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## The quasineutral limit problem in semiconductors sciences

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# THE QUASINEUTRAL LIMIT PROBLEM IN SEMICONDUCTOR SCIENCES

ABSTRACT. — The mathematical analysis on various mathematical models arisen in semiconductor science has attracted a lot of attention in both applied mathematics and semiconductor physics. It is important to understand the relations between the various models which are different kind of nonlinear system of P.D.Es. The emphasis of this paper is on the relation between the drift-diffusion model and the diffusion equation. This is given by a quasineutral limit from the DD model to the diffusion equation.

KEY WORDS: Quasineutral limit; Drift-diffusion model; Semiconductors.

The mathematical modelling and the corresponding mathematical analysis in semiconductor science have attracted a lot of attention in both applied mathematics and semiconductor physics.

Roughly speaking, we can divide semiconductor models into two classes: kinetic models and fluid dynamic models. For each of these classes there are (semi)classical models and quantum models. For instance, the Boltzmann-Poisson system and the Quantum Boltzmann-Poisson system are kinetic models, while the Hydrodynamic, the Energy-transport and the Drift-diffusion equations are fluid dynamic models for which the quantum effects can be also taken into account to get the corresponding Quantum hydrodynamic, Quantum energy-transport and Quantum drift-diffusion models respectively.

It is important to study those mathematical models since they are different kind of nonlinear systems of P.D.Es for which there are a lot of interesting problems in mathematics.

For instance, the Hydrodynamic model takes the form of Euler-Poisson equations, namely

$$\text{(1)}\qquad \begin{cases} n_t + \nabla\cdot(n\vec{u}) = 0 \\ p_t + \nabla\cdot\left(\dfrac{p\otimes p}{n}\right) + \nabla P = enE - \dfrac{p}{\tau_p} \\ w_t + \nabla\cdot(\vec{u}\,w + \vec{u}\,P) = ep\cdot E - \dfrac{w - w_0}{\tau_w} \\ \lambda^2\Delta\phi = e(n - b(x)) \quad (E = \nabla\phi) \end{cases}$$

where $n$ denotes the electron density, $\vec{u}$ is the velocity, $p$ denotes the momentum density ($p = mn\vec{u}$), $\phi$ is the negative electric potential, $P = nK_B T$, $T$ denotes the carrier temperature, $w = \dfrac{3}{2}nK_B T + \dfrac{m}{2}n|\vec{u}|$, $w_0 = \dfrac{3}{2}nK_B T^{(0)}$, $T^{(0)}$ is the ambient device

temperature, the positive constants $e$, $m$ and $K_B$ are the electron charge, the effective electron mass and the Boltzmann constants, $\lambda$ is the dielective constant, $\tau_p$ and $\tau_w$ are the momentum and energy relaxation time, and $b(x)$, called the doping profile, stands for the density of fixed, positive charged background ions.

This HD model was introduced to describe electron flow when the transport of energy plays a crucial role. It can be derived from the Boltzmann-Poisson system for semiconductors by Moment method. See [14, and the references there].

Compared to the pure Euler equation, the system (1) contains certain dissipative mechanism which makes it possible to establish the theory on globally defined smooth solutions. See, for instance, the corresponding results in [1] for one-space dimensional system, and [12] for 3-space dimensional system. However, it would be more difficult than the pure Euler equation on the study of weak entropy solutions. This is true even for the simplified HD model, namely

$$\text{(2)} \qquad \begin{cases} n_t + \nabla \cdot (n\vec{u}) = 0 \\ (n\vec{u})_t + \nabla \cdot (n\vec{u} \otimes \vec{u}) + \nabla P(n) = n\nabla \Phi - \dfrac{n\vec{u}}{\tau} \\ \Delta \Phi = n - b(x) \end{cases}$$

for which there are certain results on globally defined classical solutions for multi-dimensional system, see [10, 6, 5], but nothing on weak entropy solutions, although the one-dimensional case has been studied extensively, see [11] and the references concerned.

It is also important to understand the relations between those models mentioned above. The relations are at least formally well understood. For instance, the passage from the HD model to ET or DD models is so-called relaxation limit; the way from the DD model to the diffusion equation is given by a quasineutral limit. Classical models are obtained from quantum models in the so-called classical limit, where the scaled Plank constant tends to zero, etc. However, it is really a challenging problem to establish these limits rigorously in mathematics. This paper is concentrated on quasineutral limit, particularly the quasineutral limit of drift-diffusion models in semiconductors.

The scaled semiconductor drift-diffusion equations read

$$\text{(3)} \qquad \begin{cases} n_t = \mu_n \operatorname{div} (\nabla(n^{\gamma_n}) + nE) \\ p_t = \mu_p \operatorname{div} (\nabla(p^{\gamma_p}) - pE) \\ -\lambda^2 \operatorname{div} E = n - p - C \end{cases}$$

with $x \in \Omega \subset \mathbb{R}^d$, $\Omega$ bounded with smooth boundary, $t \geqslant 0$ and $E = -\nabla \Phi$. The unknowns $n$, $p$, $E$, $\Phi$ are the electron density, the hole density, the electric field and the electric potential, respectively. The given function $C = C(x)$ is the doping profile describing fixed background charges. The dimensionless positive parameters $\mu_n$, $\mu_p$ and $\lambda$ are the scaled mobilities of electrons, holes and the scaled Debye length, respectively.

If $\gamma_n = \gamma_p = 1$ (isothermal case), (3) is called the standard drift-diffusion model; if

$\gamma_n$, $\gamma_p \geq 1$, not equal to one together, (isentropic case), (3) is called the nonlinear drift-diffusion model.

This model was first proposed in [17] in the semiconductor context. There are different ways to obtain this model. One possibility is a relaxation limit from the hydrodynamic model. Also, the model can be derived directly from the semiconductor Boltzmann equation using the moment method for which more explanation can be found in [14].

The time-dependent and the stationary DD model have been mathematically analyzed extensively. The main interest here is the behavior of the solutions of (3) in the vanishing Debye length limit $\lambda \to 0$, namely, quasineutral limit.

Quasineutrality is a frequently used modelling assumption in charged particle transport. Formally, quasineutral models are derived in the limit as the ratio of the Debye length to a characteristic length tends to zero. In the semiconductor content, this formalized perturbation approach has been used extensively for the analysis of the qualitative behavior of semiconductor devices, see [14-16], etc., where the contributions are concerned with formal asymptotic expansions. As far as the rigorous results are concerned, very few is known. The special situation when $C \equiv 0$ is studied in [2, 13] when the initial data for $n$ and $p$ are equal. The situation of $C \not\equiv 0$ is more difficult to be treated on which the first rigorous result for the standard DD model ($\gamma_n = \gamma_p = 1$) under certain restrictive assumptions is obtained in [4]. For the general case $\gamma_n > 0$, $\gamma_p > 0$, when the doping profile is a constant or does not change sign, generalizing the results of [4] to nonlinear diffusion, we employ multiplier technique instead of the invariant region method used in [4] in order to obtain the lower and upper bounds on the densities.

Consider an insulated semiconductor modelled by the following initial-boundary value problem

$$
(4) \qquad \begin{cases} (3) \\ (\nabla(n^{\gamma_n}) + nE)\cdot \nu = 0 \\ (\nabla(p^{\gamma_p}) - pE)\cdot \nu = 0 \\ \nabla E \cdot \nu = 0, \end{cases} \quad x \in \partial\Omega, \quad t > 0
$$

$$
n(t=0, x) = n_0(x), \quad p(t=0, x) = p_0(x), \quad x \in \Omega
$$

where $\nu$ is the normal vector along the boundary $\partial\Omega$.

A necessary solvability condition for the Poisson equation, subject to the Neumann boundary condition is global charge neutrality

$$\int_\Omega (n - p - C)\, dx = 0.$$

Since the total numbers of electrons and holes are conserved, it is sufficient to require that

$$\int_\Omega (n_0 - p_0 - C)\, dx = 0.$$

Now, we explain the quasineutral limit in the DD model. We perform the Debye limit $\lambda \to 0$ formally in the system (3) to get the system

$$\begin{cases} N_t = \mu_n \operatorname{div}(\nabla N^{\gamma_n} + N\mathcal{E}) \\ P_t = \mu_p \operatorname{div}(\nabla P^{\gamma_p} - P\mathcal{E}) \\ 0 = N - P - C \end{cases} \tag{5}$$

where $N, P, \mathcal{E}$ are the formal limits of $n, p, E$ as $\lambda \to 0$.

Due to the singular perturbation character of the problem (the Poisson equation becomes an algebraic equation in the limit) we can not a priorily expect that all initial and boundary conditions hold for the limiting problem. However, by the conservation form of the continuity equations the property of zero flux through the boundary will prevail in the limit:

$$(\nabla N^{\gamma_n} + N\mathcal{E})\cdot\nu = 0, \quad (\nabla P^{\gamma_p} - P\mathcal{E})\cdot\nu = 0 \quad \text{on } \partial\Omega \tag{6}$$

while the boundary condition for the electric field $E$ does not. Initial conditions for the limiting problem are satisfied in the sense of $H^{-1}(\Omega)$.

Simple manipulations of (5) give the paraboli-elliptic system

$$\begin{cases} \left(\frac{1}{\mu_n} + \frac{1}{\mu_p}\right) P_t = \operatorname{div}(\nabla((P+C)^{\gamma_n} + P^{\gamma_p}) + C\mathcal{E}) \\ -\operatorname{div}(((\mu_n + \mu_p)P + \mu_n C)\mathcal{E}) = \operatorname{div}(\nabla(\mu_n(P+C)^{\gamma_n} - \mu_p P^{\gamma_p})). \end{cases} \tag{7}$$

If, further, $C \equiv 0$, the limiting problem becomes

$$P_t = \frac{\mu_n \mu_p}{\mu_n + \mu_p} \operatorname{div}(\nabla(P^{\gamma_n} + P^{\gamma_p}))$$

which is the case in plasma physics.

We studied the quasineutral limit rigorously when one of the following assumptions holds:

ASSUMPTION A.

(*i*) $C(x) = \text{const}$

(*ii*) *there exists a positive constant* $\delta$ *independent of* $\lambda$ *such that* $n_0^\lambda \geqslant \delta + C > 0$, $p_0^\lambda \geqslant \geqslant \delta$ *in* $\Omega$

(*iii*) $0 < \gamma_n, \gamma_p < +\infty$.

ASSUMPTION B.

(*i*) *There exists a positive constant* $\underline{C}$ *such that* $C(x) \geqslant \underline{C} > 0$ (*or* $C(x) \leqslant -\underline{C} < 0$) *and* $C(x) \in W^{1,\infty}(\Omega)$

(*ii*) $n_0^\lambda$, $p_0^\lambda$ *are bounded away from* 0 *uniformly as* $\lambda \to 0$

(*iii*) $1 \leqslant \gamma_p \leqslant \frac{3}{2}$, $\gamma_n \geqslant \frac{2d}{d+1}$ $\left(\text{or } 1 \leqslant \gamma_n \leqslant \frac{3}{2},\ \gamma_p \geqslant \frac{2d}{d+1}\right)$.

REMARK 1. The other case when B(*iii*) is replaced by

$$(B') \qquad 1 \leqslant \gamma_p \leqslant \frac{3}{2},\ \gamma_n \leqslant \frac{2d}{d+1} \left( \text{or } 1 \leqslant \gamma_n \leqslant \frac{3}{2},\ \gamma_p \leqslant \frac{2d}{d+1} \right)$$

has been investigated later in [8].

To state our results, we introduce the entropy

$$e^\lambda(t) = \int_\Omega \left( n^\lambda \frac{(n^\lambda)^{\gamma_n - 1} - 1}{\gamma_n - 1} + p^\lambda \frac{(p^\lambda)^{\gamma_p - 1} - 1}{\gamma_p - 1} + \frac{\lambda^2}{2} |E^\lambda|^2 \right) dx + e_0$$

where $\left( \frac{A^{\gamma-1} - 1}{\gamma - 1} \right) \Big|_{\gamma = 1} := \ln A$ for $A > 0$ and the constant $e_0$ is chosen such that the entropy $e^\lambda(0)$ is a nonnegative quantity.

THEOREM 1. *Assume the initial data $n_0^\lambda$, $p_0^\lambda \geqslant 0$ are such that the initial entropy $e^\lambda(0)$ is uniformly bounded as $\lambda \to 0$ and that there are functions $n_0$, $p_0 \in L^\infty(\Omega)$ such that $n_0^\lambda \to n_0$, $p_0^\lambda \to p_0$ strongly in $L^\infty(\Omega)$ as $\lambda \to 0$. Also, let one of the above assumptions (A), (B) and (B′) holds. Let $T > 0$ and $Q_T = (0, T) \times \Omega$. Then, as $\lambda \to 0$ the following convergences hold (after extracting subsequences):*

$$n^\lambda \to N \text{ strongly in } L^{q_n}(Q_T),$$
$$p^\lambda \to P \text{ strongly in } L^{q_p}(Q_T),$$
$$E^\lambda \rightharpoonup \mathcal{E} \text{ weakly in } L^s(Q_T),$$
$$n^\lambda - p^\lambda - C = O(\lambda) \text{ in } L^2(Q_T)$$

*where $q_n$, $q_p$, $s > 1$ depend on $\gamma_n$ and $\gamma_p$.*

*Furthermore, the limit $(N, P, \mathcal{E})$ satisfies the system (5) (6) in $D'(Q_T)$ and the initial data $N(t = 0, x) = n_0(x)$, $P(t = 0, x) = p_0(x)$ in the sense of $H^{-1}(\Omega)$.*

The main steps to establish the theorem.

1. To establish the uniform a priori estimates on densities by using the multiplier techniques and energy arguments.

2. To construct the entropy functional so as to get the uniform estimates related to $E^\lambda$ and etc.

3. To prove strong convergence of $n^\lambda$ and $p^\lambda$ in $L^{q_n}(Q_T)$ and $L^{q_p}(Q_T)$ respectively.

4. To establish the weak-convergence of the terms $(n^\lambda - p^\lambda - C)E^\lambda$ and $n^\lambda E^\lambda$, $p^\lambda E^\lambda$. This needs to improve the uniform $L^a$-estimates on density and electric field since we have only obtained weaker estimates on $E^\lambda$.

The detailed arguments can be found in [3].

Physically, it is more interesting when the doping profile changes sign. One of the main difficulty is the oscillatory behavior on the field. Let us consider a simple case –

the one-dimensional standard bipolar DD model

$$\begin{cases} n_t^\lambda = \mu_n (n_x^\lambda + n^\lambda E^\lambda)_x \\ p_t^\lambda = \mu_p (p_x^\lambda - p^\lambda E^\lambda)_x \\ -\lambda^2 E_x^\lambda = n^\lambda - p^\lambda - C \end{cases} \tag{8}$$

with $x \in [0, 1]$, $t \geq 0$ and $E^\lambda = -\Phi_x^\lambda$, and subject to the following boundary and initial conditions

$$n_x^\lambda + n^\lambda E^\lambda = p_x^\lambda - p^\lambda E^\lambda = E^\lambda = 0, \qquad x = 0, 1, \quad t > 0 \tag{9}$$

$$n^\lambda(t = 0, x) = n_0^\lambda(x), \qquad p^\lambda(t = 0, x) = p_0^\lambda(x), \qquad x \in [0, 1] \tag{10}$$

Introduce the entropy

$$e^\lambda(t) = \int_0^1 \left( n^\lambda \log n^\lambda + p^\lambda \log p^\lambda + \frac{\lambda^2}{2} |E^\lambda|^2 \right) dx + e_0,$$

where the constant $e_0$ is chosen such that the entropy $e^\lambda(0)$ is a nonnegative quantity. Denote

$$S^+ = \{x : C(x) > 0\}, \qquad S^0 = \{x : C(x) = 0\} \quad \text{and} \quad S^- = \{x : C(x) < 0\}.$$

For the nonnegative doping profile, we have

THEOREM 2. *Assume the initial data $n_0^\lambda$, $p_0^\lambda \geq 0$ are such that the initial entropy $e^\lambda(0)$ is uniformly bounded as $\lambda \to 0$ and that there are functions $n_0$, $p_0 \in L^\infty(\Omega)$ such that $n_0^\lambda \to n_0$, $p_0^\lambda \to p_0$ strongly in $L^\infty(\Omega)$ as $\lambda \to 0$. Also, let the following assumptions hold*:*

(i) the doping profile $C(x)$ is nonnegative and satisfies $\sqrt{C} \in H^1((0, 1))$.*

*(ii) $S^+$ is an open subset of $[0, 1]$.*

*Let $T > 0$ and $Q_T = (0, 1) \times (0, T)$. Then, as $\lambda \to 0$ the following convergences hold (after extracting subsequences)*:

$$\begin{aligned} &n^\lambda \to N \text{ strongly in } L^\alpha(Q_T), \quad 1 \leq \alpha < 2, \\ &p^\lambda \to P \text{ strongly in } L^\beta(Q_T), \quad 1 \leq \beta < 2, \\ &E^\lambda \rightharpoonup \mathcal{E} \text{ weakly in } L^2(B^+ \times (0, T)), \\ &n^\lambda - p^\lambda - C = O(\lambda) \text{ in } L^2((0, 1) \times (0, T)), \\ &n^\lambda E^\lambda \to N\mathcal{E}, \quad p^\lambda E^\lambda \to P\mathcal{E} \text{ in } D'(B^+ \times (0, T)), \\ &(n^\lambda - p^\lambda) E^\lambda \to 0 \text{ strongly in } L^{4/3}(S^0 \times (0, T)) \end{aligned}$$

*where $B^+$ is any closed subinterval of the set $S^+$. Furthermore, the limit $(N, P, \mathcal{E})$ satisfies the system (11) (12) in $D'(B^+ \times (0, T))$, and, respectively, the porous media type equation $N_t = \dfrac{2\mu_n \mu_p}{\mu_n + \mu_p} N_{xx}$ with $N = P$ in $D'(B^0 \times (0, T))$, where $B^0$ is any closed subinterval of $S^0$, and the initial data $N(t = 0, x) = n_0(x)$, $P(t = 0, x) = p_0(x)$ in the*

*sense of* $H^{-1}((0,1))$.

$$\begin{cases} N_t = \mu_n (N_x + N\mathcal{E})_x \\ P_t = \mu_p (P_x - P\mathcal{E})_x \\ 0 = N - P - C \end{cases} \tag{11}$$

$$N_x + N\mathcal{E} = P_x - P\mathcal{E} = 0, \quad x = 0, 1. \tag{12}$$

COROLLARY 3. *Under the assumption of the above theorem, we have*
(*i*) *If* $C = 0$, *then* $N = P$ *satisfies the porous media type equation*

$$N_t = \frac{2\mu_n \mu_p}{\mu_n + \mu_p} N_{xx} \qquad N(t=0, x) = n_0(x) = p_0(x)$$

*in* $D'((0,1) \times (0,T))$.
(*ii*) *If* $C(x) > 0$ *in* $(0,1)$, *then* $(N, P, \mathcal{E})$ *satisfies the system* (11) (12) *in* $D'((0,1) \times (0,T))$ *and the initial data* $N(t=0, x) = n_0(x)$, $P(t=0, x) = p_0(x)$ *in the sense of* $H^{-1}((0,1))$.

REMARK 2. A similar result holds for the case of the non-positive doping profile.

REMARK 3. In general, the field $E^\lambda$ will not be bounded in $L^s$ as $\lambda \to 0$. This yields many difficulties in establishing the weak convergence of $n^\lambda E^\lambda$ and $p^\lambda E^\lambda$. So that new techniques are needed.

The proof of theorem is based on the entropy methods and the weak compactness argument. First, by constructing the entropy functional, the uniform a priori estimates are obtained. Then, the weak compactness methods yield the desired convergence. However, the uniform a priori estimates obtained by the entropy functional is not sufficient to establish the weak convergence of $n^\lambda E^\lambda$ and $p^\lambda E^\lambda$ since the concentration-oscillation phenomena may appear in the weak-convergence. By using some new techniques of the weak-convergence method, we are able to overcome the concentration-oscillation phenomena and hence obtain the weak-convergence of $n^\lambda E^\lambda$ and $p^\lambda E^\lambda$. The detailed arguments can be found in [7].

REMARK 4. The problem is much more difficult than the above case when we turn to the doping profile which may change sign. The first rigorous result to deal with this case is given in [9] recently. In [9], the vanishing Debye length limit of the bipolar one-dimensional standard drift-diffusion models for semiconductors modelling a p-n junction device (*i.e.* with a fixed bipolar background charge) is studied. For general changing sign smooth doping profile the quasineutral limit in the well-prepared and also ill-prepared initial data cases is performed rigorously by using the multiple scaling asymptotic expansions of a singular perturbation analysis and the careful energy method. The key point of the proof is to introduce a density transform and a $\lambda$-weighted Lyapunov's functional, and to establish an entropy inequality, which yields the uniform Sobolev's energy estimates of the error functions.

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