \tag{2.4}$$

are the hole and electron flow densities, which depend on the conductivities σ_p and σ_n and the chemical potentials μ_v and μ_c in the valence and conduction bands. Here r denotes the net recombination rate and will be specified in (2.12). In this paper we restrict ourselves to the case of a drain- and source-free region without contacts, and thus obtain the boundary condition

$$\nu \cdot J_p = \nu \cdot J_n = 0 \tag{2.5}$$

on $\mathbf{R}_+ \times \partial W$, where ν denotes the outward unit normal to the boundary ∂W. We remark that the proposed approach yields corresponding assertions for situations with drains, sources, and contacts.

Since we are describing a nonequilibrium dynamics, we also need initial electron and hole concentrations n_0 and p_0.

So far the above equations look similar to the Van Roosbroeck equations, but our equations differ from them essentially in the structure of the conductivities σ_p and σ_n and in the net recombination rate r and the chemical potentials μ_v and μ_c. All these variables are related to the occupation rates in the valence and conduction bands, R_v and R_c. In particular, we have the occupation rates of the states

$$R_v = \left\{1 + \exp\left[-\frac{1}{kT}(\mu_v - E)\right]\right\}^{-1} \tag{2.6}$$

for $E \in \bar{E}_v$ in the valence band and

$$R_c = \left\{1 + \exp\left[-\frac{1}{kT}(\mu_c - E)\right]\right\}^{-1} \tag{2.7}$$

for $E \in \bar{E}_c$ in the conduction band on $\mathbf{R}_+ \times \bar{W}$. Here k is the Boltzmann constant and T the absolute temperature. Obviously, in both bands we have Fermi–Dirac statistics characterized by the corresponding chemical potentials. We remark that Van Roosbroeck's equations are based on the Boltzmann approximation.

Using the occupation rates R_v and R_c and the density of states λ, we can write the concentration of holes as

$$p = \int_{\bar{E}_v} (1 - R_v)\, \lambda \, dE \tag{2.8}$$

and the concentration of electrons as

$$n = \int_{\bar{E}_c} R_c \lambda \, dE \tag{2.9}$$

An important result from our approach is the nonlinear logistic structure of the conductivities σ_p and σ_n. These have the following form:

$$\sigma_p = \psi \int_{\bar{E}_v} \frac{1}{kT} R_v (1 - R_v)\, \lambda^2 \, dE \tag{2.10}$$

and

$$\sigma_n = \psi \int_{\bar{E}_c} \frac{1}{kT} R_c (1 - R_c)\, \lambda^2 \, dE \tag{2.11}$$

where ψ is a material parameter which will be specified in (4.30). We remark that the conductivities are bounded and vanish for zero or full occupation, $R = 0$ or $R = 1$. The above conductivities also give a good natural model for the degenerate case when the chemical potentials are located within the bands. For nearly constant density of states in the non-degenerate case the following form follows from (2.10) and (2.8) for the conductivity σ_p:

$$\sigma_p \approx \frac{\psi}{kT} \lambda \int_{\bar{E}_v} (1 - R_v)\, \lambda \, dE = \frac{\psi}{kT} \lambda p$$

which is the Van Roosbroeck conductivity of the valence band. An analogous result holds for the conductivity of the conduction band.

Here we specify the net recombination rate r in the form

$$\begin{aligned} r &= C_r \left\{ R_c(\underline{e}_c)[1 - R_v(\bar{e}_v)] \exp\left(\frac{\Delta E}{2kT}\right) \right. \\ &\quad \left. - R_v(\bar{e}_v)[1 - R_c(\underline{e}_c)] \exp\left(-\frac{\Delta E}{2kT}\right) \right\} \\ &= C_r \left\{ 1 + \exp\left[\frac{1}{kT}(\mu_v - \bar{e}_v)\right] \right\}^{-1} \left\{ 1 + \exp\left[\frac{1}{kT}(\mu_c - \underline{e}_c)\right] \right\}^{-1} \\ &\quad \times \left\{ \exp\left[\frac{1}{kT}\left(\mu_c - \frac{1}{2}\Delta E\right)\right] - \exp\left[\frac{1}{kT}\left(\mu_v - \frac{1}{2}\Delta E\right)\right] \right\} \end{aligned} \tag{2.12}$$

We note that for equal chemical potentials $\mu_v = \mu_c$ a vanishing net recombination rate $r = 0$ follows. The above nonlinear structure of r then drives the whole system from any initial electron and hole concentration into an equilibrium with equal chemical potentials $\mu_v = \mu_c$.

Finally, we remark that the proposed approach can also be applied to other electronic materials and yields quite interesting natural charge transport equations.

3. THE MICROSCOPIC STOCHASTIC MODEL

We suppose that microscopic objects exist (e.g., localized states, atoms) which we call states. At these states the electrons may stay and they are allowed to jump from state to state. We suppose that the duration of a jump itself is small in comparison with the mean waiting time until the next jump of the electron.

Our microscopic stochastic model is based on an interacting particle system which is called an exclusion process in ref. 5. These particles represent electrons which are jumping according to a Markov kernel on a given set of states. However, any jump which would take an electron to an already occupied state is excluded.

Many properties of the semiconducting material are modeled by a random counting measure N_n representing the states. The external and internal influences on the microscopic stochastic motion of electrons are modeled via the jump intensities of the Markov kernel.

To introduce the microscopic stochastic model, we use the results in ref. 10 and refer for notation and definitions to refs. 3 and 4.

To be mathematically precise, let $(\Omega, \mathbf{F}, P)$ denote the basic probability space, which is complete, and let $\mathbf{F} = (\mathbf{F}_t)$, $t \geqslant 0$, be an increasing right-continuous family of complete sub-σ-fields of $\mathbf{F}$. Let E represent the expectation with respect to the probability measure P and $\mathbf{B}(G)$ the Borel σ-field of a topological space G.

For $K \in (0, \infty)$ we denote by LC_K the set of bounded Lipschitz-continuous functions

$$f \mid \mathbf{R}^4 \to [-K, K]$$

with

$$|f(u) - f(q)| \leqslant K |q - u| \tag{3.1}$$

for all $u, q \in \mathbf{R}^4$, using the usual Euclidean norm.

3.1. The Set of States

Recall from Section 1 that $W \subset \mathbf{R}^3$ denotes an open connected bounded domain with smooth boundary, which represents the spatial extension of the semiconductor.

Let us denote the open energy intervals of the valence and conduction bands by

$$E_v = (\underline{e}_v, \bar{e}_v) \qquad \text{and} \qquad E_c = (\underline{e}_c, \bar{e}_c)$$

Now, we introduce the set

$$Q = W \times (E_v \cup E_c) \subset \mathbf{R}^4 \tag{3.2}$$

and interpret its closure $\bar{Q}$ as the state domain, where a state $q = (q_1, q_2, q_3, q_4) \in \bar{Q}$ is characterized by the three spatial coordinates

$$\tilde{q} = (q_1, q_2, q_3) \in \bar{W}$$

and its energy coordinate

$$q_4 \in \bar{E}_v \cup \bar{E}_c$$

We model the motion of electrons as jumps from states to other states. The set of states may have an ordered or disordered structure.

We introduce a family $(N_n)_{n>1}$ of $\mathbf{F}_0$-measurable counting measures on $\mathbf{B}(\bar{Q})$ which we call counting measures of states. For fixed $n > 1$ we assume that two states do not have the same location in $\bar{Q}$. This means N_n must be a simple point process. Obviously, for each set $A \in \mathbf{B}(\bar{Q})$ the random variable $N_n(A)$ counts the number of states in A. Because N_n is assumed to be $\mathbf{F}_0$-measurable, the realization of N_n remains fixed from the beginning.

We interpret the parameter n, for which

$$n = EN_n(\bar{Q}) \left(\int_{\bar{Q}} dq \right)^{-1} \tag{3.3}$$

as the mean number of states per unit volume in $\mathbf{R}^4$. Since n is extremely large for semiconductors, we will later investigate the limiting behavior for $n \to \infty$.

Let the given density of states λ be a twice continuously differentiable function on $\bar{Q}$ which is strictly positive in $\bar{W} \times (E_v \cup E_c)$. We assume at the band edges $\bar{e}_v$ and $\underline{e}_c$ that λ together with its first derivative in the energy direction vanishes, but the second derivative in the energy direction is

strictly positive. We remark that by a slight modification of our approach one can also handle other shapes of the band edges.

Now, for each $K \in (0, \infty)$ we suppose that the following condition holds for the random medium N_n:

$$\lim_{n \to \infty} E \sup_{f \in LC_K} \left[\int_{\bar{Q}} f(q) \frac{1}{n} N_n(dq) - \int_{\bar{Q}} f(q)\, \lambda(q)\, dq \right]^2 = 0 \tag{3.4}$$

That is, the difference of the two functionals converges as $n \to \infty$ in the mean square sense to zero uniformly in the test functions in LC_k. Furthermore, we assume that the fourth moment of the normalized number of states in $\bar{Q}$ is bounded by a constant $K_1 < \infty$:

$$\sup_{n>1} E\left(\frac{1}{n} N_n(\bar{Q})\right)^4 = K_1 \tag{3.5}$$

There exists a wide class of stochastic point processes N_n which satisfy the above conditions. For instance, this is shown in ref. 10 for the Poisson point process and holds also for many deterministic grids. It seems that most important semiconducting materials of practical interest can be modeled by the above counting measures N_n.

3.2. The Markovian Jump Mechanism

To model the Markovian jump mechanism, we introduce for each $n > 1$ an **F**-adapted cadlag (right continuous with left-hand limits) Poisson jump measure μ_n on $\mathbf{B}([0, \infty)) \otimes \mathbf{B}(\bar{Q}) \otimes \mathbf{B}(\bar{Q})$ which generates the possible jumps of the electrons on the set of states. We emphasize that these possible jumps do not depend on the actual configuration of the electrons. Later, within the dynamics of our model only those jumps from occupied into vacant states will be allowed, with the others excluded.

We can thus say that the process

$$\{\mu_n([0, t], A, B)\}_{t \geq 0}$$

is the Poisson process which counts the possible jumps from A into B for any pair of subsets $A, B \in \mathbf{B}(\bar{Q})$.

The Poisson jump measure μ_n is characterized by its intensity measure, which is also defined on $\mathbf{B}([0, \infty)) \otimes \mathbf{B}(\bar{Q}) \otimes \mathbf{B}(\bar{Q})$ and has the form

$$\nu_n(dt, du, dq) = n^{-1} w_t(u, q)\, N_n(du)\, N_n(dq)\, dt \tag{3.6}$$

where the jump rate $w_t(u, q)$ will be specified below in (3.7).

If the jump rate w_t does not depend on the time t, then in our model an electron at a state at u waits an exponential time with parameter

$$\rho(u) = \int_{\bar{Q}\setminus\{u\}} w_t(u, q) \frac{1}{n} N_n(dq)$$

At the end of this time it chooses a state q with probability

$$n^{-1} w_t(u, q)/\rho(u)$$

if q is vacant, then it jumps to q, whereas if q is occupied, then it stays at u. Therefore, we will have at most one particle at each site at any given time instant. We incorperate the assumptions about the microscopic behavior of the electrons within the given semiconducting material into the specification of the jump rate w_t. Similarly to the hopping probabilities suggested by Miller and Abrahams[6] and Mott,[1,8] we propose for $t \geqslant 0$ and $u, q \in \bar{Q}$ the following jump rate:

$$w_t(u, q) = \gamma \exp\left\{ -\frac{2}{\alpha} |\tilde{q} - \tilde{u}| - \frac{e}{2kT} [V(t, \tilde{q}) - V(t, \tilde{u})] \right.$$
$$\left. - \frac{2}{\beta} |q_4 - u_4| - \frac{1}{2kT} (q_4 - u_4) \right\} \tag{3.7}$$

with the notation $u = (u_1, u_2, u_3, u_4)$, $\tilde{u} = (u_1, u_2, u_3)$ also for q and $\tilde{q}$.

Here β is the energetic scattering width, which in our case is assumed to be much smaller than the gap width ΔE.

Therefore, we set

$$\beta = y \Delta E \tag{3.8}$$

where $y \ll 1$ is a small parameter. Later we let y tend to zero.

Analogously, α denotes the spatial scattering width. To obtain in the later asymptotics for $y \to 0$ a limiting charge transport dynamics simultaneously between and within the bands, we have to set

$$\alpha = S y^{5/2} \exp(-y^{-1}) \tag{3.9}$$

where S is a macroscopic reference length which we call the relative spatial scattering width. To scale the dynamics in a proper way, we also have to choose the preexponential factor γ in (3.7) in the form

$$\gamma = \tilde{\gamma} y^{-27/3} \exp(5y^{-1}) \tag{3.10}$$

where $\tilde{\gamma}$ plays the role of a time scaling parameter and is a material constant like ΔE and S.

Let us remark that one can approximately write

$$V(t, \tilde{q}) - V(t, \tilde{u}) \approx \text{grad } V(t, \tilde{u}) \cdot (\tilde{q} - \tilde{u})$$

for sufficiently small $\tilde{q} - \tilde{u}$.

We have to assume that in reality the parameter y is small enough ($y < \bar{y} \ll 1$) for the given material so that the jump rate w_t decreases in all directions. This means that the relations

$$\frac{2}{\beta} > \frac{1}{2kT} \tag{3.11}$$

and

$$\frac{2}{\alpha} > \frac{e}{2kT} \sup_{t \geq 0, \tilde{q} \in \bar{W}} |\text{grad } V(t, \tilde{q})| \tag{3.12}$$

should be satisfied.

We note from (3.7) that jumps into lower energy levels have a higher jump rate than those into higher ones. Further, we have the highest spatial jump rate in the opposite direction of the gradient of the electrostatic potential V, which is that of the electrical field.

The assumptions (3.11) and (3.12) exclude the cases of extremely low temperatures T or very strong electrical fields, which we do not consider here.

The jump rate (3.7) applies to an isotropic material, but the approach can be generalized also to the anisotropic case.

3.3. The Initial Condition

We denote by $L_{n,t}$ the counting measure of electrons at time $t \geq 0$ and assume that $L_{n,0}$ is $\mathbf{F}_0$-measurable.

The function $\varphi \mid \bar{Q} \to [0, 1]$ will be called the initial occupation rate of the states. We assume at time $t = 0$ that at most one electron occupies each state and for all $K \in (0, \infty)$ the following condition holds:

$$\lim_{n \to \infty} E \sup_{f \in LC_K} \left[\int_{\bar{Q}} f(q) \frac{1}{n} L_{n,0}(dq) - \int_{\bar{Q}} f(q)\, \varphi(q)\, \lambda(q)\, dq \right]^2 = 0 \tag{3.13}$$

The above condition supposes that the normalized initial counting measure of electrons $(1/n)\, L_{n,0}(dq)$ converges in the above mean square sense to the measure $\varphi(q)\, \lambda(q)\, dq$. Obviously, a wide class of initial electron configurations satisfy this condition. For instance, it holds if the states are independently occupied with probability φ at the beginning.

For a simpler presentation of the results we assume that $\varphi \in \mathbf{C}^3(\bar{Q})$, that there is no electron or hole current through the boundary ∂W at the beginning, and that φ follows Fermi–Dirac statistics [see (2.8), (2.9)] in both bands.

3.4. The Stochastic Equation

Let δ_u denote the Dirac measure at $u \in \bar{Q}$ and $L_{n,t-}$ the left-hand limit of the electron counting measure $L_{n,t}$ at time $t > 0$.

Now, for $n > 1$ we define the measure-valued process

$$L_n = \{L_{n,t}\}_{t \geq 0}$$

as the unique solution of the following stochastic equation:

$$L_{n,t} = L_{n,0} + \int_0^t \int_{\bar{Q}} \int_{\bar{Q}} (\delta_f - \delta_u)\, L_{n,s-}(\{u\}) \times [1 - L_{n,s-}(\{q\})]\, \mu_n(ds, du, dq) \tag{3.14}$$

$t \geq 0$, which describes the evolution of the electron counting measure $L_{n,t}$ driven by the Poisson jump measure μ_n.

It can be seen that the Dirac measure changes its position from u to q at time t if such a possible jump is generated at t by μ_n where just before t the state at u is occupied and that at q is vacant. Thus, we have only jumps from occupied into vacant states. The exclusion of jumps into occupied states creates the interaction of our microscopic stochastic particle system.

3.5. The Occupation Rate

Now, we introduce the occupation rate $H(t, q)$, which we may later interpret as the asymptotic probability ($n \to \infty$) that a state at $q \in \bar{Q}$ will be occupied at time $t \geq 0$.

We define H as the unique solution of the following integrodifferential equation:

$$\frac{\partial}{\partial t} H(t, q) = [1 - H(t, q)] \int_{\bar{Q}} w_t(u, q)\, H(t, u)\, \lambda(u)\, du - H(t, q) \int_{\bar{Q}} w_t(q, u)[1 - H(t, u)]\, \lambda(u)\, du \tag{3.15}$$

for all $t>0$ and $q\in\bar{Q}$ with initial condition

$$H(0, q)=\varphi(q) \tag{3.16}$$

for all $q\in\bar{Q}$.

It is shown in ref. 10 that we have

$$H(t, q)\in[0, 1] \tag{3.17}$$

for all $t\geqslant 0$ and $q\in\bar{Q}$.

Equation (3.15) describes the evolution of the occupation rate H. It shows how $H(t, q)$ changes in relation to the values of H in $\bar{Q}$ and the jump rate w_t at time t. In some sense it can be interpreted as a kind of Boltzmann equation.

3.6. The Law of Large Numbers

The mean number n of states per unit volume is extremely large for most semiconducting materials and structures. Therefore, we study a suitable limit of the normalized counting measure of electrons $n^{-1}L_{n,t}$ for the case $n\to\infty$. We will formulate in the following a law of large numbers which shows that the random measure $n^{-1}L_{n,t}(dq)$ converges in a suitable sense to the deterministic measure $H(t, q)\,\lambda(q)\,dq$.

In our case the jump rate w_t does not depend on n. Under the above assumptions the law of large numbers

$$\lim_{n\to\infty} E \sup_{f\in CL_K} E\Bigg(\sup_{0\leqslant t\leqslant t_0} \Bigg[\int_{\bar{Q}} f(q)\frac{1}{n} L_{n,t}(dq) - \int_{\bar{Q}} f(q)\,H(t, q)\,\lambda(q)\,dq \Bigg]^2 \Bigg| \mathsf{F}_0 \Bigg) = 0 \tag{3.18}$$

holds for fixed t_0 and $K\in(0, \infty)$.

The choice of the class of test functions LC_K and the inner conditional expectation is crucial for the proof of this result, which uses semimartingale methods. The proof is omitted here because it is almost the same as in ref. 10.

We remark that the conditional expectation in (3.18) relates to the driving Poisson jump measure μ_n and the remaining expectation corresponds to the F_0-measurable random medium N_n and the initial configuration of electrons $L_{n,0}$.

4. THE MACROSCOPIC NONEQUILIBRIUM DYNAMICS

Equation (3.15) describes the evolution of the occupation rate H driven by the jump rate w_t given in (3.7). The jump rate has a local charac-

ter, that is, for smaller and smaller values of the parameter y [see (3.8)] the jumps of electrons become smaller and smaller. Therefore it makes sense to look for a suitable limit of the occupation rate H for $y \to 0$ to obtain instead of the integrodifferential equation (3.15) partial differential equations which describe the asymptotic occupation rate. Now, it is our aim to derive the structure of these partial differential equations, which will turn out to be that of the continuity equations described in Section 2.

Because the jump rate w_t defined in (3.7) depends on the parameter $y \in (0, 1)$, we can write

$$H(t, q) = H_y(t, q) \tag{4.1}$$

for all $t \in [0, t_0]$ and $q \in \bar{Q}$.

In the following we derive the asymptotic occupation rate R as the limit of the occupation rate H_y for $y \to 0$. We choose strong smoothness and convergence assumptions to obtain the characterization of R in a straightforward way. These assumptions seem to hold under quite natural conditions, which we do not try to specify in this paper, but this represents an interesting problem.

We assume for all $y \in (0, 1)$ that

$$H_y \in \mathbf{C}^{1,3}([0, t], \bar{Q}) \tag{4.2}$$

where the third derivative should be uniformly bounded with respect to $y \in (0, \bar{y})$.

Further, we suppose that

$$R \in \mathbf{C}^{1,2}([0, t_0], \bar{Q}) \tag{4.3}$$

and that H_y together with its time derivative $(\partial H/\partial t)$ and the other first- and second-order derivatives

$$\frac{\partial}{\partial q_i} H_y, \frac{\partial^2}{\partial q_i \partial q_k} H_y, \qquad i, k \in \{1,..., 4\} \tag{4.4}$$

converges pointwise for all $t \in [0, t_0]$ and $q \in \bar{Q}$ to R.

4.1. Fermi–Dirac Statistics

For all $t \in [0, t_0]$ and $\tilde{q} \in \bar{W}$ we introduce the concentration of electrons ρ_v in the valence band by

$$\rho_v(t, \tilde{q}) = \int_{\bar{E}_v} R(t, q)\, \lambda(q)\, dq_4 \tag{4.5}$$

and the concentration of electrons ρ_c in the conduction band by

$$\rho_c(t, \tilde{q}) = \int_{\bar{E}_c} R(t, q)\, \lambda(q)\, dq_4 \tag{4.6}$$

According to (2.8) and (2.9), we obtain

$$p(t, \tilde{q}) = \int_{\bar{E}_v} \lambda(q)\, dq_4 - \rho_v(t, \tilde{q}) \tag{4.7}$$

for the hole concentration and

$$n(t, \tilde{q}) = \rho_c(t, \tilde{q}) \tag{4.8}$$

for the electron concentration.

For all $t \in [0, t_0]$ and $\tilde{q} \in \bar{W}$ we introduce the chemical potential $\mu_v(t, \tilde{q})$ of the valence band as the unique solution of the implicit equation

$$\int_{\bar{E}_v} \left(1 + \exp\left\{-\frac{1}{kT}[\mu_v(t, \tilde{q}) - q_4]\right\}\right)^{-1} \lambda(q)\, dq_4 = \rho_v(t, \tilde{q}) \tag{4.9}$$

and analogously the chemical potential $\mu_c(t, \tilde{q})$ of the conduction band as the unique solution of the equation

$$\int_{\bar{E}_c} \left(1 + \exp\left\{-\frac{1}{kT}[\mu_c(t, \tilde{q}) - q_4]\right\}\right)^{-1} \lambda(q)\, dq_4 = \rho_c(t, \tilde{q}) \tag{4.10}$$

Now, we can formulate the following assertion, which shows that the asymptotic occupation rate R follows in the energy direction within each band a Fermi–Dirac statistics [see (2.8) and (2.9)].

Proposition 4.1. Under the above assumptions, for each $t \geqslant 0$ it follows that

$$R(t, q) = R_v(t, q) = \left(1 + \exp\left\{-\frac{1}{kT}[\mu_v(t, \tilde{q}) - q_4]\right\}\right)^{-1} \tag{4.11}$$

for all $q = (q_1, q_2, q_3, q_4) \in \bar{W} \times \bar{E}_v$, and

$$R(t, q) = R_c(t, q) = \left(1 + \exp\left\{-\frac{1}{kT}[\mu_c(t, \tilde{q}) - q_4]\right\}\right)^{-1} \tag{4.12}$$

for all $q \in \bar{W} \times \bar{E}_c$.

Proof. 1. For shorter notation in the sequel, for $t \geqslant 0$, $q = (q_1, q_2, q_3, q_4) \in \mathbf{R}^4$, and $u = (u_1, u_2, u_3, u_4) \in \mathbf{R}^4$, we write

$$\tilde{q} = (q_1, q_2, q_3), \qquad \tilde{u} = (u_1, u_2, u_3) \tag{4.13}$$

$$d_{\tilde{u},\tilde{q}} = \exp\left\{ -\frac{e}{2kT} [V(t, \tilde{q}) - V(t, \tilde{u})] \right\} \tag{4.14}$$

$$g_{u,q} = \exp\left[-\frac{1}{2kT} (q_4 - u_4) \right] \tag{4.15}$$

$$e_1 = \exp\left(-\frac{2}{\alpha} |\tilde{q} - \tilde{u}| \right) \tag{4.16}$$

$$e_2 = \exp\left(-\frac{2}{\beta} |q_4 - u_4| \right) \tag{4.17}$$

$$H_q = H_y(t, q) \tag{4.18}$$

$$\hat{q} = (q_1, q_2, q_3, u_4) \tag{4.19}$$

and

$$\eta = \tilde{\gamma} S^5 \, \Delta E \tag{4.20}$$

2. Now, using the special form of the jump rate w_t given in (3.7) and the definitions of α and β in (3.8) and (3.9), we obtain from Eq. (3.15), in terms of the above notations, for all $y \in (0, \bar{y})$, $t > 0$, and $q \in \bar{Q}$ the relation

$$\begin{aligned}
\frac{\partial}{\partial t} H_y(t, q) &= \frac{\partial}{\partial t} H_q \\
&= \eta \alpha^{-5} \beta^{-1} \int_{\bar{Q}} [(1 - H_q) H_u d_{\tilde{u},\tilde{q}} g_{u,q} \\
&\quad - H_q (1 - H_u) d_{\tilde{q},\tilde{u}} g_{q,u}] e_1 e_2 \lambda(u) \, du \\
&= \eta \alpha^{-5} \beta^{-1} \int_{\bar{Q}} [(1 - H_q)[H_{\hat{q}} + (H_u - H_{\hat{q}})] d_{\tilde{u},\tilde{q}} g_{u,q} \\
&\quad - H_q [1 - H_{\hat{q}} - (H_u - H_{\hat{q}})] \\
&\quad \times [d_{\tilde{u},\tilde{q}} + (d_{\tilde{q},\tilde{u}} - d_{\tilde{u},\tilde{q}})] g_{q,u}] \lambda(u) e_1 e_2 \, du \\
&= \eta \alpha^{-5} \beta^{-1} \int_{\bar{Q}} \Big([1 - H_q) H_{\hat{q}} g_{u,q} - H_q (1 - H_{\hat{q}}) g_{q,u}] \\
&\quad + (H_u - H_{\hat{q}}) \{ [(1 - H_q) g_{u,q} + H_q g_{q,u}] d_{\tilde{u},\tilde{q}} \\
&\quad + H_q g_{q,u} (d_{\tilde{q},\tilde{u}} - d_{\tilde{u},\tilde{q}}) \} \\
&\quad - H_q (1 - H_{\hat{q}}) (d_{\tilde{q},\tilde{u}} - d_{\tilde{u},\tilde{q}}) g_{q,u} \Big) \lambda(u) e_1 e_2 \, du
\end{aligned}$$

$$
\begin{aligned}
&= \eta\alpha^{-5}\beta^{-1}\int_{\bar{Q}}\Big(\{(1-H_{\hat{q}})\,H_q(g_{u,q}-g_{q,u}) \\
&\quad + (H_{\tilde{q}}-H_q)[(1-H_q)\,g_{u,q}+H_q\,g_{q,u}]\}\,d_{\tilde{u},\tilde{q}} \\
&\quad + (H_u-H_{\tilde{q}})\{[(1-H_q)\,g_{u,q}+H_q\,g_{q,u}]\,d_{\tilde{u},\tilde{q}} \\
&\quad + H_q\,g_{q,u}(d_{\tilde{q},\tilde{u}}-d_{\tilde{u},\tilde{q}})\} \\
&\quad - H_q(1-H_{\hat{q}})(d_{\tilde{q},\tilde{u}}-d_{\tilde{u},\tilde{q}})\,g_{q,u}\Big)\,\{\lambda(q)+[\lambda(u)-\lambda(q)]\}\,e_1 e_2\,du
\end{aligned}
\tag{4.21}
$$

3. It can be shown for all $q\in Q$ and $l_r\in\{0, 1, 2,\dots\}$ with $r\in\{1, 2, 3, 4\}$ that

$$
\begin{aligned}
&\lim_{y\to 0}\int_{\bar{Q}}\prod_{i=1}^{4}(u_i-q_i)^{l_i}\,\alpha^{-3}e_1\beta e_2\,du \\
&\qquad = \begin{cases}\pi/2 & \text{for } l_1=l_2=l_3=0,\quad l_4=2\\ 0 & \text{for } l_1=l_2=l_3=0,\quad l_4\in\{1,3,4,\dots\}\\ 0 & \text{for } (l_1,l_2,l_3)\neq(0,0,0)\end{cases}
\end{aligned}
\tag{4.22}
$$

Further, because of (3.8) and (3.9) we have

$$
\lim_{y\to 0}\alpha^2\beta^{-2}=0 \tag{4.23}
$$

From truncated Taylor expansions with (4.23), (4.2)–(4.4), and (4.22) for all $t>0$ and $q\in Q$ it follows from (4.22) that

$$
\begin{aligned}
0 &= \lim_{y\to 0}\alpha^2\beta^{-2}\lambda(q)\frac{\partial}{\partial t}H_q \\
&= \lim_{y\to 0}\eta\alpha^{-3}\beta^{-3}\lambda(q)\int_{\bar{Q}}\Bigg(\Bigg\{(1-H_{\hat{q}})\,H_q\left[-\frac{1}{kT}(q_4-u_4)\right] \\
&\quad + \left[\frac{\partial}{\partial q_4}H_q(u_4-q_4)+\frac{1}{2}\frac{\partial^2}{\partial q_4^2}H_q(u_4-q_4)^2\right]\Bigg\} \\
&\quad \times\left[1-\frac{1}{2kT}(1-2H_q)(q_4-u_4)\right] \\
&\quad \times\left[1+\frac{e}{2kT}\sum_{i=1}^{3}\frac{\partial}{\partial q_i}V(t,\tilde{q})(u_i-q_i)\right]
\end{aligned}
$$

$$+\left[\sum_{i=1}^{3}\frac{\partial}{\partial q_i}H_{\hat{q}}(u_i-q_i)\right]\{[(1-H_q)\,g_{u,q}+H_q\,g_{q,u}]\,d_{\tilde{u},\tilde{q}}$$

$$+H_q\,g_{q,u}(d_{\tilde{q},\tilde{u}}-d_{\tilde{u},\tilde{q}})\}$$

$$-H_q(1-H_{\hat{q}})\left[-\frac{e}{kT}\sum_{i=1}^{3}\frac{\partial}{\partial q_i}V(t,\tilde{q})(q_i-u_i)\right]g_{q,u}\Bigg)$$

$$\times\left[\lambda(q)+\sum_{i=1}^{4}\frac{\partial}{\partial q_i}\lambda(q)(u_i-q_i)\right]e_1e_2\,du$$

$$=\eta\lambda(q)\frac{\pi}{2}\Bigg([1-R(t,q)]\,R(t,q)\frac{1}{kT}\frac{\partial}{\partial q_4}\lambda(q)$$

$$+\frac{\partial}{\partial q_4}R(t,q)\left\{\frac{\partial}{\partial q_4}\lambda(q)+\frac{1}{2kT}[1-2R(t,q)]\,\lambda(q)\right\}$$

$$+\frac{1}{2}\frac{\partial^2}{\partial q_4^2}R(t,q)\,\lambda(q)\Bigg)$$

$$=\eta\frac{\pi}{4}\frac{\partial}{\partial q_4}\left(\lambda^2(q)\left\{\frac{\partial}{\partial q_4}R(t,q)+\frac{1}{kT}R(t,q)[1-R(t,q)]\right\}\right) \tag{4.24}$$

4. In view of the smoothness properties of R in (4.3) there exists a function c_v on $(0,t_0]\times W$ such that for all $(t,q)\in(0,t_0]\times(\bar{W}\times[\underline{e}_v,\bar{e}_v])$ we have from (4.25) the assertion

$$c_v(t,\tilde{q})=\lambda^2(q)\left\{\frac{\partial}{\partial q_4}R(t,q)+\frac{1}{kT}R(t,q)[1-R(t,q)]\right\} \tag{4.25}$$

This equation can only be valid with $c_v(t,\tilde{q})=0$ because λ becomes smaller than any $\varepsilon>0$ within the neighborhood of the band edge $\bar{e}_v$ and the expression

$$\frac{\partial}{\partial q_4}R(t,q)+\frac{1}{kT}R(t,q)[1-R(t,q)]$$

is uniformly bounded.

Therefore, for each $t\in(0,t_0]$ and $q\in\bar{W}\times\bar{E}_v$, R should be a solution of the differential equation

$$0=\frac{\partial}{\partial q_4}R(t,q)+\frac{1}{kT}R(t,q)[1-R(t,q)] \tag{4.26}$$

For a given concentration of electrons in the valence band

$$\rho_v(t,\tilde{q})=\int_{\bar{E}_v}R(t,q)\,\lambda(q)\,dq_4$$

[see (4.5)] it follows that the differential equation (4.26) has the unique solution

$$R(t, q) = \left(1 + \exp\left\{-\frac{1}{kT}[\mu_v(t, \tilde{q}) - q_4]\right\}\right)^{-1} \tag{4.27}$$

where the chemical potential of the valence band $\mu_v(t, \tilde{q})$ is defined as the implicit solution of Eq. (4.9).

In the same way we can also prove the corresponding result for the conductivity band. ▮

4.2. The Continuity Equations

In the following we investigate within the valence band the evolution of the concentration of electrons. It turns out to be characterized by a similar continuity equation as we will obtain for the conduction band.

We will now derive the continuity equations which describe the evolution of the concentration of electrons in the valence and electron bands. We recall that we also have then automatically from (4.7) and (4.8) the evolution of the densities of holes and electrons.

We introduce for each $t > 0$ and $\tilde{q} \in \bar{W}$ quantities which we will later interpret as the electron current density vector in the valence band,

$$j_v(t, \tilde{q}) = -\sigma_p(t, \tilde{q}) \operatorname{grad}[\mu_v(t, \tilde{q}) + eV(t, \tilde{q})] \tag{4.28}$$

and the electron current density vector in the conduction band,

$$j_c(t, \tilde{q}) = -\sigma_n(t, \tilde{q}) \operatorname{grad}[\mu_c(t, \tilde{q}) + eV(t, \tilde{q})] \tag{4.29}$$

where the condiuctivities σ_p and σ_n are defined as in (2.10) and (2.11), respectively, and the material parameter ψ has the form

$$\psi = \tilde{\gamma} S^5 \Delta E \frac{\pi}{2} \tag{4.30}$$

Further, for the parameter $C_r = C_r(\tilde{q})$ in the net recombination rate $r(t, \tilde{q})$ in (2.12) let us choose for all $\tilde{q} \in \bar{W}$ the form

$$C_r(\tilde{q}) = \tilde{\gamma} \frac{\pi}{16} S^3 \Delta E^6 \frac{\partial^2}{\partial q_4^2} \lambda(q_c) \frac{\partial^2}{\partial q_4^2} \lambda(q_v) \tag{4.31}$$

where $q_c = (q_1, q_2, q_3, \underline{e}_c)$ and $q_v = (q_1, q_2, q_3, \bar{e}_v)$.

Proposition 4.2. Under the above assumptions, we have for each $t>0$ and $\tilde{q}\in W$ the equations

$$\frac{\partial}{\partial t}\rho_v(t,\tilde{q}) = -\operatorname{div} j_v(t,\tilde{q}) + r(t,\tilde{q}) \tag{4.32}$$

and

$$\frac{\partial}{\partial t}\rho_c(t,\tilde{q}) = -\operatorname{div} j_c(t,\tilde{q}) - r(t,\tilde{q}) \tag{4.33}$$

with reflecting boundary conditions for $\tilde{q}\in\partial W$:

$$j_v(t,\tilde{q})\cdot v_{\tilde{q}} = 0 \tag{4.34}$$

and

$$j_c(t,\tilde{q})\cdot v_{\tilde{q}} = 0 \tag{4.35}$$

and initial conditions for $\tilde{q}\in\bar{W}$

$$\rho_v(0,\tilde{q}) = \int_{\bar{E}_v} \varphi(q)\,\lambda(q)\,dq_4 \tag{4.36}$$

$$\rho_c(0,\tilde{q}) = \int_{\bar{E}_c} \varphi(q)\,\lambda(q)\,dq_4 \tag{4.37}$$

Recall that for $\tilde{q}\in\partial W$ the vector $v_{\tilde{q}}$ denotes the outward unit normal to the boundary ∂W at the point $\tilde{q}$, and φ is the initial occupation rate.

From the comparison of Eqs. (4.32) and (4.33) with the well-known structure of a continuity equation we interpret the quantities j_v and j_c as electron current density vectors in the corresponding bands.

Further, we have from (2.3), (2.4), (4.28), and (4.29) the relations

$$J_p = -j_v \tag{4.38}$$

$$J_n = j_c \tag{4.39}$$

on $(0, t_0]\times\bar{W}$, and can easily verify from the above proposition and (4.7) and (4.8), Eqs. (2.1)–(2.5) in Section 2 for the flow of electrons and holes.

Proof. 1. From (4.5), (4.4), and (3.15) we obtain for $t\in(0,t_0]$ and $\tilde{q}\in W$

$$\frac{\partial}{\partial t}\rho_v(t,\tilde{q}) = \lim_{y\to 0}\int_{\bar{E}_v}\frac{\partial}{\partial t}H_q\lambda(q)\,dq_4$$

$$= \lim_{y\to 0}\{G_y(t,q) + P_y(t,q)\} \tag{4.40}$$

with

$$G_y(t,\tilde{q}) = \eta\alpha^{-5}\beta^{-1}\int_{\bar{E}_v}\int_{\bar{W}\times\bar{E}_v}[(1-H_q)\,H_u d_{\tilde{u},\tilde{q}}\,g_{u,q} - H_q(1-H_u)\,d_{\tilde{q},\tilde{u}}\,g_{q,u}]\,e_1 e_2\lambda(u)\,\lambda(q)\,du\,dq_4 \tag{4.41}$$

and

$$P_y(t,\tilde{q}) = \eta\alpha^{-5}\beta^{-1}\int_{\bar{E}_v}\int_{\bar{W}\times\bar{E}_c}[(1-H_q)\,H_u d_{\tilde{u},\tilde{q}}\,g_{u,q} - H_q(1-H_u)\,d_{\tilde{q},\tilde{u}}\,g_{q,u}]\,e_1 e_2\lambda(u)\,\lambda(q)\,du\,dq_4 \tag{4.42}$$

2. It can be shown for all $q\in W\times E_v$ and $l_r\in\{0,1,\ldots\}$ with $r\in\{1,2,3,4\}$ that for $l_1+l_2+l_3\geqslant 1$

$$\lim_{y\to 0}\int_{\bar{W}\times\bar{E}_v}\prod_{i=1}^{4}(u_i-q_i)^{l_i}\,\alpha^{-5}e_1\beta^{-1}e_2\,du\,dq_4 = \begin{cases}\pi & \text{for } (l_1,l_2,l_3,l_4)\in\{(2,0,0,0),(0,2,0,0),(0,0,2,0)\}\\ 0 & \text{otherwise}\end{cases} \tag{4.43}$$

We note that we have for all $t>0$ and $\tilde{q}\in\bar{W}$

$$D(t,\tilde{q}) = \int_{\bar{E}_v}\int_{\bar{E}_v}[(1-H_q)\,H_{\hat{q}}\,g_{u,q} - H_q(1-H_{\hat{q}})\,g_{q,u}]\,\lambda(q)\,\lambda(q)\,e_2\,du_4\,dq_4 = 0 \tag{4.44}$$

Thus, using the method in (4.21) and applying (4.44) and (4.43), it follows from (4.41) for all $t>0$ and $\tilde{q}\in\bar{W}$ that

$$\begin{aligned}\lim_{y\to 0} G_y(t,\tilde{q}) &= \eta\lim_{y\to 0}\alpha^{-5}\beta^{-1}\Bigg[\int_{\bar{W}} D(t,\tilde{q})\,e_1 d_{\tilde{u},\tilde{q}}\,d\tilde{u}\\ &+\int_{\bar{W}}\int_{\bar{E}_v}\int_{\bar{E}_v}\{[(1-H_q)\,H_{\hat{q}}\,g_{u,q} - H_q(1-H_{\hat{q}})\,g_{q,u}]\,\lambda(q)[\lambda(u)-\lambda(\hat{q})]\\ &+((H_u-H_{\hat{q}})\{[(1-H_q)\,g_{u,q}+H_q\,g_{q,u}]\,d_{\tilde{u},\tilde{q}}+H_q g_{q,u}(d_{\tilde{q},\tilde{u}}-d_{\tilde{u},\tilde{q}})\}\\ &-H_q(1-H_{\hat{q}})(d_{\tilde{q},\tilde{u}}-d_{\tilde{u},\tilde{q}})\,g_{q,u})\,\lambda(q)\,\lambda(u)\,e_1 e_2\,du_4\,dq_4\,d\tilde{u}\end{aligned}$$

$$= \eta \lim_{y \to 0} \alpha^{-5} \beta^{-1} \int_{\bar{W}} \int_{\bar{E}_v} \int_{\bar{E}_v} \left(\sum_{i=1}^{3} \left[\frac{\partial}{\partial q_i} H_{\hat{q}}(u_i - q_i) + \frac{1}{2} \frac{\partial^2}{\partial q_i^2} H_{\hat{q}}(u_i - q_i)^2 \right] \right.$$
$$\times \left\{ \left[1 + \frac{e}{2kT} \sum_{i=1}^{3} \frac{\partial}{\partial q_i} V(t, \tilde{q})(u_i - q_i) \right] \right.$$
$$\left. - H_q \frac{e}{kT} \sum_{i=1}^{3} \frac{\partial}{\partial q_i} V(t, \tilde{q})(u_i - q_i) \right\}$$
$$+ H_q (1 - H_{\hat{q}}) \frac{e}{kT} \sum_{i=1}^{3} \left[\frac{\partial}{\partial q_i} V(t, \tilde{q})(u_i - q_i) \right.$$
$$\left. \left. + \frac{1}{2} \frac{\partial^2}{\partial q_i^2} V(t, \tilde{q})(u_i - q_i)^2 \right] \right) \lambda(q)$$
$$\times \left[\lambda(q) + \sum_{i=1}^{4} \frac{\partial}{\partial q_i} \lambda(q)(u_i - q_i) \right] e_1 e_2 \, du_4 \, dq_4 \, d\tilde{u} \tag{4.45}$$

Now, we obtain from (4.45) with (4.43) and (4.2)–(4.3)

$$\lim_{y \to 0} G_y(t, \tilde{q}) = \eta \pi \int_{\bar{E}_v} \sum_{i=1}^{3} \left(\frac{\partial}{\partial q_i} R(t, q) \left\{ \lambda(q) \frac{\partial}{\partial q_i} \lambda(q) \right. \right.$$
$$\left. + \frac{e}{2kT} \frac{\partial}{\partial q_i} V(t, \tilde{q})[1 - 2R(t, q)] \, \lambda(q)^2 \right\}$$
$$+ \frac{1}{2} \frac{\partial^2}{\partial q_i^2} R(t, q) \, \lambda(q)^2 + R(t, q)[1 - R(t, q)] \frac{e}{kT}$$
$$\left. \times \left[\frac{\partial}{\partial q_i} V(t, \tilde{q}) \frac{\partial}{\partial q_i} \lambda(q) \, \lambda(q) + \frac{1}{2} \frac{\partial^2}{\partial q_i^2} V(t, \tilde{q}) \, \lambda(q)^2 \right] \right) dq_4$$
$$= \frac{\pi}{2} \eta \int_{\bar{E}_v} \sum_{i=1}^{3} \frac{\partial}{\partial q_i} \left\{ \lambda(q)^2 \left(\frac{\partial}{\partial q_i} R(t, q) \right. \right.$$
$$\left. \left. + \frac{e}{kT} R(t, q)[1 - R(t, q)] \frac{\partial}{\partial q_i} V(t, \tilde{q}) \right\} dq_4 \tag{4.46}$$

We note from (4.11) for $i \in \{1, 2, 3\}$, $t \geqslant 0$, and $q \in \bar{W} \times \bar{E}_v$ that

$$\frac{\partial}{\partial q_i} R(t, q) = \frac{1}{kT} R(t, q)[1 - R(t, q)] \frac{\partial}{\partial q_i} \mu_v(t, \tilde{q})$$

Therefore, from (4.46), (2.10), and (4.28) for $t > 0$ and $\tilde{q} \in W$ we get

$$\lim_{y\to 0} G_y(t,\tilde{q}) = \eta \frac{\pi}{2kT} \sum_{i=1}^{3} \frac{\partial}{\partial q_i} \left\{ \int_{\bar{E}_v} \lambda(q)^2 R(t,q)[1-R(t,q)]\, dq_4 \right.$$
$$\left. \times \frac{\partial}{\partial q_i} [\mu_v(t,\tilde{q}) + eV(t,\tilde{q})] \right\}$$
$$= -\mathrm{div}(j_v(t,\tilde{q})) \tag{4.47}$$

3. For all $\tilde{q} \in W$, $l_i \in \{0, 1, \ldots\}$, $i \in \{1, \ldots, 5\}$, with $l_4 + l_5 \geqslant 4$, we have

$$\lim_{y\to 0} \int_{\bar{E}_v} \int_{\bar{E}_c} \int_{\bar{W}} \prod_{i=1}^{3} (u_i - q_i)^{l_i} \alpha^{-3} e_1 (u_4 - \underline{e}_c)^{l_4}$$
$$\times \beta^{-3} \exp\left(-\frac{2}{\beta} |u_4 - \underline{e}_c| \right)$$
$$\times (\bar{e}_v - q_4)^{l_5} \beta^{-3} \exp\left(-\frac{2}{\beta} |\bar{e}_v - q_4| \right) d\tilde{u}\, du_4\, dq_4$$
$$= \begin{cases} \dfrac{\pi}{4} & \text{for} \quad l_1 = l_2 = l_3 = 0 \quad \text{and} \quad l_4 = l_5 = 2 \\ 0 & \text{otherwise} \end{cases} \tag{4.48}$$

Further, from (4.20) and (3.8) and (3.9),

$$\eta \alpha^{-5} \beta^{-1} \exp\left(-\frac{2}{\beta} \Delta E \right) = \tilde{\gamma} y^{-25/2} y^{-1} \exp[(5-2)\, y^{-1}]$$
$$= \tilde{\gamma} y^{-15/2} \exp(3y^{-1})\, y^{-6}$$
$$= \tilde{\gamma} S^3 \Delta E^6 \alpha^{-3} \beta^{-6} \tag{4.49}$$

According to our assumptions in Section 3.1, λ and $(\partial/\partial q_4)\lambda$ vanish at the band edges and with $q_v = (q_1, q_2, q_3, \bar{e}_v)$ and $q_c = (q_1, q_2, q_3, \underline{e}_c)$ we have the expansions

$$\lambda(q) = \frac{1}{2} \frac{\partial^2}{\partial q_4^2} \lambda(q_v)(\bar{e}_v - q_v)^2 + \cdots \tag{4.50}$$

and

$$\lambda(u) = \frac{1}{2} \frac{\partial^2}{\partial q_4^2} \lambda(q_c)(u_4 - \underline{e}_c)^2 + \cdots \tag{4.51}$$

Therefore, for all $t \in (0, t_0]$ and $\tilde{q} \in W$, from (4.42) by similar arguments as used above with (4.48)–(4.51), (4.27), (4.15), and (2.12), we get

$$\begin{aligned}
\lim_{y \to 0} P_y(t, \tilde{q}) = \lim_{y \to 0} \tilde{\gamma} S^3 \Delta E^6 \int_{\bar{E}_v} \int_{\bar{E}_c} \int_{\bar{W}} & \\
& \times [(1 - H_q) H_u d_{\tilde{u}\tilde{q}} g_{u,q} - H_q (1 - H_u) d_{\tilde{q},\tilde{u}} g_{q,u}] \\
& \times \frac{1}{2} \frac{\partial^2}{\partial q_4^2} \lambda(q_c)(u_4 - \underline{e}_c)^2 \frac{1}{2} \frac{\partial^2}{\partial q_4^2} \lambda(q_v)(\bar{e}_v - q_v)^2 \\
& \times \alpha^{-3} e_1 \beta^{-3} \exp\left(- \frac{2}{\beta} |u_4 - \underline{e}_c| \right) \\
& \times \beta^{-3} \exp\left(- \frac{2}{\beta} |\bar{e}_v - q_4| \right) d\tilde{u}\, du_4\, dq_4 \\
= \quad \tilde{\gamma} S^3 \Delta E^6 \frac{\pi}{16} \frac{\partial^2}{\partial q_4^2} \lambda(q_c) \frac{\partial^2}{\partial_{q_4}^2} \lambda(q_v) & \\
& \times \{[1 - R(t, q_v)]\, R(t, q_c)\, g_{q_c, q_v} \\
& - R(t, q_v)[1 - R(t, q_c)]\, g_{q_v, q_c}\} \\
= \quad r(t, \tilde{q}) & \qquad (4.52)
\end{aligned}$$

Combining (4.47) and (4.52) then gives the continuity equation (4.32) and Eq. (4.33) follows in an analogous manner.

4. Since the initial conditions (4.36) and (4.37) are obvious, it remains to show the reflecting boundary conditions (4.34) and (4.35).

For simplicity, let us choose a point $\tilde{p} = (p_1, p_2, p_3) \in \partial W$, which is a maximal point of ∂W in the direction of the first spatial coordinate. From the smoothness of the boundary ∂W we can conclude that the outward unit normal $v_{\tilde{q}}$ of ∂W at $\tilde{p}$ is parallel to the direction of the first spatial coordinate.

It can be shown for $l_i \in \{0, 1, \ldots\}$, $i \in \{1, \ldots, 4\}$, with $l_1 + l_2 + l_3 \geqslant 1$ that

$$\begin{aligned}
& \lim_{y \to 0} \int_{\bar{E}_v} \int_{\bar{Q}} \left[\prod_{i=1}^{3} (u_i - p_i)^{l_i} \right] (u_4 - q_4)^{l_4} \alpha^{-4} \beta^{-1} e_1 e_2\, du\, dq_4 \\
& = \begin{cases} \frac{3}{4}\pi & \text{for} \quad l_1 = 1, \quad l_2 = l_3 = l_4 = 0 \\ 0 & \text{otherwise} \end{cases} \qquad (4.53)
\end{aligned}$$

Now it follows from (4.5) and (3.15) as in (4.40)–(4.52) for all $t \in (0, t_0]$

$$\begin{aligned} 0 &= \lim_{y \to 0} \alpha \frac{\partial}{\partial t} \rho_v(t, \tilde{p}) \\ &= \lim_{y \to 0} \alpha \int_{\bar{E}_v} \frac{\partial}{\partial t} H_q \lambda(q)\, dq_4 \\ &= \lim_{y \to 0} \alpha \{G_y(t, q) + P_y(t, q)\} \\ &= \lim_{y \to 0} \alpha G_y(t, q) + 0 \end{aligned} \tag{4.54}$$

With the notation $p = (p_1, p_2, p_3, q_4)$ and $\hat{p} = (p_1, p_2, p_3, u_4)$ we get from (4.54) with (4.53) [similar to (4.35)–(4.37)]

$$\begin{aligned} 0 &= \eta \lim_{y \to 0} \alpha^{-4} \beta^{-1} \int_{\bar{E}_v} \int_{\bar{W} \times \bar{E}_v} \left\{ \frac{\partial}{\partial q_1} H_p(u_1 - p_1) \right. \\ &\quad \left. + H_p(1 - H_{\hat{p}}) \frac{e}{kT} \frac{\partial}{\partial q_1} V(t, \tilde{p})(u_1 - p_1)\, \lambda(p)\, \lambda(\hat{p})\, e_1 e_2\, du\, dq_4 \right. \\ &= \eta \frac{3}{4} \pi \int_{\bar{E}_v} \left\{ \frac{\partial}{\partial q_1} R(t, p) + R(t, p)[1 - R(t, p)] \frac{e}{kT} \right. \\ &\quad \left. \times \frac{\partial}{\partial q_1} V(t, \tilde{p}) \right\} \lambda(p)^2\, dq_4 \\ &= \eta \frac{3}{4} \pi \int_{\bar{E}_v} R(t, p)[1 - R(t, p)] \frac{1}{kT} \frac{\partial}{\partial q_1} \\ &\quad \times [\mu_v(t, \tilde{p}) + eV(t, \tilde{p})]\, \lambda^2(p)\, dq_4 \\ &= \frac{3}{2} j_v(t, \tilde{p}) \cdot \nu_{\tilde{p}} \end{aligned} \tag{4.55}$$

From (4.16) it follows that e_1 is translation and rotation invariant in $\mathbf{R}^3$. Therefore, we can conclude for all $\tilde{q} \in \partial W$ and $t \in (0, t_0]$ that

$$j_v(t, \tilde{q}) \cdot \nu_{\tilde{q}} = 0 \tag{4.56}$$

Analogously, we can also show that

$$j_c(t, \tilde{q}) \cdot \nu_{\tilde{q}} = 0 \tag{4.57}$$

for all $t \in (0, t_0]$ and $\tilde{q} \in \partial W$.

Since the assertions (4.56) and (4.57) are already assumed to be valid for the starting point $t=0$ in our initial condition, Proposition 4.2 is now proved. ▮

We note from the above proofs that we have different time scales of the dynamics in the energy direction, at the boundary, and in the spatial direction.

We remark that our approach works also for other shapes of the density of states at the band edges. For instance, if we assume that λ is zero and $|(\partial/\partial q_4)\,\lambda|$ is strictly positive at the band edges, then we obtain, with

$$\alpha = Sy^{3/2} \exp(-y^{-1})$$
$$\gamma = \tilde{\gamma} y^{-17/2} \exp(5y^{-1})$$

and

$$C_r(\tilde{q}) = \tilde{\gamma} 4\pi S^3\, \Delta E^4 \frac{\partial}{\partial q_4} \lambda(q_c) \frac{\partial}{\partial q_4} \lambda(q_v)$$

analogous formulas to those above.

Further, we can also allow small gaps within the bands as long as they are smaller than ΔE.

Under such assumptions, similar results to those above can be established. This means the donator and acceptor energy levels can be modeled within the corresponding bands as long as the gap with size ΔE remains the maximum gap.

There is no major difficulty in applying our approach to a dynamics with drain and source or to modeling the behaviour at contacts, even for semiconductors with strong electrical fields or very low temperatures.

ACKNOWLEDGMENTS

I thank A. Liemant, K. Groeger, H. Gajewski, U. Wuensche, and L. Brehmer for stimulating discussions on the subject of this paper, which also includes results from ref. 11.

REFERENCES

1. W. Fichtner and D. Rose, eds. *IEEE Trans. Electron. Devices* **ED-30** (1983).
2. H. K. Henisch, *Phil. Mag. B* **52**(3):379–389 (1985).
3. N. Ikeda and S. Watanabe, *Stochastic Differential Equations and Diffusion Processes.* (North-Holland, Amsterdam, 1981).
4. J. Jacod and A. N. Shirjajew, *Limit Theorems for Stochastic Processes* (Springer, 1987).
5. T. Liggett, *Interacting Particle Systems* (Springer, 1985).

6. A. Miller and B. Abrahams, *Phys. Rev.* **120**:745 (1960).
7. N. F. Mott, *Non-crystall. Solids* **11** (1968).
8. N. F. Mott, *Phil. Mag. B* **19**:835 (1969).
9. G. Pfister and H. Scher, *Phys. Rev. B* **15**:2062 (1977).
10. E. Platen, A law of large numbers for wide range exclusion processes in random media, *Stoch. Proc. Appl.*, to appear.
11. E. Platen, A. Liemant, L. Brehmer, I. Mueller, and W. Wagner, A stochastic approach to electronic charge transport in ordered and disordered semiconducting materials, Preprint P-Math-08/88, AdW der DDR, Berlin.
12. F. W. Schmidlin, *Phys. Rev. B* **16**:2362 (1977).
13. W. Van Roosbroeck, *Bell Syst. Tech. J.* **29**:560–607 (1950).