DERIVATION OF THE DRIFT DIFFUSION SHOCKLEY-READ-HALL MODEL FOR SEMICONDUCTORS*

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Abstract. The Shockley-Read-Hall model for recombination-generation of electron-hole pairs in semiconductors based on a quasistationary approximation for electrons in a trapped state is generalized to distributed trapped states in the forbidden band. Existence of solutions has been proven, and the quasistationary limit is rigorously justified.

Key words. Semiconductor, drift-diffusion model, collision operators

1. Introduction. The Shockley-Read-Hall (SRH-)model was introduced in 1952 [14], [7] to describe the statistics of recombination and generation of holes and electrons in semiconductors occurring through the mechanism of trapping.

The transfer of electrons from the valence band to the conduction band is referred to as the generation of electron-hole pairs (or pair-generation process), since not only a free electron is created in the conduction band, but also a hole in the valence band which can contribute to the charge current. The inverse process is termed recombination of electron-hole pairs. The bandgap between the upper edge of the valence band and the lower edge of the conuction band is very large in semiconductors, which means that a big amount of energy is needed for a direct band-to-band generation event. The presence of trap levels within the forbidden band caused by crystal impurities facilitates this process, since the jump can be split into two parts, each of them 'cheaper' in terms of energy. The basic mechanisms are illustrated in Figure 1.1: (a) hole emission, (b) hole capture, (c) electron emission, (d) electron capture.



FIG. 1.1. The four basic processes of electron-hole recombination.

Models for this process involve equations for the densities of electrons in the conduction band, holes in the valence band, and trapped electrons. Basic for the SRH model are

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the drift-diffusion assumption for the transport of electrons and holes, the assumption of one trap level in the forbidden band, and the assumption that the dynamics of the trapped electrons is quasistationary, which can be motivated by the smallness of the density of trapped states compared to typical carrier densities. This model is an important ingredient of simulation models for semiconductor devices (see [9]).

In this work, generalization of the classical SRH model is considered: Instead of a single trapped state, a distribution of trapped states across the forbidden band is allowed. For this model existence result and rigorous result concerning the quasistationary limit is proven. The essential estimate is derived similarly to [5], where the quasineutral limit has been carried out.

In the following section, the drift-diffusion based model is formulated and nondimensionalized, and the SRH-model is formally derived. Section 3 contains the rigorous justification of the passage to the quasistationary limit.

2. Formal derivation of the Shockley-Read-Hall model. We consider a semiconductor crystal represented by the bounded domain $\Omega \subseteq \mathbb{R}^3$ (all our results are easily extended to the one and two-dimensional situations) with a constant (in space) number density of traps N_{tr} , where

$$N_{tr} = \int_{E_v}^{E_c} M_{tr}(E) \, \mathrm{d}E.$$
 (2.1)

We denote by E_v and E_c valence band edge and the conduction band edge, respectively, whereas $M_{tr}(E)$ is the density of available trapped states, and it depends on energy E. The position density of occupied traps is given by

$$n_{tr}(x,t) = \int_{E_v}^{E_c} M_{tr}(E) f_{tr}(x,E,t) \, \mathrm{d}E, \qquad (2.2)$$

where $f_{tr}(x, E, t)$ is the fraction of occupied trapped states at position $x \in \Omega$, energy $E \in (E_v, E_c)$, and time $t \ge 0$. Note that $0 \le f_{tr} \le 1$ should hold from a physical point of view.

The governing equations are given by

$$\partial_t f_{tr} = S_p - S_n, \qquad S_p = \frac{1}{\tau_p N_{tr}} \left[p_0 (1 - f_{tr}) - p f_{tr} \right] \qquad (2.3)$$

$$S_n = \frac{1}{\tau_n N_{tr}} \left[n_0 f_{tr} - n(1 - f_{tr}) \right] \qquad J_n = \mu_n (U_T \nabla n - n \nabla V), \qquad (2.4)$$

$$R_n = \int_{E_v}^{E_c} S_n M_{tr} dE \qquad J_p = -\mu_p (U_T \nabla p + p \nabla V), \qquad (2.5)$$

$$R_p = \int_{E_v}^{E_c} S_p M_{tr} dE$$

$$\varepsilon_s \Delta V = q(n + n_{tr} - p - C). \tag{2.6}$$

Here $n \ge 0$ denotes the density of electrons in the conduction band, whereas $p \ge 0$ is the density of holes in the valence band, with p, n being oppositly charged. For the

current densities J_n, J_p we use the simplest possible model, the drift diffusion ansatz, with constant mobilities μ_n, μ_p , and with thermal voltage U_T . Moreover, since the trapped states have fixed positions, there is no flux in (2.3).

By R_n and R_p we denote the recombination-generation rates for n and p, respectively. The rate constants are $\tau_n(E)$, $\tau_p(E)$, $n_0(E)$, $p_0(E)$, where $n_0(E)p_0(E) = n_i^2$ with the energy independent intrinsic density n_i .

In the Poisson equation (2.6), V(x,t) is the electrostatic potential, ε_s the permittivity of the semiconductor, q the elementary charge, and C = C(x) the doping profile.

Note that if τ_n, τ_p, n_0, p_0 are independent from E, or if there exists only one trap level E_{tr} with $M_{tr}(E) = N_{tr}\delta(E - E_{tr})$, then $R_n = \frac{1}{\tau_n} [n_0 \frac{n_{tr}}{N_{tr}} - n(1 - \frac{n_{tr}}{N_{tr}})], R_p = \frac{1}{\tau_p} [p_0(1 - \frac{n_{tr}}{N_{tr}}) - p \frac{n_{tr}}{N_{tr}}]$, and the system for n, p, and n_{tr} is closed by integration of (2.3):

$$\partial_t n_{tr} = R_p - R_n. \tag{2.7}$$

We now introduce a scaling of n, p, and f_{tr} in order to render the equations (2.4)–(2.6) dimensionless:

Scaling of parameters:

$$M_{tr} \to \frac{N_{tr}}{E_c - E_v} M_{tr}, \quad \tau_{n,p} \to \bar{\tau} \tau_{n,p}, \quad \mu_{n,p} \to \bar{\mu} \mu_{n,p}, \quad (n_0, p_0, C) \to \bar{C}(n_0, p_0, C).$$

Scaling of unknowns:

 $(n,p) \to \overline{C}(n,p), \quad n_{tr} \to N_{tr}n_{tr}, \quad V \to U_T V, \quad f_{tr} \to f_{tr}.$

Scaling of independent variables:

$$E \to E_v + (E_c - E_v)E, \quad x \to \sqrt{\frac{\bar{\mu}U_T\bar{C}\bar{\tau}}{N_{tr}}}x, \quad t \to \frac{\bar{C}}{N_{tr}}\bar{\tau}t.$$

Dimensionless parameters:

$$\lambda = \sqrt{\frac{\varepsilon_s N_{tr}}{q\bar{C}^2 \bar{\mu} \bar{\tau}}} = \frac{1}{\bar{x}} \sqrt{\frac{\varepsilon_s U_T}{q\bar{C}}} \text{ is the scaled Debye length, } \varepsilon = \frac{N_{tr}}{\bar{C}} \text{ is the ratio of the density}$$
of traps to the typical doping density, and will be assumed to be small: $\varepsilon \ll 1$.

The scaled system reads:

$$\varepsilon \partial_t f_{tr} = S_p(p, f_{tr}) - S_n(n, f_{tr}), \qquad S_p = \frac{1}{\tau_p} [p_0(1 - f_{tr}) - pf_{tr}],$$

$$S_n = \frac{1}{\tau_n} [n_0 f_{tr} - n(1 - f_{tr})],$$
(2.8)

$$\partial_t n = \nabla \cdot J_n + R_n, \qquad J_n = \mu_n (\nabla n - n \nabla V), \qquad R_n = \int_0^1 S_n M_{tr} \, \mathrm{d}E \qquad (2.9)$$

$$\partial_t p = -\nabla \cdot J_p + R_p, \qquad J_p = -\mu_p (\nabla p + p \nabla V), \qquad R_p = \int_0^1 S_p M_{tr} \, \mathrm{d}E \qquad (2.10)$$

$$\lambda^2 \Delta V = n + \varepsilon n_{tr} - p - C. \tag{2.11}$$

By letting $\varepsilon \to 0$ in (2.8) formally, we obtain $f_{tr} = \frac{\tau_n p_0 + \tau_p n}{\tau_n (p+p_0) + \tau_p (n+n_0)}$, and the reduced system has the following form

$$\partial_t n = \nabla \cdot J_n + R,\tag{2.12}$$

$$\partial_t p = -\nabla \cdot J_p + R,\tag{2.13}$$

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$$R(n,p) = (n_i^2 - np) \int_0^1 \frac{M_{tr}(E)}{\tau_n(E)(p + p_0(E)) + \tau_p(E)(n + n_0(E))} \, \mathrm{d}E,$$
(2.14)

$$\lambda^2 \Delta V = n - p - C. \tag{2.15}$$

Note that if τ_n, τ_p, n_0, p_0 are independent from E or if there exists only one trap level, then we would have the standard Shockley-Read-Hall model, with $R = \frac{n_i^2 - np}{\tau_n(p+p_0) + \tau_p(n+n_0)}$. Existence and uniqueness of solutions of the system (2.12)–(2.15) has been shown in [9].

3. Rigorous derivation of the drift diffusion Shockley-Read-Hall model. We consider initial-boundary value problems with initial conditions

$$n(x,0) = n_I(x),$$
 $p(x,0) = p_I(x),$ $f_{tr}(x,E,0) = f_{tr,I}(x,E)$ (3.1)

satisfying

$$N \ge n_I, p_I \ge 0, \qquad 0 \le f_{tr,I} \le 1$$
 (3.2)

and with mixed Dirichlet-Neumann boundary conditions on $\partial\Omega$, i.e., let

$$n(x,t) = n_D(x,t), \quad p(x,t) = p_D(x,t), \quad V(x,t) = V_D(x,t) \quad x \in \partial\Omega_D \subset \partial\Omega \quad (3.3)$$

and

$$\frac{\partial n}{\partial \nu} = \frac{\partial p}{\partial \nu} = \frac{\partial V}{\partial \nu} = 0 \quad \text{on } \partial \Omega_N := \partial \Omega \setminus \partial \Omega_D, \tag{3.4}$$

where ν is the outward unit normal vector along $\partial \Omega_N$.

The following assumptions on the data will be used: For the boundary data

$$n_D, p_D \in W^{1,\infty}_{loc}(\Omega \times \mathbb{R}^+_t), \quad V_D \in L^{\infty}_{loc}(\mathbb{R}^+_t, W^{1,6}(\Omega)),$$
(3.5)

for the initial data

$$n_I, p_I \in H^1(\Omega) \cap L^{\infty}(\Omega), \qquad \qquad 0 \le f_{tr,I} \le 1, \qquad (3.6)$$

$$\int_{\Omega} (n_I + \varepsilon n_{tr}(f_{tr,I}) - p_I - C) \, \mathrm{d}x = 0, \qquad \text{if } \partial\Omega = \partial\Omega_N, \qquad (3.7)$$

for the doping profile

$$C \in L^{\infty}(\Omega), \qquad (3.8)$$

for the recombination-generation rate constants

$$n_0, p_0, \tau_n, \tau_p \in L^{\infty}((0,1)), \qquad \tau_n, \tau_p \ge \tau_{min} > 0.$$
 (3.9)

We permit the special cases that either $\partial \Omega_D$ or $\partial \Omega_N$ are empty. In particular, we assume that either $\partial \Omega_D$ has positive (d-1)-dimensional measure, or it is empty. In the second situation ($\partial \Omega_D$ empty) we have to assume total charge neutrality, i.e.,

$$\int_{\Omega} (n + \varepsilon n_{tr} - p - C) \, \mathrm{d}x = 0.$$
(3.10)

The potential is then only determined up to a (physically irrelevant) additive constant.

We shall first prove local existence of solutions for fixed positive ε by a contraction argument, following the lines of [4], [9]. We define the fixed point map $F : \{n, p, f_{tr}\} \rightarrow \{u, v, u_{tr}\}$ by the following:

<u>Step 1</u>: For n, p, f_{tr} given (satisfying (3.10) if $\partial \Omega = \partial \Omega_N$), we obtain V by solving the problem (2.11), (3.3), (3.4); if $\partial \Omega_D$ has a positive measure, the solution exists and it is unique for all t. For empty $\partial \Omega_D$ the assumption (3.10) implies solvability and uniqueness up to a constant, whose value is unimportant for the following.

Step 2: We obtain the new trap occupancy u_{tr} from

$$\varepsilon \partial_t u_{tr} = \frac{1}{\tau_p} \left[p_0 (1 - u_{tr}) - p u_{tr} \right] - \frac{1}{\tau_n} \left[n_0 u_{tr} - n(1 - u_{tr}) \right], \qquad (3.11)$$
$$u_{tr}|_{t=0} = f_{tr,I},$$

the new electron density u from

$$\partial_t u = \nabla \cdot (\mu_n (\nabla u - n \nabla V)) + R_n (n, u_{tr}), \qquad (3.12)$$
$$u|_{\partial\Omega_D} = n_D, \quad \frac{\partial u}{\partial\nu}|_{\partial\Omega_N} = 0, \quad u|_{t=0} = n_I,$$

and the new hole density v from

$$\partial_t v = \nabla \cdot \left(\mu_p (\nabla v + p \nabla V) + R_p(p, u_{tr}) \right),$$
$$v|_{\partial \Omega_D} = p_D, \quad \frac{\partial v}{\partial \nu}|_{\partial \Omega_N} = 0, \quad v|_{t=0} = p_I$$

For the fixed point argument we shall use the following norm:

$$\begin{aligned} \|(n, p, f_{tr})\|_{T} &= \max_{0 \le t \le T} \left\{ \|n(t)\|_{L^{2}(\Omega)} + \|p(t)\|_{L^{2}(\Omega)} + \|f_{tr}(t)\|_{L^{2}(\Omega \times (0, 1))} \right\} \\ &+ \left(\int_{0}^{T} \left(\|\nabla n(t)\|_{L^{2}(\Omega)}^{2} + \|\nabla p(t)\|_{L^{2}(\Omega)}^{2} \right) dt \right)^{1/2}. \end{aligned}$$
(3.13)

Note that the property (3.10) is preserved in case of a pure Neumann problem. We now show that the map F is contractive for a sufficiently small time interval (0, T) on a ball with sufficiently large radius a around the initial data (considered as constant functions of time):

$$M_a := \{ (n, p, f_{tr}) : 0 \le f_{tr} \le 1, \| (n - n_I, p - p_I, f_{tr} - f_{tr,I}) \|_T \le a \}.$$
(3.14)

First, let us show that F maps M_a into itself. We observe that the equation for u_{tr} preserves the natural bounds for the initial data: $0 \le u_{tr} \le 1$. Multiplication of (3.11) by $u_{tr} - f_{tr,I}$ and straightforward estimation gives

$$\max_{[0,T]} \|u_{tr} - f_{tr,I}\|_{L^2(\Omega \times (0,1))} \le \frac{T\gamma(a)}{\varepsilon} \le \frac{a}{5},$$
(3.15)

for any a by choosing T small enough.

Multiplication of (3.12) by $u - n_D$ ($n_D = 0$ for the pure Neumann problem) and integration by parts gives

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} (u-n_D)^2 \,\mathrm{d}x = -\mu_n \int_{\Omega} |\nabla u|^2 \,\mathrm{d}x + \mu_n \int_{\Omega} \nabla u \cdot (n\nabla V + \nabla n_D) -\mu_n \int_{\Omega} n\nabla V \cdot \nabla n_D \,\mathrm{d}x + \int_{\Omega} (u-n_D)(R_n - \partial_t n_D) \,\mathrm{d}x$$
(3.16)

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For estimating the right hand side we use the Cauchy-Schwarz inequality, the assumptions on boundary and initial data, the estimate $|R_n(n, u_{tr})| \leq C(n+1)$, and the fact that $(n, p, f_{tr}) \in M_a$:

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|u - n_D\|_{L^2(\Omega)}^2 \leq -\frac{\mu_n}{2} \|\nabla(u - n_I)\|_{L^2(\Omega)}^2 + C(\gamma(a) + \|n\nabla V\|_{L^2(\Omega)}^2 + \|u - n_D\|_{L^2(\Omega)}^2).$$
(3.17)

For estimating the nonlinear term $n\nabla V$ we employ the Hölder inequality, the Gagliardo-Nirenberg inequality, the Poisson equation, and the Sobolev imbedding theorem:

$$\|n\nabla V\|_{L^{2}(\Omega)} \leq \|n\|_{L^{3}(\Omega)} \|\nabla V\|_{L^{6}(\Omega)} \\ \leq (C(\delta)\|n\|_{L^{2}(\Omega)} + \delta \|\nabla n\|_{L^{2}(\Omega)})(\|n+p\|_{L^{2}(\Omega)} + \|f_{tr}\|_{L^{2}(\Omega \times (0,1))} + 1),$$
(3.18)

for any $\delta > 0$, which leads to the estimate (using the definition of M_a)

$$\int_0^T \|n\nabla V\|_{L^2(\Omega)}^2 dt \le \gamma(a)(TC(\delta) + \delta).$$
(3.19)

As a consequence, the Gronwall lemma applied to (3.17) implies

$$\max_{[0,T]} \|u - n_D\|_{L^2(\Omega)}^2 \le \|n_I - n_D\|_{L^2(\Omega)}^2 + \gamma(a)(r(T)C(\delta) + \delta), \qquad (3.20)$$

with $r(T) \to 0$ for $T \to 0$, and, therefore,

$$\max_{[0,T]} \|u - n_I\|_{L^2(\Omega)}^2 \le 2\|n_I - n_D\|_{L^2(\Omega)}^2 + \gamma(a)(r(T)C(\delta) + \delta) \le \frac{a^2}{25}, \qquad (3.21)$$

where the last inequality is achieved by first choosing a big enough, then δ small enough, and then T small enough.

Analogously, we prove

$$\max_{[0,T]} \|v - p_I\|_{L^2(\Omega)} \le \frac{a}{5}.$$
(3.22)

As for the integral terms in the norm, we obtain from (3.17) after integration with respect to time

$$\frac{\mu_n}{2} \int_0^T \|\nabla(u - n_I)\|_{L^2(\Omega)}^2 \, \mathrm{d}t \le \frac{1}{2} \|n_I - n_D\|_{L^2(\Omega)}^2 + T\gamma(a) \le \frac{\mu_n}{2} \frac{a^2}{25},$$

such that

$$\left(\int_0^T \|\nabla(u - n_I)\|_{L^2(\Omega)}^2 \,\mathrm{d}t\right)^{1/2} \le \frac{a}{5}.$$
(3.23)

Note that again a has to be chosen big enough, and T small enough. The same estimate holds for $\nabla(v - p_I)$. Combining it with (3.15), (3.21), (3.22), and (3.23), $F: M_a \to M_a$ has been proven.

The next step is to prove that F is a contraction. For the components of the difference

$$(\delta u, \delta v, \delta u_{tr}) = F(n_1, p_1, f_{tr,1}) - F(n_2, p_2, f_{tr,2})$$
(3.24)

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we obtain the problems

$$\varepsilon \partial_t \delta u_{tr} = -\kappa \delta u_{tr} + A_n \delta n + A_p \delta p, \qquad (3.25)$$
$$\delta u_{tr}|_{t=0} = 0,$$

with $\kappa = \frac{p_0 + p_1}{\tau_p} + \frac{n_0 + n_1}{\tau_n}, A_n = \frac{1 - u_{tr,2}}{\tau_n}, A_p = -\frac{u_{tr,2}}{\tau_p}, \delta n = n_1 - n_2$ etc., for δu_{tr} , $\partial_t \delta u = \nabla \cdot (\mu_n (\nabla \delta u - n_1 \nabla \delta V - \delta n \nabla V_2)) + R_n (n_1, u_{tr,1}) - R_n (n_2, u_{tr,2})$ (3.26) $\delta u|_{\partial \Omega_D} = 0, \quad \frac{\partial \delta u}{\partial \nu}|_{\partial \Omega_N} = 0, \quad \delta u|_{t=0} = 0,$

for δu , and

$$\partial_t \delta v = \nabla \cdot \left(\mu_p (\nabla \delta v + p_1 \nabla \delta V + \delta p \nabla V_2)\right) + R_p(p_1, u_{tr,1}) - R_p(p_2, u_{tr,2}) \quad (3.27)$$
$$\delta v|_{\partial \Omega_D} = 0, \quad \frac{\partial \delta v}{\partial \nu}|_{\partial \Omega_N} = 0, \quad \delta v|_{t=0} = 0,$$

for δv .

The following estimates are very similar to the above. Multiplication of (3.25) by δu_{tr} and a simple estimation shows that

$$\max_{[0,T]} \|\delta u_{tr}\|_{L^{2}(\Omega \times (0,1))} \leq \frac{r(T)}{\varepsilon} \|(\delta n, \delta p, \delta f_{tr})\|_{T}, \qquad (3.28)$$

with $\lim_{T\to 0} r(T) = 0.$

Multiplying (3.26) with δu , integrating with respect to x and t, we obtain

$$\frac{1}{2} \|\delta u(t)\|_{L^{2}(\Omega)}^{2} + \frac{\mu_{n}}{2} \int_{0}^{t} \|\nabla \delta u(s)\|_{L^{2}(\Omega)}^{2} ds \\
\leq C \int_{0}^{t} \left(\|\delta n \nabla V_{2}\|_{L^{2}(\Omega)}^{2} + \|n_{1} \nabla \delta V\|_{L^{2}(\Omega)}^{2} \\
+ \|\delta n\|_{L^{2}(\Omega)}^{2} + \|\delta f_{tr}\|_{L^{2}(\Omega)}^{2} + \|\delta u\|_{L^{2}(\Omega)}^{2} \right) ds.$$
(3.29)

The first two terms on the right hand side we estimate analogously to (3.18), leading to

$$\int_{0}^{t} \left(\|\delta n \nabla V_{2}\|_{L^{2}(\Omega)}^{2} + \|n_{1} \nabla \delta V\|_{L^{2}(\Omega)}^{2} + \|\delta n\|_{L^{2}(\Omega)}^{2} + \|\delta f_{tr}\|_{L^{2}(\Omega)}^{2} \right) ds$$

$$\leq (r(T)C(\delta) + \delta) \|(\delta n, \delta p, \delta f_{tr})\|_{T}.$$

Application of the Gronwall lemma to (3.29), the analogous estimate for δv , and a combination of these results with (3.28) finally lead to

$$\|(\delta u, \delta v, \delta u_{tr})\|_T \le \left(\frac{r(T)C(\delta)}{\epsilon} + \delta\right) \|(\delta n, \delta p, \delta f_{tr})\|_T.$$
(3.30)

By choosing first δ and then T sufficiently small, F can be made contractive in M_a . Summarizing, the following local existence result has been proven.

THEOREM 3.1. Let the assumptions (3.5)–(3.9) hold. Then there exists T > 0, such that the problem (2.8)–(2.11), (3.1)–(3.4) has a unique solution with $n, p \in C([0,T], L^2(\Omega)) \cap L^2((0,T), H^1(\Omega)), f_{tr} \in C([0,T], L^2(\Omega \times (0,1))), 0 \le f_{tr} \le 1.$

It is obvious from (3.30) that the local existence result does not come with a uniform in ϵ estimate. Even the guaranteed existence time tends to zero with ϵ . The following global existence result with uniform (in ϵ) bounds is a generalization of [5, Lemma 3.1], where the case of homogeneous Neumann boundary conditions and vanishing recombination was treated. Our proof uses a similar approach and can be found in [10].

LEMMA 3.2. Let the assumptions of THEOREM 3.1 be satisfied. Then, the solution of (2.8)-(2.11), (3.1)-(3.4) exists for all times and satisfies $n, p \in L^{\infty}_{loc}((0,\infty), L^{\infty}(\Omega)) \cap L^{2}_{loc}((0,\infty), H^{1}(\Omega)))$ uniformly in ε as $\varepsilon \to 0$ as well as $0 \leq f_{tr} \leq 1$.

Finally, we write the main theorem, and the proof is also to be found in [10]:

THEOREM 3.3. Let the assumptions of THEOREM 3.1 be satisfied. Then, as $\varepsilon \to 0$, for every T > 0, the solution (f_{tr}, n, p, V) of (2.8)–(2.11), (3.1)–(3.4) converges with convergence of f_{tr} in $L^{\infty}((0, T) \times \Omega \times (0, 1))$ weak*, n and p in $L^{2}((0, T) \times \Omega)$, and V in $L^{2}((0, T), H^{1}(\Omega))$. The limits of n, p, and V satisfy (2.12)–(3.4).

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