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Weak solutions to one-dimensional quantum drift-diffusion equations for semiconductors

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Abstract: The weak solutions to the stationary quantum drift-diffusion equations (QDD) for semiconductor devices are investigated in one space dimension. The proofs are based on a reformulation of the system as a fourth-order elliptic boundary value problem by using an exponential variable transformation. The techniques of *a priori* estimates and Leray-Schauder's fixed-point theorem are employed to prove the existence. Furthermore, the uniqueness of solutions and the semiclassical limit $\delta \to 0$ from QDD to the classical drift-diffusion (DD) model are studied.

Key words: semiconductor device; quantum drift-diffusion equations; existence and uniqueness; exponential variable transformation; semiclassical limit

During recent years there has been rapid progress in the miniaturization of semiconductor devices, reaching a length scale at which quantum effects play a dominant role. This paper is concerned with the analysis of the steady state of the quantum drift-diffusion model (QDD) for semiconductors. The QDD describes electron transport in semiconductors as a quantum fluid and it is of considerable physical and practical importance. It is an extension of the classical drift-diffusion model including quantum corrections. These quantum terms allow a description of quantum effects. For an overview of the classical drift-diffusion model, refer to Refs. [1 – 3]. More details and a derivation of the QDD can be found in Ref. [4]. In Ref. [5], a bipolar quantum drift-diffusion model including generation-recombination terms is considered. To our knowledge, there is no uniqueness result for multi-dimensional stationary QDD equations[6]. This is why we consider the stationary quantum drift-diffusion equations in one space dimension.

The macroscopic quantum equations in a one-dimensional stationary version have been developed in the past years. The existence and uniqueness of strong solutions with positive electron density to a one-dimensional quantum Euler-Poisson system for semiconductors was considered in Ref. [7]. Gualdani and Jüngel[8] studied the steady-state viscous quantum hydronamic model in a one space dimension, which consists of the continuity equations for the electron and current densities, coupled to the Poisson equation for the electrostatic potential.

1 Reformulation of the Equations

The scaled equations of the QDD in a one space dimension read:

$$n_t = J_x,\ J = T_0 n_x - nV_x - \delta^2 n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x,\ \lambda^2 V_{xx} = n - C(x) \qquad x \in (0,1),\ t>0$$

where $n(x,t)$ is the election density, $V(x,t)$ the electrostatic potential, and $J(x,t)$ the current density. The doping profile $C(x)$ models fixed background charges. We assume that the ambient temperature T_0 be positive. The dimensionless constants δ and λ are the scaled Planck constant and the scaled Debye length, respectively.

The objective of this paper is to analyze the one-dimensional stationary version of the quantum drift-diffusion model:

$$T_0 n_x - nV_x - \delta^2 n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x = J_0 \tag{1}$$

$$\lambda^2 V_{xx} = n - C(x) \qquad x \in (0,1) \tag{2}$$

where the current density J_0 is a positive constant. We choose the physically motivated boundary conditions:

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$$n(0)=n(1)=1,\ n_x(0)=n_x(1)=0,\ V(0)=V_0 \tag{3}$$

Dividing (1) by n and taking the derivative gives

$$T_0\left(\frac{n_x}{n}\right)_x-\frac{n-C(x)}{\lambda^2}-\delta^2\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_{xx}=\left(\frac{J_0}{n}\right)_x$$

After an exponential transformation $n=\mathrm{e}^u$, we obtain

$$-\frac{\delta^2}{2}\left(\frac{u_x^2}{2}+u_{xx}\right)_{xx}+T_0u_{xx}+J_0\mathrm{e}^{-u}u_x=\lambda^{-2}(\mathrm{e}^u-C) \tag{4}$$

With boundary conditions for u:

$$u(0)=u(1)=0,\qquad u_x(0)=u_x(1)=0 \tag{5}$$

As usual, we call $u\in H_0^2(0,1)$ a weak solution of (4) and (5), if for all $\psi\in H_0^2(0,1)$ it holds:

$$-\frac{\delta^2}{2}\int_0^1\left(\frac{u_x^2}{2}+u_{xx}\right)\psi_{xx}\mathrm{d}x-T_0\int_0^1u_x\psi_x\mathrm{d}x+J_0\int_0^1\mathrm{e}^{-u}u_x\psi\mathrm{d}x=\lambda^{-2}\int_0^1(\mathrm{e}^u-C)\psi\mathrm{d}x$$

The nonlinear fourth-order equation (4) with boundary condition (5) is the problem to be analyzed in this paper, which is organized in the following way.

2 *A Priori* Estimates

In order to use the Leray-Schauder fixed-point theorem[9-10] to prove the existence, we need the following lemma 1; to prove the uniqueness, we need lemma 2.

Lemma 1 Suppose that $C\in L^\infty(0,1)$ be such that $C>0$ and $u\in H_0^2(0,1)$ be a solution of (4) and (5). Then estimate

$$\frac{\delta^2}{2}\|u_{xx}\|_{L^2(0,1)}^2+T_0\|u_x\|_{L^2(0,1)}^2\leqslant C_1 \tag{6}$$

holds. In particular, it follows that $\|u\|_{L^\infty(0,1)}\leqslant C_2$, where $C_2=\sqrt{C_1/T_0}$.

Proof We use $\psi=u$ as a test function in the weak formulation of (4) to obtain

$$\frac{\delta^2}{2}\int_0^1\left(\frac{u_x^2u_{xx}}{2}+u_{xx}^2\right)\mathrm{d}x+T_0\int_0^1u_x{}^2-J_0\int_0^1\mathrm{e}^{-u}u_xu\mathrm{d}x=-\lambda^{-2}\int_0^1(\mathrm{e}^u-C)u\mathrm{d}x \tag{7}$$

It is not difficult to see that $\mathrm{e}^{-1}+\|C\log C\|_{L^\infty(0,1)}$ is an upper bound for the function $\varphi(u)=-u(\mathrm{e}^u-C(x))$, $u\in\mathbf{R}$, for every $x\in(0,1)$. Furthermore, the boundary conditions give

$$\int_0^1u_x{}^2u_{xx}\mathrm{d}x=\frac{1}{3}(u_x^3(1)-u_x^3(0))=0$$

and

$$\int_0^1\mathrm{e}^{-u}u_xu\mathrm{d}x=-u(x)\mathrm{e}^{-u(x)}\Big|_0^1+\int_0^1\mathrm{e}^{-u(x)}\mathrm{d}u(x)=0$$

So we conclude that (7) can be estimated as

$$\frac{\delta^2}{2}\int_0^1u_{xx}{}^2\mathrm{d}x+T_0\int_0^1u_x^2\mathrm{d}x\leqslant\lambda^{-2}(\mathrm{e}^{-1}+\|C\log C\|_{L^\infty(0,1)})$$

or

$$\frac{\delta^2}{2}\|u_{xx}\|_{L^2(0,1)}^2+T_0\|u_x\|_{L^2(0,1)}^2\leqslant C_1$$

where $C_1=\lambda^{-2}(\mathrm{e}^{-1}+\|C\log C\|_{L^\infty(0,1)})$. Finally, from the Sobolev imbedding theorem, $\|u\|_{L^\infty(0,1)}\leqslant\|u_x\|_{L^2(0,1)}\leqslant C_2$, where $C_2=\sqrt{C_1/T_0}$. This proves lemma 1.

Lemma 2 Let $\delta\leqslant T_0/2$ hold and $u\in H_0^2(0,1)$ be a weak solution of (4) and (5). Then $\|u_x\|_{L^\infty(0,1)}\leqslant C_3$ holds.

Proof We observe that, due to the boundary conditions for u_x,

$$u_x^2(x)=2\int_0^xu_x(s)u_{xx}(s)\mathrm{d}s\leqslant2\left(\int_0^xu_x^2(s)\right)^{\frac{1}{2}}\left(\int_0^xu_{xx}^2(s)\right)^{\frac{1}{2}}\leqslant2\|u_x\|_{L^2(0,1)}\|u_{xx}\|_{L^2(0,1)} \tag{8}$$

and thus,

$$|u_x(x)|\leqslant\sqrt{2}\|u_x\|_{L^2(0,1)}^{\frac{1}{2}}\|u_{xx}\|_{L^2(0,1)}^{\frac{1}{2}}\leqslant\frac{\sqrt{2}\varepsilon}{2}\|u_x\|_{L^2(0,1)}+\frac{\sqrt{2}}{2\varepsilon}\|u_{xx}\|_{L^2(0,1)}$$

taking $\varepsilon = \alpha/\sqrt{2}$, we obtain

$$\|u_x\|_{L^\infty(0,1)} \leqslant \frac{\alpha}{2}\|u_x\|_{L^2(0,1)} + \frac{1}{\alpha}\|u_{xx}\|_{L^2(0,1)}$$

for all $\alpha > 0$. Choosing $\alpha = \dfrac{T_0}{\delta\sqrt{C_1}}$ and lemma 1 gives

$$\|u_x\|_{L^\infty(0,1)} \leqslant \frac{\sqrt{T_0}}{2\delta} + \frac{\sqrt{T_0}}{2\delta}\sqrt{\frac{8\delta^3}{T_0^{\ 3}}} \leqslant C_3$$

where $C_3 = \sqrt{T_0}/\delta$, we have employed $\delta \leqslant T_0/2$.

3 Existence and Uniqueness of Weak Solutions

Theorem 1 Let $C \in L^\infty(0,1)$ be such that $C > 0$, there exists a weak solution $u \in H_0^2(0,1)$ of (4) and (5).

Proof Consider the problem

$$-\frac{\delta^2}{2}\int_0^1 u_{xx}\psi_{xx} - \frac{\delta^2}{4}\sigma\int_0^1 w_x^2\psi_{xx}\mathrm{d}x - T_0\int_0^1 u_x\psi_x\mathrm{d}x + \sigma J_0\int_0^1 \mathrm{e}^{-w}w_x\psi\mathrm{d}x = \frac{\sigma}{\lambda^2}\int_0^1(\mathrm{e}^w - C)\psi\mathrm{d}x \tag{9}$$

where $\sigma \in [0,1]$, with boundary conditions:

$$u(0) = u(1) = 0, \quad u_x(0) = u_x(1) = 0$$

and $w \in H_0^1(0,1)$, the test functions $\psi \in H_0^2(0,1)$.

Defining the bilinear form:

$$a(u,\psi) = \frac{\delta^2}{2}\int_0^1 u_{xx}\psi_{xx} + T_0\int_0^1 u_x\psi_x\mathrm{d}x \qquad u,\psi \in H_0^{\ 2}(0,1)$$

and the linear functional:

$$F(\psi) = -\frac{\delta^2}{4}\sigma\int_0^1 w_x^{\ 2}\psi_{xx}\mathrm{d}x - \frac{\sigma}{\lambda^2}\int_0^1(\mathrm{e}^w - C)\psi\,\mathrm{d}x + \sigma J_0\int_0^1 \mathrm{e}^{-w}w_x\psi\mathrm{d}x$$

for $\psi \in H_0^2(0,1)$. Then there is a constant $m > 0$ such that $a(u,u) > m\|u\|_{H^2(0,1)}$, i. e., the form $a(\cdot,\cdot)$ is coercive on $H_0^2(0,1) \times H_0^2(0,1)$. Moreover, $a(\cdot,\cdot)$ is continuous and the linear functional F is continuous on $H_0^{\ 2}(0,1)$. By the Lax-Milgram theorem, there exists a unique solution $u \in H_0^2(0,1)$ to $a(u,\psi) = F(\psi)$ for $\psi \in H_0^{\ 2}(0,1)$, i. e., u solves (9). Thus, the operator

$$S: H_0^1(0,1) \times [0,1] \to H_0^1(0,1), \quad (w,\sigma) \mapsto u$$

is well-defined. It can be seen easily that the operator S is continuous. Due to the compact imbedding of $H_0^2(0,1)$ in $H_0^1(0,1)$, it is compact. Additionally, we have $S(w,0) = 0$ for any $w \in H_0^1(0,1)$. Following the steps of the proof of lemma 1, we can know that $\|u\|_{H_0^1} \leqslant$ constant for all $(u,\sigma) \in H_0^1(0,1) \times [0,1]$ satisfying $S(u,\sigma) = u$.

All conditions of the Leray-Schauder fixed-point theorem for the compact operator S are satisfied. The existence of a fixed point $T(u,1) = u$ follows.

Remark 1 By the embedding theorem, we have $u \in L^\infty(0,1)$, so we can conclude the existence of a positive lower bound for $n = \mathrm{e}^u$. Notice that this yields positives without the use of a maximum principle.

Remark 2 Obviously, with $u \in H_0^2(0,1)$, the evaluation of the potential V is straightforward.

In the sequel, the uniqueness result is established. Here we also need $\delta \leqslant T_0/2$.

Theorem 2 If $J_0 > 0$ is sufficiently small and $u, v \in H^2(0,1)$ are two weak solutions of (4) and (5), then $u = v$ holds.

Proof Take difference of the weak formulations of (4) for u and for v with test function $u - v \in H_0^2(0,1)$,

$$\frac{\delta^2}{2}\int_0^1(u_{xx} - v_{xx})^2\mathrm{d}x + \frac{\delta^2}{4}\int_0^1(u_x^{\ 2} - v_x^{\ 2})(u-v)_{xx}\mathrm{d}x + T_0\int_0^1(u_x - v_x)^2\mathrm{d}x =$$
$$-\frac{1}{\lambda^2}\int_0^1(\mathrm{e}^u - \mathrm{e}^v)(u-v)\mathrm{d}x + J_0\int_0^1(\mathrm{e}^{-u}u_x - \mathrm{e}^{-v}v_x)(u-v)\mathrm{d}x \tag{10}$$

The monotonicity of $x \mapsto \mathrm{e}^x$ implies $-\lambda^{-2}\int_0^1(\mathrm{e}^u - \mathrm{e}^v)(u-v)\mathrm{d}x \leqslant 0$ and we have

$$\left|J_0\int_0^1(\mathrm{e}^{-u}u_x - \mathrm{e}^{-v}v_x)(u-v)\mathrm{d}x\right| \leqslant J_0\int_0^1\mathrm{e}^{-u}|u_x - v_x||u-v|\mathrm{d}x + J_0\int_0^1 v_x|\mathrm{e}^{-u} - \mathrm{e}^{-v}||u-v|\mathrm{d}x \leqslant$$

$$J_0(4e^{C_2}C_2C_3+4C_3e^{C_2}C_2)=8J_0C_2C_3e^{C_2}$$

We conclude from (10)

$$\frac{\delta^2}{2}\int_0^1(u_{xx}-v_{xx})^2\mathrm{d}x+\frac{\delta^2}{4}\int_0^1(u_x^{\ 2}-v_x^{\ 2})(u-v)_{xx}\mathrm{d}x+T_0\int_0^1(u_x-v_x)^2\mathrm{d}x\leqslant 8J_0C_2C_3e^{C_2}$$

or

$$\frac{\delta^2}{4}\int_0^1(u_{xx}-v_{xx})^2\mathrm{d}x+\frac{3T_0}{4}\int_0^1(u_x-v_x)^2\mathrm{d}x+\int_0^1\left(\frac{\delta}{2}|u_{xx}-v_{xx}|-\frac{\sqrt{T_0}}{2}|u_x-v_x|\right)^2\mathrm{d}x+$$

$$\frac{\delta}{2}\int_0^1|u_{xx}-v_{xx}||u_x-v_x|\left(\sqrt{T_0}-\frac{\delta}{2}|u_x+v_x|\right)\mathrm{d}x\leqslant 8J_0C_2C_3e^{C_2}$$

By lemma 2, we conclude $\sqrt{T_0}-\frac{\delta}{2}|u_x+v_x|\geqslant 0$. For sufficiently small $J_0>0$, we obtain

$$\frac{\delta^2}{4}\int_0^1(u_{xx}-v_{xx})^2\mathrm{d}x+\frac{3T_0}{4}\int_0^1(u_x-v_x)^2\mathrm{d}x\leqslant 0$$

This implies $u-v=0$ in $H^2(0,1)$ and therefore in $(0,1)$.

4 Semiclassical Limit

In this section, we prove the following theorem, the proof of which is a consequence of the key estimate (6) and the compact embedding $H^1(0,1)$ into $L^\infty(0,1)$.

Theorem 3 Let u_δ be a solution to (4) and (5). u_δ denotes the δ-dependent of u. Then as $\delta\to 0$, maybe for a subsequence,

$$u_\delta\to u \text{ weakly in } H^1 \text{ and strongly in } L^\infty \tag{11}$$

and u is a weak solution of

$$T_0u_{xx}+J_0e^{-u}u_x=\lambda^{-2}(e^u-C) \tag{12}$$

subject to the boundary condition

$$u(0)=u(1)=0$$

Proof From lemma 1 and Sobolev embedding theorem, we obtain

$$\|u_\delta\|_{H^1(0,1)}\leqslant c$$

where c is a δ-independent constant. Therefore, we have a subsequence of u_δ (not relabeled), such that (11) holds. After integration by parts, the weak formulation of (4) reads

$$-\frac{\delta^2}{4}\int_0^1u_{\delta,x}\psi_{xx}\mathrm{d}x-\frac{\delta^2}{2}\int_0^1u_\delta\psi_{xxxx}\mathrm{d}x=T_0\int_0^1u_{\delta,x}\psi_x\mathrm{d}x-J_0\int_0^1e^{-u_\delta}u_{\delta,x}\psi\mathrm{d}x+\lambda^{-2}\int_0^1(e^{u_\delta}-C)\psi\mathrm{d}x$$

The convergences (11) allow us to pass to the limit $\delta\to 0$ in the above equation, observing that the left-hand side vanishes in the limit:

$$0=T_0\int_0^1u_x\psi_x\mathrm{d}x-J_0\int_0^1e^{-u}u_x\psi\mathrm{d}x+\lambda^{-2}\int_0^1(e^u-C)\psi\mathrm{d}x$$

This shows the weak form of (12) holds.

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一维半导体量子漂移-扩散方程的弱解

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摘要：研究了半导体器件中量子漂移-扩散模型（QDD）的一维稳态模型. 通过指数变量代换，把原问题转化成一个非线性四阶方程的边值问题，然后利用不动点定理的理论方法和先验估计的技巧，证明了问题弱解的存在性. 在此基础上，还证明了电流充分小的情形下该问题的解的惟一性和当 Planck 常数 $\delta\to 0$ 时，QDD 的解收敛于经典的漂移-扩散模型（DD）的解.

关键词：半导体器件；量子漂移-扩散方程；存在惟一性；指数函数代换；半古典极限

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