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ABSTRACT

The existence of weak solutions to the stationary quantum drift-diffusion equations for semiconductor devices is investigated. The proof is based on minimization procedure of non-linear functional and Schauder fixed-point theorem. Furthermore, the semiclassical limit $\varepsilon \rightarrow 0$ from the quantum drift-diffusion model to the classical drift-diffusion model is discussed.

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1. Introduction

Due to the ongoing miniaturization of electronic devices, mathematical models of ultra small semiconductors have to incorporate the quantum mechanical effects [1,2,6]. This paper is concerned with quantum drift-diffusion models. In Ref. [3], Jüngel and Pinnau have proved the existence of solution in one dimension, the proof is finished by introducing a positivity-preserving numerical scheme. Then the conclusion is extended to multi-dimensions in Ref. [4]. The solutions they have got are all strong solutions, but the assumptions they imposed are somewhat strict.

The scaled equations of the quantum drift-diffusion model read:

$$\begin{aligned} n_t - \nabla \cdot J &= 0, \\ n \nabla V + \nabla r(n) - \varepsilon^2 n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) &= J, \\ -\lambda^2 \Delta V &= n - C \end{aligned} \quad (1)$$

where $n(x, t)$ is the electron density, $J(x, t)$ the current density, and $V(x, t)$ the electrostatic potential. The dimensionless constants ε and λ are the scaled Planck constant and the scaled Debye length, respectively. The doping profile $C(x)$ models fixed background charges, $r(n)$ is the pressure function.

We assume $\Omega \subset \mathbb{R}^N$ ($N = 1, 2, 3$) is a bounded domain, and the boundary $\partial\Omega$ splits into two disjoint parts Γ_D and Γ_N , where Γ_D models the Ohmic contacts of the device and Γ_N represents the insulating parts of the boundary. Assuming $\partial\Omega \in C^{0,1}$, Γ_D has nonvanishing $(N-1)$ -dimensional Lebesgue measure. Let γ denote the unit outward normal vector along $\partial\Omega$.

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The objective of this paper is to analyze the stationary version

$$\begin{aligned} \nabla \cdot J &= 0, \quad J = n \nabla F, \\ F &= V + h(n) - \varepsilon^2 \frac{\Delta \sqrt{n}}{\sqrt{n}}, \\ -\lambda^2 \Delta V &= n - C \end{aligned} \quad (2)$$

subject to the boundary conditions

$$\begin{aligned} n &= n_D, \quad V = V_D, \quad F = F_D \quad \text{on } \Gamma_D, \\ \frac{\partial n}{\partial \gamma} &= \frac{\partial V}{\partial \gamma} = \frac{\partial F}{\partial \gamma} = 0 \quad \text{on } \Gamma_N. \end{aligned}$$

We shall make use of the following assumptions.

(A1) $n_D, V_D, F_D, C \in L^\infty(\Omega) \cap H^1(\Omega)$, $\inf n_D > 0$.

(A2) The enthalpy function $h(s)$ ($s \geq 0$) is strictly monotone increasing, locally Lipschitz continuous, and

$$\lim_{s \rightarrow 0^+} h(s) = -\infty, \quad \lim_{s \rightarrow +\infty} h(s) = +\infty.$$

We introduce a new variable $\rho = \sqrt{n}$, then from (2) we obtain

$$\begin{aligned} \nabla \cdot (\rho^2 \nabla F) &= 0, \\ \varepsilon^2 \Delta \rho &= \rho(V + h(\rho^2) - F), \\ -\lambda^2 \Delta V &= \rho^2 - C \end{aligned} \quad (3)$$

subject to the boundary conditions

$$\begin{aligned} \rho &= \rho_D, \quad V = V_D, \quad F = F_D \quad \text{on } \Gamma_D, \\ \frac{\partial \rho}{\partial \gamma} &= \frac{\partial V}{\partial \gamma} = \frac{\partial F}{\partial \gamma} = 0 \quad \text{on } \Gamma_N, \end{aligned} \quad (4)$$

where $\rho_D = \sqrt{n_D}$.

2. Preliminaries

Given $f \in L^2(\Omega)$, assume $\Phi \in L^\infty(\Omega) \cap H^1(\Omega)$ is the unique weak solution of

$$-\lambda^2 \Delta \Phi = f, \quad \Phi = 0 \quad \text{on } \Gamma_D, \quad \frac{\partial \Phi}{\partial \gamma} = 0 \quad \text{on } \Gamma_N.$$

Define $\tilde{\Phi}[f] = \Phi$, then $\tilde{\Phi}[\cdot]$ is a continuous linear mapping [7].

Let $\Phi_e \in L^\infty(\Omega) \cap H^1(\Omega)$ be the unique weak solution of

$$-\Delta \Phi_e = 0, \quad \Phi_e = V_D \quad \text{on } \Gamma_D, \quad \frac{\partial \Phi_e}{\partial \gamma} = 0 \quad \text{on } \Gamma_N.$$

Given $\rho \in L^2(\Omega)$, then $V = \tilde{\Phi}[\rho^2 - C] + \Phi_e$ is the unique weak solution of

$$-\lambda^2 \Delta V = \rho^2 - C, \quad V = V_D \quad \text{on } \Gamma_D, \quad \frac{\partial V}{\partial \gamma} = 0 \quad \text{on } \Gamma_N.$$

Let $B = \{f \in L^2(\Omega) \mid \inf F_D \leq f \leq \sup F_D\}$. Given $F \in B$, $\delta \in (0, \infty)$, for all $\rho \in L^2(\Omega)$, define

$$E_\delta(\rho) = \varepsilon^2 \int_\Omega |\nabla \rho|^2 dx + \int_\Omega H_\delta(\rho^2) dx + \frac{\lambda^2}{2} \int_\Omega |\nabla \tilde{\Phi}[\rho^2 - C]|^2 dx + \int_\Omega \rho^2 \Phi_e dx - \int_\Omega F \rho^2 dx,$$

where $H_\delta(s) = \int_1^s h_\delta(u) du$, $h_\delta(u) = \max\{h(u), h(\delta)\}$.

Assuming $\rho_c \in L^\infty(\Omega) \cap H^1(\Omega)$ and $\rho_c = \rho_D$ on Γ_D , we set $\mathcal{X} = \rho_c + H_0^1(\Omega)$.

Lemma 1. Given $F \in B$, if there exists a minimizer ρ_δ of $E_\delta(\rho)$ in \mathcal{X} , we set $V = \tilde{\Phi}[\rho^2 - C] + \Phi_e$. Then ρ_δ is a weak solution of

$$\varepsilon^2 \Delta \rho = \rho(V + h_\delta(\rho^2) - F), \quad \rho = \rho_D \quad \text{on } \Gamma_D, \quad \frac{\partial \rho}{\partial \nu} = 0 \quad \text{on } \Gamma_N.$$

Proof. For all $\varphi \in H_0^1(\Omega)$, $\rho \in \mathcal{X}$, $s \in \mathbb{R}$ satisfying $\rho + s\varphi \in \mathcal{X}$, it holds

$$\begin{aligned} E_\delta(\rho + s\varphi) - E_\delta(\rho) &= \varepsilon^2 \left(\int_{\Omega} |\nabla \rho + s \nabla \varphi|^2 dx - \int_{\Omega} |\nabla \rho|^2 dx \right) + \int_{\Omega} (H_\delta((\rho + s\varphi)^2) - H_\delta(\rho^2)) dx \\ &\quad + \frac{\lambda^2}{2} \int_{\Omega} (|\nabla \tilde{\Phi}[(\rho + s\varphi)^2 - C]|^2 - |\nabla \tilde{\Phi}[\rho^2 - C]|^2) dx \\ &\quad + \left(\int_{\Omega} (\rho + s\varphi)^2 \Phi_e dx - \int_{\Omega} \rho^2 \Phi_e dx \right) + \left(\int_{\Omega} F(\rho + s\varphi)^2 dx - \int_{\Omega} F\rho^2 dx \right) \\ &= I_1 + I_2 + I_3 + I_4 + I_5. \end{aligned}$$

According to mean value theorem of integral, we obtain

$$I_2 = \int_{\Omega} \left(\int_{\rho^2}^{(\rho+s\varphi)^2} h_\delta(u) du \right) dx = \int_{\Omega} 2\rho s\varphi h_\delta(\rho^2) dx + o(s).$$

By integration by parts and the linear property of $\tilde{\Phi}[\cdot]$, we get

$$\begin{aligned} I_3 &= \frac{\lambda^2}{2} \int_{\Omega} \tilde{\Phi}[(\rho + s\varphi)^2 - C] \frac{(\rho + s\varphi)^2 - C}{\lambda^2} dx - \frac{\lambda^2}{2} \int_{\Omega} \tilde{\Phi}[\rho^2 - C] \frac{\rho^2 - C}{\lambda^2} dx \\ &= \frac{\lambda^2}{2} \int_{\Omega} \tilde{\Phi}[(\rho + s\varphi)^2 - C] \left(\frac{(\rho + s\varphi)^2 - C}{\lambda^2} - \frac{\rho^2 - C}{\lambda^2} \right) dx + \frac{\lambda^2}{2} \int_{\Omega} \tilde{\Phi}[2\rho s\varphi + s^2\varphi^2] \frac{\rho^2 - C}{\lambda^2} dx \\ &= \frac{\lambda^2}{2} \left(\int_{\Omega} \tilde{\Phi}[\rho^2 - C] \frac{2\rho s\varphi}{\lambda^2} dx + o(s) \right) + \frac{\lambda^2}{2} \int_{\Omega} \tilde{\Phi}[\rho^2 - C] \frac{2\rho s\varphi + s^2\varphi^2}{\lambda^2} dx \\ &= \frac{\lambda^2}{2} \left(\frac{4}{\lambda^2} \int_{\Omega} \tilde{\Phi}[\rho^2 - C] \rho s\varphi dx + o(s) \right) \\ &= 2 \int_{\Omega} \tilde{\Phi}[\rho^2 - C] \rho s\varphi dx + o(s). \end{aligned}$$

By simply calculating, we get

$$I_1 = \varepsilon^2 \int_{\Omega} 2\nabla \rho \cdot s \nabla \varphi dx + o(s), \quad I_4 = \int_{\Omega} 2\rho s\varphi \Phi_e dx + o(s), \quad I_5 = \int_{\Omega} 2\rho s\varphi F dx + o(s).$$

To sum up, we obtain

$$E_\delta(\rho + s\varphi) - E_\delta(\rho) = 2 \left(\int_{\Omega} \varepsilon^2 \nabla \rho \cdot s \nabla \varphi dx + \int_{\Omega} \rho(h_\delta + V - F)s\varphi dx \right) + o(s).$$

If ρ_δ is a minimizer of $E_\delta(\rho)$ in \mathcal{X} , then as $s \rightarrow 0$,

$$E_\delta(\rho_\delta + s\varphi) - E_\delta(\rho_\delta) = 2 \left(\int_{\Omega} \varepsilon^2 \nabla \rho_\delta \cdot s \nabla \varphi dx + \int_{\Omega} \rho_\delta(h_\delta + V - F)s\varphi dx \right) + o(s) \geq 0.$$

Let $s \rightarrow 0^+$ and $s \rightarrow 0^-$, respectively. Then

$$\int_{\Omega} \varepsilon^2 \nabla \rho_\delta \cdot \nabla \varphi dx + \int_{\Omega} \rho_\delta(h_\delta + V - F)\varphi dx = 0. \quad \square$$

Lemma 2 (Pseudo-convexity inequality). For all $s \in (0, 1)$, $\rho_1, \rho_2 \in L^2(\Omega)$ and $|\rho_1| \neq |\rho_2|$, one has

$$E_\delta(\sqrt{s\rho_1^2 + (1-s)\rho_2^2}) < sE_\delta(\rho_1) + (1-s)E_\delta(\rho_2).$$

Proof. Set $\rho = \sqrt{s\rho_1^2 + (1-s)\rho_2^2}$, then

$$\begin{aligned} \nabla \rho &= \frac{s\rho_1 \nabla \rho_1 + (1-s)\rho_2 \nabla \rho_2}{\rho}, \\ s|\nabla \rho_1|^2 + (1-s)|\nabla \rho_2|^2 - \left| \frac{s\rho_1}{\rho} \nabla \rho_1 + \frac{(1-s)\rho_2}{\rho} \nabla \rho_2 \right|^2 \\ &= \frac{s(1-s)\rho_2^2}{\rho^2} |\nabla \rho_1|^2 + \frac{s(1-s)\rho_1^2}{\rho^2} |\nabla \rho_2|^2 - 2s(1-s) \frac{\rho_1 \rho_2}{\rho^2} \nabla \rho_1 \cdot \nabla \rho_2 \\ &= s(1-s) \left| \frac{\rho_2}{\rho} \nabla \rho_1 - \frac{\rho_1}{\rho} \nabla \rho_2 \right|^2 \geq 0. \end{aligned}$$

So we get

$$|\nabla \rho|^2 \leq s|\nabla \rho_1|^2 + (1-s)|\nabla \rho_2|^2.$$

Next, we prove that for all $x_0 \in \Omega$, $H_\delta(\rho^2(x_0)) < H_\delta(\rho_1^2(x_0)) + H_\delta(\rho_2^2(x_0))$.

We just need to prove

$$\int_1^{\rho^2(x_0)} h_\delta(u) \, du \leq s \int_1^{\rho_1^2(x_0)} h_\delta(u) \, du + (1-s) \int_1^{\rho_2^2(x_0)} h_\delta(u) \, du$$

or

$$\int_{\rho_1^2(x_0)}^{\rho^2(x_0)} h_\delta(u) \, du \leq (1-s) \int_{\rho_1^2(x_0)}^{\rho_2^2(x_0)} h_\delta(u) \, du.$$

There is no loss in generality in assuming that $\rho_1(x_0) < \rho_2(x_0)$. According to the mean value theorem, there exist $\xi_1 \in (\rho_1^2(x_0), \rho^2(x_0))$, $\xi_2 \in (\rho^2(x_0), \rho_2^2(x_0))$ satisfying

$$\begin{aligned} (1-s) \int_{\rho_1^2(x_0)}^{\rho_2^2(x_0)} h_\delta(u) \, du &= (1-s)(\rho^2(x_0) - \rho_1^2(x_0))h_\delta(\xi_1) + (1-s)(\rho_2^2(x_0) - \rho^2(x_0))h_\delta(\xi_2) \\ &\geq (1-s)(\rho_2^2(x_0) - \rho_1^2(x_0))h_\delta(\xi_1) \\ &= (\rho^2(x_0) - \rho_1^2(x_0))h_\delta(\xi_1) \\ &= \int_{\rho_1^2(x_0)}^{\rho^2(x_0)} h_\delta(u) \, du. \end{aligned}$$

Then from $|\rho_1| \neq |\rho_2|$, we get $H_\delta(\rho^2(x_0)) < H_\delta(\rho_1^2(x_0)) + H_\delta(\rho_2^2(x_0))$.

According to the linear property of $\tilde{\Phi}[\cdot]$, we obtain

$$\nabla \tilde{\Phi}[\rho^2 - C] = s\nabla \tilde{\Phi}[\rho_1^2 - C] + (1-s)\nabla \tilde{\Phi}[\rho_2^2 - C].$$

So we conclude

$$s|\nabla \tilde{\Phi}[\rho_1^2 - C]|^2 + (1-s)|\nabla \tilde{\Phi}[\rho_2^2 - C]|^2 - |\nabla \tilde{\Phi}[\rho^2 - C]|^2 = s(1-s)|\nabla \tilde{\Phi}[\rho_1^2 - C] - \nabla \tilde{\Phi}[\rho_2^2 - C]|^2 \geq 0. \quad \square$$

Lemma 3. Given $F \in B$, there exists a unique nonnegative minimizer of $E_\delta(\rho)$ in \mathcal{X} .

Proof. From $\lim_{u \rightarrow \infty} h_\delta(u) = \infty$, we know that the functional E_δ is coercive with respect to the $L^2(\Omega)$ norm. \mathcal{X} is a translate of a Hilbert space, thus the existence of minimizers of $E_\delta(\rho)$ follows from the $H^1(\Omega)$ -weakly sequentially lower semicontinuity of $E_\delta(\rho)$ (which is easy to see).

By the using of Lemma 2, we get that when $|\rho_1| \neq |\rho_2|$, one has

$$E_\delta\left(\sqrt{\frac{1}{2}\rho_1^2 + \frac{1}{2}\rho_2^2}\right) < \frac{1}{2}E_\delta(\rho_1) + \frac{1}{2}E_\delta(\rho_2).$$

So we obtain the uniqueness of the nonnegative minimizer.

Due to the above analysis, we obtain that given $F \in L^\infty(\Omega)$, $\delta \in (0, \infty)$, there exists a unique solution (V_δ, ρ_δ) satisfying $V_\delta \in L^\infty(\Omega) \cap H^1(\Omega)$, $\rho_\delta \in H^1(\Omega)$, and the equations

$$\varepsilon^2 \Delta \rho = \rho(V + h_\delta(\rho^2) - F), \quad -\lambda^2 \Delta V = \rho^2 - C, \quad (5)$$

with the boundary condition

$$\rho = \rho_D, \quad V = V_D \quad \text{on } \Gamma_D, \quad \frac{\partial \rho}{\partial \gamma} = \frac{\partial V}{\partial \gamma} = 0 \quad \text{on } \Gamma_N. \quad \square \quad (6)$$

Lemma 4. Let (A1), (A2) hold. Given $F \in L^\infty(\Omega)$, then there exists $\delta_0 > 0$ such that, for all $\delta \in (0, \delta_0)$, there exists a unique solution (V_δ, ρ_δ) to (5)–(6), which satisfies $V_\delta \in L^\infty(\Omega) \cap H^1(\Omega)$, $\rho_\delta \in H^1(\Omega)$, $\rho_\delta > c$, $c > 0$ is independent of δ .

Proof. Assuming $h(s_0) = 0$, we obtain from the monotonicity of the enthalpy function, that for all $\delta \in (0, s_0)$, one has

$$\int_{s_0}^{\rho^2} h_\delta(u) \, du \geq 0.$$

So we get

$$H_\delta(\rho^2) = \int_1^{\rho^2} h_\delta(u) \, du \geq \int_1^{s_0} h_\delta(u) \, du \geq (s_0 - 1)h_\delta(1) \geq (s_0 - 1)h(1).$$

Then from the definition of $E_\delta(\rho)$, we know E_δ is bounded from below uniformly for δ in \mathcal{X} . So $\|\rho_\delta\|_{H^1(\Omega)} \leq c_1$, with $c_1 > 0$ independent of δ .

From the second equation of (5), we get $\|V_\delta\|_{L^\infty(\Omega)} \leq c_2$, and $c_2 > 0$ is independent of δ .

Using $(\rho_\delta - c)^- = \min\{0, \rho_\delta - c\}$ as a test function for the first equation of (5) for $0 < c \leq \inf \rho_D$, we get

$$\varepsilon^2 \int_{\Omega} |\nabla(\rho_\delta - c)^-|^2 \, dx = \int_{\Omega} \rho_\delta (V_\delta + h_\delta(\rho_\delta^2) - F)(-(\rho_\delta - c)^-) \, dx \leq \int_{\Omega} \rho_\delta (V_\delta + h_\delta(c^2) - F)(-(\rho_\delta - c)^-) \, dx.$$

From $\lim_{s \rightarrow 0^+} h(s) = -\infty$, we get that there exists $(c, \bar{\delta})$, with $c > 0$, $\bar{\delta} > 0$, such that for $0 < \delta \leq \bar{\delta}$, one has

$$\varepsilon^2 \int_{\Omega} |\nabla(\rho_\delta - c)^-|^2 \, dx \leq 0.$$

Hence $\rho_\delta \geq c$ when $0 < \delta \leq \bar{\delta}$. Set $\delta_0 = \min\{\bar{\delta}, c^2\}$. Then when $\delta < \delta_0$, it holds $h(\rho_\delta^2) \geq h(\delta)$. This gives $h_\delta(\rho_\delta^2) = h(\rho_\delta^2)$. \square

Lemma 4 immediately implies the following lemma.

Lemma 5. Let (A1), (A2) hold, given $F \in L^\infty(\Omega)$, there exists a unique solution (V, ρ) , with $V \in L^\infty(\Omega) \cap H^1(\Omega)$, $\rho \in H^1(\Omega)$, to the equations

$$\varepsilon^2 \Delta \rho = \rho(V + h(\rho^2) - F), \quad -\lambda^2 \Delta V = \rho^2 - C, \quad (7)$$

with the boundary conditions

$$\rho = \rho_D, \quad V = V_D \quad \text{on } \Gamma_D, \quad \frac{\partial \rho}{\partial \gamma} = \frac{\partial V}{\partial \gamma} = 0 \quad \text{on } \Gamma_N.$$

Lemma 6. Let ρ be the solution in Lemma 5. Then $\rho \in L^\infty(\Omega)$.

Proof. We just need to prove ρ is bounded from above.

Using $(\rho - a)^+ = \max\{0, \rho - a\}$, for some $a \geq \sup_{\Gamma_D} \rho_D > 0$ to be determined, as a test function in the first equation of (7), we get

$$\varepsilon^2 \int_{\Omega} |\nabla(\rho - a)^+|^2 dx = \int_{\Omega} \rho(F - V - h(\rho^2))(\rho - a)^+ dx.$$

Following from $\lim_{s \rightarrow +\infty} h(s) = +\infty$, we know that there exists a positive constant $a \geq \sup_{\Gamma_D} \rho_D$ such that when $\rho > a$, one has $F - V - h(\rho^2) < 0$. Hence we get

$$\varepsilon^2 \int_{\Omega} |\nabla(\rho - a)^+|^2 dx \leq 0.$$

This gives $\rho \leq a$. \square

3. Existence of weak solutions

Theorem 1. Let (A1), (A2) hold. Then there exists a solution $(\rho, V, F) \in L^\infty(\Omega) \cap H^1(\Omega)$ to (3)–(4).

Proof. We set $F = f \in B$ in the second equation of (3) to get

$$\begin{aligned} \nabla \cdot (\rho^2 \nabla F) &= 0, \\ \varepsilon^2 \Delta \rho &= \rho(V + h(\rho^2) - f), \\ -\lambda^2 \Delta V &= \rho^2 - C. \end{aligned} \quad (8)$$

By Lemmas 5, 6, there exists a unique solution $(\rho, V, F) \in (L^\infty(\Omega) \cap H^1(\Omega))^3$ of (8) satisfying the boundary condition

$$\begin{aligned} \rho &= \rho_D, \quad V = V_D, \quad F = F_D \quad \text{on } \Gamma_D, \\ \frac{\partial \rho}{\partial \gamma} &= \frac{\partial V}{\partial \gamma} = \frac{\partial F}{\partial \gamma} = 0 \quad \text{on } \Gamma_N. \end{aligned} \quad (9)$$

Using the maximum principle we get

$$\inf F_D \leq F \leq \sup F_D.$$

Hence $F \in B$.

Thus the mapping $T : B \rightarrow B$, $T(f) = F$, is well defined. Moreover, it is not difficult to check that T is compact, noting the compact embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$. Next we prove T is continuous.

Assume $f_n \in B$ is convergent to f as $n \rightarrow \infty$ in $L^2(\Omega)$, $(\rho, V, F) \in (L^\infty(\Omega) \cap H^1(\Omega))^3$ is a solution to (8)–(9), and $(\rho^{(n)}, V^{(n)}, F^{(n)}) \in (L^\infty(\Omega) \cap H^1(\Omega))^3$ is a solution to (8)–(9) in which we have substituted f_n for f .

Replace F with f_n in the definition of $E_\delta(\rho)$ and define it as $E_\delta^{(n)}(\rho)$. It is not difficult to conclude

$$\lim_{n \rightarrow \infty} E_\delta^{(n)}(\rho) = E_\delta(\rho).$$

Thus one has

$$\lim_{n \rightarrow \infty} \inf_{\rho \in \mathcal{X}} E_\delta^{(n)}(\rho) = \inf_{\rho \in \mathcal{X}} E_\delta(\rho).$$

$E_\delta(\rho)$ is continuous, so we get from Lemma 3

$$\lim_{n \rightarrow \infty} \|\rho^{(n)} - \rho\| = 0.$$

From the first equation of (8) we obtain

$$\lim_{n \rightarrow \infty} \|F^{(n)} - F\| = 0.$$

Hence T is continuous.

Finally we can finish the proof by Schauder fixed-point theorem. \square

4. Semiclassical limit

We analyze the semiclassical limit in the isothermal condition. The isothermal quantum drift-diffusion equations read:

$$\begin{aligned}\nabla \cdot (\rho_\varepsilon^2 \nabla F_\varepsilon) &= 0, \\ \varepsilon^2 \Delta \rho_\varepsilon &= \rho_\varepsilon (V_\varepsilon + \ln(\rho_\varepsilon^2) - F_\varepsilon), \\ -\lambda^2 \Delta V_\varepsilon &= \rho_\varepsilon^2 - C\end{aligned}\tag{10}$$

with the boundary condition

$$\begin{aligned}\rho_\varepsilon &= \sqrt{n_D^\varepsilon}, \quad V_\varepsilon = V_D^\varepsilon, \quad F_\varepsilon = F_D^\varepsilon \quad \text{on } \Gamma_D, \\ \frac{\partial \rho_\varepsilon}{\partial \gamma} &= \frac{\partial V_\varepsilon}{\partial \gamma} = \frac{\partial F_\varepsilon}{\partial \gamma} = 0 \quad \text{on } \Gamma_N.\end{aligned}\tag{11}$$

We impose the following assumptions.

(A3) $n_D^\varepsilon, V_D^\varepsilon, F_D^\varepsilon \in L^\infty(\Omega) \cap H^1(\Omega)$, and there exists a $K > 0$ such that $n_D^\varepsilon \geq K$ for all $\varepsilon > 0$. F_D^ε is uniformly bounded.

(A4) $n_D^\varepsilon \rightarrow n_D, V_D^\varepsilon \rightarrow V_D, F_D^\varepsilon \rightarrow F_D$ in $H^1(\Omega)$ as $\varepsilon \rightarrow 0$.

Theorem 2. Let (A1)–(A4) hold, then there exist functions $n, F, V \in L^\infty(\Omega) \cap H^1(\Omega)$ satisfying

$$\nabla \cdot (n \nabla F) = 0, \quad F = V + \ln(n), \quad -\lambda^2 \Delta V = n - C,\tag{12}$$

subject to the boundary condition

$$\begin{aligned}n &= n_D, \quad V = V_D, \quad F = F_D \quad \text{on } \Gamma_D, \\ \frac{\partial n}{\partial \gamma} &= \frac{\partial V}{\partial \gamma} = \frac{\partial F}{\partial \gamma} = 0 \quad \text{on } \Gamma_N.\end{aligned}\tag{13}$$

Assuming $\rho_\varepsilon, F_\varepsilon, V_\varepsilon \in L^\infty(\Omega) \cap H^1(\Omega)$ solve (10)–(11), then there exists a subsequence of $(\rho_\varepsilon, F_\varepsilon, V_\varepsilon)$ (not relabeled) such that

$$\rho_\varepsilon^2 \rightarrow n, \quad F_\varepsilon \rightarrow F, \quad V_\varepsilon \rightarrow V \quad \text{weakly in } H^1(\Omega), \text{ strongly in } L^2(\Omega) \text{ as } \varepsilon \rightarrow 0.$$

Proof. Set $H(s) = \int_1^s \ln(u) du$, and define

$$\begin{aligned}I(n) &\triangleq \int_\Omega H(n) dx + \frac{\lambda^2}{2} \int_\Omega |\nabla \tilde{\Phi}[n - C]|^2 dx + \int_\Omega n \tilde{\Phi}_e dx - \int_\Omega F n dx, \\ E^\varepsilon(\rho) &\triangleq \varepsilon^2 \int_\Omega |\nabla \tilde{\rho}|^2 dx + \int_\Omega H(\rho^2) dx + \frac{\lambda^2}{2} \int_\Omega |\nabla \tilde{\Phi}[\rho^2 - C]|^2 dx + \int_\Omega \rho^2 \Phi_e dx - \int_\Omega F_\varepsilon \rho^2 dx.\end{aligned}$$

Similarly as in Section 3, we can prove that there exist functions $n, F, V \in L^\infty(\Omega) \cap H^1(\Omega)$ satisfying (12)–(13), where n is also the unique minimizer of $I(n)$ in \mathcal{X} . Furthermore, ρ_ε is the unique minimizer of $E^\varepsilon(\rho)$ in $\mathcal{Y} \triangleq \rho_D + H_0^1(\Omega)$.

By using maximum principle, we obtain from (A3) that F_ε is bounded uniformly for ε . This yields a uniform bound on $E^\varepsilon(\rho)$. Hence we get the uniform bound on ρ_ε . From the third equation of (10) we get the uniform bound on V_ε . So there exists a subsequence of $(\rho_\varepsilon, F_\varepsilon, V_\varepsilon)$ (not relabeled) such that

$$\rho_\varepsilon^2 \rightarrow n^*, \quad F_\varepsilon \rightarrow F^*, \quad V_\varepsilon \rightarrow V^* \quad \text{weakly in } H^1(\Omega), \text{ strongly in } L^2(\Omega)$$

as $\varepsilon \rightarrow 0$.

From $\sqrt{n^*} \in \mathcal{Y}$ we obtain $\lim_{\varepsilon \rightarrow 0} \sup E^\varepsilon(\rho_\varepsilon) \leq \lim_{\varepsilon \rightarrow 0} \sup E^\varepsilon(\sqrt{n^*})$. Hence $\lim_{\varepsilon \rightarrow 0} \sup E^\varepsilon(\rho_\varepsilon) \leq I(n^*)$,

$$E^\varepsilon(\rho_\varepsilon) = I(\rho_\varepsilon^2) + \varepsilon^2 \int_\Omega |\nabla \rho_\varepsilon|^2 dx + \int_\Omega (F - F_\varepsilon) \rho_\varepsilon^2 dx.$$

Then by the weakly lower semicontinuity of $I(n)$ (which is easy to see) we get

$$\liminf_{\varepsilon \rightarrow 0} E^\varepsilon(\rho_\varepsilon) \geq I(n).$$

So $I(n^*) \geq I(n)$. n^* is the unique minimizer of $I(n)$, hence $I(n) = I(n^*)$, $n = n^*$.

Then it's not difficult to prove $F = F^*, V = V^*$. \square

5. Conclusions

By the employing of the non-linear functional

$$E_\delta(\rho) = \varepsilon^2 \int_{\Omega} |\nabla \rho|^2 dx + \int_{\Omega} H_\delta(\rho^2) dx + \frac{\lambda^2}{2} \int_{\Omega} |\nabla \Phi[\rho^2 - C]|^2 dx + \int_{\Omega} \rho^2 \Phi_e dx - \int_{\Omega} F \rho^2 dx,$$

we obtain the relations between its unique nonnegative minimizer and the weak solution to the stationary quantum drift-diffusion equations. Note the means we employ to remove the variable δ . Then the existence of weak solutions is proved by the Schauder fixed point theorem. This method works well for the stationary problem, but not for the transient equations. Therefore, seeking a new method for the transient quantum drift-diffusion equations will be our next work. Moreover, latest studies of quantum semiconductor models are all related to two kinds of particles, namely electrons and holes [5]. So we need to transfer our work focus to bipolar models in future.

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