

http://www.aimspress.com/journal/mine

Research article

Stationary solutions to a hybrid viscous hydrodynamic model with classical boundaries †

Federica Di Michele^{1,*,§}, Bruno Rubino², Rosella Sampalmieri² and Kateryna Stiepanova³

¹ Istituto Nazionale di Geofisica e Vulcanologia, via Alfonso Corti 12, Milan, Italy

- ² Department of Information Engineering, Computer Science and Mathematics, University of L'Aquila via Vetoio, L'Aquila, Italy
- ³ V. N. Karazin Kharkiv National University, Kharkiv, Ukraine
- [†] This contribution is part of the Special Issue: Math aspects of classical and quantum fluid dynamics
 Guest Editors: Paolo Antonelli; Luigi Forcella
 Link: www.aimspress.com/mine/article/6556/special-articles
- * Correspondence: Email: federica.dimichele@ingv.it.

Abstract: In this paper we present a quantum-classical hybrid model based on the hydrodynamic equations in steady state form. The approach presented here, which has already been proposed in previous works, consists in considering an intrinsically hybrid version of the Bohm potential, which acts only in the region of the domain where quantum effects play an important role, while it disappears where the quantum contribution is essentially negligible and the operation of the device can be well described by using a classical model. Compared to previous results from the same line of research, here we assume that the device at the boundaries of the domain behaves classically, while quantum effects are localised in the central part of it. This is the case of greatest scientific interest, since, in real devices, quantum effects are generally localized in a small area within the device itself. The well posedness of the problem is ensured by adding a viscous term necessary for the convergence of the hybrid limit to an appropriate weak solution. Some numerical tests are also performed for different values of the viscous coefficient, in order to evaluate the effects of the viscosity, especially on the boundaries of the device.

Keywords: hybrid model; quantum models; hydrodynamic; viscous terms; quantum devices

Mathematics in Engineering, 6(5): 705–725. DOI:10.3934/mine.2024027 Received: 24 April 2024 Revised: 13 August 2024 Accepted: 26 August 2024 Published: 12 September 2024

[§]Past affiliation: Gran Sasso Science Institute (GSSI), via M. Iacobucci 2, L'Aquila, Italy

1. Introduction

Many modern semiconductor devices base their operation on quantum phenomena. These effects, often difficult to describe from a mathematical point of view, are localized only in a specific region of the device, therefore, it seems reasonable to use a hybrid approach, which involves the use of both quantum [1, 2, 8, 20, 31] and classical models [10, 21, 23, 24, 28–30]. Several interesting results are available in the literature, starting from the pioneering work by N. Ben Abdallah [4], where a set of physically reasonable conditions is prescribed at the interface between classical and quantum domains to link the Boltzmann equation and the stationary Schrödinger equations. A similar approach has been employed in [3, 5, 7, 11, 12, 17, 25, 32]. The interface conditions used in these works are somewhat arbitrary since there are no direct measurements of the physical variables on the surface between classical and quantum domains. Furthermore, the transition between the classical and the quantum system does not take place abruptly in a precise section of the device but rather, there is a transition zone where the system behaves in a *semi-classical* way. Following this idea, in [9, 13] an alternative approach was proposed for the first time. A smooth quantum function Q(x) which multiplies the Bohm potential is introduced and it drives the classical system to become quantum and vice versa. Namely Q(x) = 0 in the classical part and Q(x) = 1 in the quantum one, but physically reasonable transition regions, where 0 < Q(x) < 1, are also included. In this way, no artificial interface condition are required, and the model naturally evolves from the classical to the quantum regimes [14–16, 18].

Unfortunately, the term Q(x) adds some difficulties, especially in the treatment of the boundaries of the device. In our previous works in this line, to allow the existence of the weak hybrid solution, we necessarily had to consider boundary conditions in the quantum domain. Indeed, considering only quantum boundaries is the main limitation of the original model since the boundaries usually act as Ohmic contacts and they are well described by classical equations. To overcome this problem, here we introduce a suitable viscous term that regularizes the equations allowing us to consider classical boundaries. A similar viscosity has been employed by [19] to prove the existence of a solution to the quantum hydrodynamic model (QHD) for any positive values of the current density J.

In more detail, the aim of this paper is to study the existence of steady-state weak solutions to the following visco-hybrid quantum hydrodynamical equation (VH-QHD):

$$\begin{cases} 2\varepsilon^2 \left(Q \frac{(\sqrt{n})_{xx}}{\sqrt{n}} + Q' \frac{(\sqrt{n})_x}{\sqrt{n}} \right)_x - \left(T \ln n + \frac{J^2}{2n^2} \right)_x + V_x = \frac{J}{\tau n} + \nu (\sqrt{n})_{xx}, \\ J = constant, \end{cases}$$
(1.1)

for $x \in \Omega = [0, 1]$ and $t \ge 0$.

In the system above *n* is a strictly positive function modelling the electron density, $Q: \Omega \rightarrow [0, 1]$ is a regular function as introduced in [9, 13]. In more detail the function Q(x) is such that Q = 0 in the (classical) outer part of the device and Q > 0 in the central part, where the quantum effect normally occurs.

The system (1.1) must be coupled with another equation, named the Poisson equation, which describes the behavior of the self-consistent electrical potential V:

$$\lambda^2 V_{xx} = n - C. \tag{1.2}$$

Mathematics in Engineering

In (1.1) and (1.2) several positive scaled constants appear: τ , λ , ν , and T; they represent the relaxation time, the Debye length, the viscosity coefficient, and the temperature, respectively. Finally $0 < \varepsilon << 1$ is the scaled Plank's constant. The function C(x) assigns the distribution of the fixed charge background of ions, that is the doping profile. Here we assume that *C* is non-negative and in $C^0(\Omega)$.

The following boundary conditions for the stationary problem (1.1)-(1.2) are quite standard and have been already employed in many papers such as [13, 16, 22]; we have

$$contact \ boundary: \ n(0) = n(1) = 1, \tag{1.3}$$

insulation boundary :
$$n_x(0) = n_x(1) = 0,$$
 (1.4)

and

electric potential condition : $V(0) = V_0, J = J_0$ (1.5)

where

$$V_0 = -2\varepsilon^2 Q(0)(\sqrt{n})_{xx}(0) + \frac{J^2}{2}.$$
(1.6)

Integrating $(1.1)_1$, from (1.5) and (1.6), it follows that

$$V(x) = -2\varepsilon^2 Q \frac{(\sqrt{n})_{xx}}{\sqrt{n}} - 2\varepsilon^2 Q' \frac{(\sqrt{n})_x}{\sqrt{n}} + \frac{J^2}{2n^2} + T \ln n - \frac{J}{\tau} \int_0^x \frac{1}{n} dx + \nu(\sqrt{n})_x, \quad (1.7)$$

and, in view of the above boundary conditions (1.3)–(1.5), we have

$$V(1) = -2\varepsilon^2 Q(1)(\sqrt{n})_{xx}(1) + \frac{J^2}{2} - \frac{J}{\tau} \int_0^1 \frac{1}{n} dx.$$
 (1.8)

We just point out that in the BVP above the condition $J = J_0$ replaces one of the two boundary conditions on the electric potential V, which are necessary to solve the Poisson equation. The equivalence between the two conditions is proved in [22].

The subject of this paper is therefore the following boundary problem associated with the steadystate VH-QHD model (1.1)-(1.2):

$$\begin{cases} 2\varepsilon^2 \left(\frac{Q(\sqrt{n})_{xx}}{\sqrt{n}} + \frac{Q'(\sqrt{n})_x}{\sqrt{n}}\right)_x - \left(T\ln n + \frac{J^2}{2n^2}\right)_x + V_x = \frac{J}{\tau n} + \nu(\sqrt{n})_{xx}, \\ \lambda^2 V_{xx} = n - C, \\ n(0) = n(1) = 1, \ n_x(0) = n_x(1) = 0, \ V(0) = V_0, \ J = J_0. \end{cases}$$
(1.9)

Here is the outline of the paper: In Section 2, in order to simplify the reading of the article, we state the main theorems that will be proved in the following sections. In Section 3 we study the approximating problem obtained from (1.9) assuming $Q(x) \ge q > 0$, for a given positive constant q. Then, in Section 4, the limit $q \rightarrow 0$ is considered. Finally, in Section 5, some simple numerical experiments are performed to analyze the effect of the viscosity on the classical boundaries.

2. Main results

The main results of the paper will be presented in this section. We are looking for a solution to the visco-hybrid QHD (1.9) assuming with Q = 0 close to the boundaries and Q > 0 in the central part of the domain.

We remark that both the quantum function and the doping profile are assumed to be continuous functions.

We focus on the following fourth-order boundary value problem (BVP)

$$\begin{cases} 2\varepsilon^{2} \left(Q \frac{(\sqrt{n})_{xx}}{\sqrt{n}} + Q' \frac{(\sqrt{n})_{x}}{\sqrt{n}} \right)_{xx} - \left(\left(\frac{T}{n} - \frac{J^{2}}{n^{3}} \right) n_{x} \right)_{x} + \frac{1}{\lambda^{2}} (n - C) = -\frac{J}{\tau n^{2}} n_{x} + \nu (\sqrt{n})_{xxx}, \\ \lambda^{2} V_{xx} = n - C, \\ n(0) = n(1) = 1, \ n_{x}(0) = n_{x}(1) = 0, \ V(0) = V_{0}, \ J = J_{0}, \end{cases}$$
(2.1)

obtained differentiating $(1.9)_1$ in view of the Poisson equation (1.2).

In order to prove the existence of the solution to the system above we need to assume that the flow is subsonic, since this condition guarantees the uniform ellipticity of the problem, that is

velocity of the flow :=
$$\frac{|J|}{n} < \sqrt{p'(n)} = \sqrt{T}$$
 =: sound speed, (2.2)

and then

$$n > \frac{|J_0|}{\sqrt{T}} =: n_{\star}.$$
 (2.3)

Remark 2.1. Similarly, on the boundary of the domain and for the doping profile C(x), we must have

$$n(0) = n(1) = 1 > \frac{|J_0|}{\sqrt{T}},$$
(2.4)

$$C_0 := \min_{x \in [0,1]} C(x) > n_\star = \frac{|J_0|}{\sqrt{T}}.$$
(2.5)

The 3rd order elliptic equation (2.1) is degenerate close to the boundaries where the quantum effects disappear. To overcome this technical difficulty we prove the existence of solutions for a regularized problem obtained assuming $Q = Q_q$ in (2.1), where $0 < q \le Q_q \le 1$. As a consequence, we obtain a sequence of smooth functions $\{Q_q\}, q \in \mathbb{R}_+$, and require that this sequence satisfies the following set of conditions:

$$\begin{cases} Q_q \to Q, \quad Q'_q \to Q' \quad \text{uniformly in } \Omega, \quad \text{for } q \to 0, \\ \|Q'_q\|_{L^2} \le \bar{K}, \text{ uniformly in } q, \\ \varepsilon^2 |Q'_q|^2 < Q_q \left(T - \frac{J^2}{\underline{n}^2}\right) \text{ for all } x \in [0, 1] \text{ and for all } q \in \mathbb{R}_+, \end{cases}$$

$$(2.6)$$

where $\underline{n} := \min\{1, C_0\} > n_{\star}$ and n_{\star} as in (2.3). Now we consider the following modified visco-hybrid QHD equations (VH-Q_qHD) where we set $w_q = \sqrt{n_q}$ and replace Q(x) by $Q_q(x)$. We will look for

Mathematics in Engineering

 $(w_q, V_q)(x)$, as solutions to the following VH-Q_qHD system:

$$\begin{cases} 2\varepsilon^{2} \left(Q_{q} \frac{(w_{q})_{xx}}{w_{q}} + Q_{q}' \frac{(w_{q})_{x}}{w_{q}} \right)_{xx} - 2 \left(\left(T - \frac{J^{2}}{w_{q}^{4}} \right) \frac{(w_{q})_{x}}{w_{q}} \right)_{x} + \frac{1}{\lambda^{2}} (w_{q}^{2} - C) = -\frac{2J}{\tau w_{q}^{3}} (w_{q})_{x} + \nu (w_{q})_{xxx}, \\ \lambda^{2} (V_{q})_{xx} = w_{q}^{2} - C, \\ w_{q}(0) = w_{q}(1) = 1, \ (w_{q})_{x}(0) = (w_{q})_{x}(1) = 0, \ V_{q}(0) = V_{0}, \ J = J_{0}. \end{cases}$$

$$(2.7)$$

As in [13], we start by proving the following theorem to asses the existence of solutions to (2.7).

Theorem 2.2 (Existence of VH-Q_qHD solution). Assume (2.4) and (2.5) are fulfilled, that $Q_q(x)$ is a non-negative, bounded smooth function on $\Omega = [0, 1]$ such that

$$0 < q \le Q_q \le 1, \quad \alpha := \max(\|Q'_q\|_{\infty}, \|Q''_q\|_{\infty}) < \infty \quad \text{for all} \quad x \in \Omega,$$

$$(2.8)$$

and

$$\varepsilon^2 \max_{x \in \Omega} \frac{|Q'_q|^2}{Q_q} < 4 \Big(T - \frac{J_0^2}{\underline{n}^2} \Big),$$
 (2.9)

where $\underline{n} := \min\{1, C_0\}$. Then there exists at least one solution to (2.7) such that $(w_q, V_q) \in H^4(\Omega) \times H^2(\Omega)$.

Remark 2.3. Condition (2.6)₃ essentially means that $|Q'_q|^2/Q_q$ remains bounded when $Q_q \to 0$. We observe that this condition is verified when Q_q behaves as $|x - x_0|^m$, for $m \ge 2$, when $x \to x_0$. Finally, we notice that the assumption (2.6)₃ is stronger than (2.9), required in the first part of the paper for q > 0.

To better assess the existence of the solution to a more realistic visco-hybrid QHD model, namely where Q = 0 on the classical part of the domain, we need to define what solution means in this contest. In this case, we do not expect a classical solution to exist and we look just for a weak solution defined as follows:

Definition 2.4. The couple (w, V)(x) is a weak solution of (2.1) (where $w = \sqrt{n}$), if, for any $\phi \in C_0^{\infty}(\Omega)$ the following relations are verified

$$2\varepsilon^{2} \int_{0}^{1} \left(Q \frac{w_{xx}}{w} + Q' \frac{w_{x}}{w} \right) \phi_{xx} dx + 2 \int_{0}^{1} \left(\left(T - \frac{J^{2}}{w^{4}} \right) \frac{w_{x}}{w} \right) \phi_{x} dx$$

$$+ \int_{0}^{1} \frac{1}{\lambda^{2}} (w^{2} - C) \phi dx + \int_{0}^{1} \frac{J}{\tau w^{2}} \phi_{x} dx + \nu \int_{0}^{1} w_{x} \phi_{xx} dx = 0,$$
(2.10)

and

$$\int_{0}^{1} V\phi \, dx = -2\varepsilon^{2} \int_{0}^{1} Q \frac{w_{xx}}{w} \phi \, dx - 2\varepsilon^{2} \int_{0}^{1} Q' \frac{w_{x}}{w} \phi \, dx \tag{2.11}$$
$$+ \int_{0}^{1} \frac{J^{2}}{2w^{4}} \phi \, dx + 2T \int_{0}^{1} (\ln w)\phi \, dx - \frac{J}{\tau} \int_{0}^{1} (\int_{0}^{x} \frac{1}{w^{2}(s)} \, ds) \phi \, dx + \nu \int_{0}^{1} w_{x} \phi \, dx.$$

Mathematics in Engineering

Since the limit problem behaves classically close to the boundaries, when we perform the hybrid limit we pass from the quantum to the classical regime then the quantum term disappears. Therefore we need to assume that

$$\left(Q_q \frac{(w_q)_{xx}}{w_q} + Q'_q \frac{(w_q)_x}{w_q}\right)_x \to 0 \quad \text{in} \quad L^2 \quad \text{as} \quad q \to 0,$$
(2.12)

in a neighborhood of the boundaries x = 0 and x = 1.

The main result of this paper is the following theorem:

Theorem 2.5 (Hybrid limits and existence of VH-QHD solution). Assume (2.4), (2.5) and $Q \in C^1[0, 1]$ with $0 \le Q \le 1$ and $C \in C^0[0, 1]$. Let $\{Q_q\}$ be a sequence satisfying (2.6), (2.12) and $(w_q, V_q)(x)$ be a solution to (2.7) corresponding to the approximating function Q_q . Then there exists a convergent subsequence of $(w_q, V_q)(x)$, which is not relabelled, with limit (w, V), namely

$$\begin{cases} w_q \to w \text{ in } H^1(\Omega), \\ w_q \to w \text{ in } C^0(\Omega), & \text{ as } q \to 0. \\ V_q \to V \text{ in } L^2(\Omega), \end{cases}$$
(2.13)

Such a pair (w, V)(x) is the weak solution to the VH-QHD system (2.1), where $w = \sqrt{n}$.

3. Existence of a solution to the VH-Q_qHD problem

In this section, we prove that, under a suitable set of conditions, the BVP (2.7) admits a weak solution (w_q, V_q) . For this purpose, we rewrite (2.7) in the following equivalent form

$$2\varepsilon^{2} \left(Q_{q} \frac{(w_{q})_{xx}}{w_{q}} + Q_{q}' \frac{(w_{q})_{x}}{w_{q}} \right)_{xx} - 2T (\ln w_{q})_{xx} - \left(\frac{J^{2}}{2w_{q}^{4}} \right)_{xx} = -\frac{w_{q}^{2} - C}{\lambda^{2}} + \left(\frac{J}{\tau w_{q}^{2}} \right)_{x} + \nu (w_{q})_{xxx}, \quad (3.1)$$

$$(w_q)_x(0) = (w_q)_x(1) = 0, \qquad w_q(0) = w_q(1) = 1, \qquad J = J_0.$$
 (3.2)

In the next result we prove a set of useful *a priori* estimates, which allow to properly construct the fixed point theorem which guarantees the existence result for (3.1)-(3.2).

Lemma 3.1 (A priori estimates). Assume the subsonic conditions (2.4), (2.5) and Q_q such that (2.8) and (2.9) are both satisfied. Let $w_q \in H^2(\Omega)$ be a solution of the BVP (3.1)-(3.2). Then w_q verifies the following properties:

Adjoint subsonic condition

$$w_q(x) \ge \sqrt{\underline{n}} > \sqrt{n_\star} \quad for \ x \in [0, 1]. \tag{3.3}$$

• L^{∞} bound

$$\|w_q\|_{L^{\infty}(\Omega)} \le w_M. \tag{3.4}$$

Mathematics in Engineering

• H^2 bound

$$\varepsilon^{2} \underline{c_{1}} \int_{0}^{1} (w_{q})_{xx}^{2} dx + \underline{c_{2}} \int_{0}^{1} (w_{q})_{x}^{2} dx \le K,$$
(3.5)

where $w_M \ge \sqrt{\underline{n}}, \underline{c}_1 > 0, \underline{c}_2 > 0$, and K > 0 are constants with \underline{c}_2 independent of q. *Proof.* Let

$$\begin{aligned} &2\varepsilon^2 \int_0^1 Q_q \frac{(w_q)_{xx}^2}{w_q} \, dx + 2 \int_0^1 \left(T - \frac{J^2}{w_q^4} \right) \frac{(w_q)_x^2}{w_q} \, dx + 2\varepsilon^2 \int_0^1 Q_q' \frac{(w_q)_x (w_q)_{xx}}{w_q} \, dx \\ &= -\frac{1}{\lambda^2} \int_0^1 (w_q^2 - 1)(w_q - 1) \, dx + \frac{1}{\lambda^2} \int_0^1 (C - 1)(w_q - 1) \, dx \\ &- \int_0^1 \frac{J}{\tau w_q^2} (w_q)_x \, dx + \nu \int_0^1 (w_q - 1)(w_q)_{xxx} \, dx \\ &=: I_1 + I_2 + I_3 + I_4, \end{aligned}$$

obtained multiplying (3.1) by $(w_q - 1) \in H_0^1(\Omega)$, and integrating by parts. The integrals I_1 and I_2 can be estimated as follows:

$$I_{1} + I_{2} \leq -\frac{1}{\lambda^{2}} \int_{0}^{1} (w_{q} - 1)^{2} (w_{q} + 1) dx + \frac{1}{2\lambda^{2}} \int_{0}^{1} (C - 1)^{2} dx + \frac{1}{2\lambda^{2}} \int_{0}^{1} (w_{q} - 1)^{2} dx$$
$$\leq -\frac{1}{\lambda^{2}} \int_{0}^{1} (w_{q} - 1)^{2} \left(w_{q} + \frac{1}{2} \right) dx + \frac{1}{2\lambda^{2}} \int_{0}^{1} (C - 1)^{2} dx.$$

Moreover, both I_3 and I_4 are equal to zero, indeed

$$I_3 = \int_0^1 \frac{J}{\tau w_q^2} (w_q)_x dx = -\frac{J}{\tau w_q} \Big|_{x=0}^{x=1} = 0,$$
(3.6)

$$I_4 = -\nu \int_0^1 (w_q)_x (w_q)_{xx} dx = \frac{1}{2} (w_q)_x^2 \Big|_{x=0}^{x=1} = 0.$$
(3.7)

In view of the estimate above, we get

$$2\varepsilon^{2} \int_{0}^{1} Q_{q} \frac{(w_{q})_{xx}^{2}}{w_{q}} dx + 2\varepsilon^{2} \int_{0}^{1} Q_{q}' \frac{(w_{q})_{x}(w_{q})_{xx}}{w_{q}} dx$$

$$+ 2 \int_{0}^{1} \left(T - \frac{J^{2}}{w_{q}^{4}}\right) \frac{(w_{q})_{x}^{2}}{w_{q}} dx + \frac{1}{\lambda^{2}} \int_{0}^{1} (w_{q} - 1)^{2} \left(w_{q} + \frac{1}{2}\right) dx$$

$$\leq \frac{1}{2\lambda^{2}} \int_{0}^{1} (C - 1)^{2} dx.$$
(3.8)

Observing (3.8), we can see that the first three terms on the left side can be read as a quadratic form, namely

Mathematics in Engineering

$$\int_{0}^{1} \left[2\varepsilon^{2} Q_{q} \frac{(w_{q})_{xx}^{2}}{w_{q}} + 2\varepsilon^{2} Q_{q}' \frac{(w_{q})_{x}(w_{q})_{xx}}{w_{q}} + 2\left(T - \frac{J^{2}}{w_{q}^{4}}\right) \frac{(w_{q})_{x}^{2}}{w_{q}} \right] dx$$
(3.9)
=: $\int_{0}^{1} \left(\mathcal{A}_{1} \frac{(w_{q})_{xx}^{2}}{w_{q}} + \mathcal{B}_{1} \frac{(w_{q})_{x}(w_{q})_{xx}}{w_{q}} + C_{1} \frac{(w_{q})_{x}^{2}}{w_{q}} \right) dx$
 $\geq c_{1} \int_{0}^{1} \frac{(w_{q})_{xx}^{2}}{w_{q}} dx + c_{2} \int_{0}^{1} \frac{(w_{q})_{x}^{2}}{w_{q}} dx,$

where c_1 and c_2 are positive constants. We notice that (3.9) is positive definite if and only if $\mathcal{B}_1^2 - 4\mathcal{A}_1C_1 < 0$. From (2.9), we get

$$\begin{aligned} \mathcal{B}_1^2 - 4\mathcal{A}_1 C_1 &= 4\varepsilon^2 \Big[\varepsilon^2 |Q_q'|^2 - 4Q_q \left(T - \frac{J^2}{w_q^4} \right) \Big] \\ &< 4\varepsilon^2 \Big[\varepsilon^2 |Q_q'|^2 - 4Q_q \left(T - \frac{J^2}{\underline{n}^2} \right) \Big] < 0, \quad \text{for } w_q \ge \sqrt{\underline{n}}, \end{aligned}$$

that is always true, at least for a small (positive) values of ε .

Then, in view of (3.9) and (3.8), we get

$$c_1 \int_0^1 \frac{(w_q)_{xx}^2}{w_q} dx + c_2 \int_0^1 \frac{(w_q)_x^2}{w_q} dx \le \frac{1}{2\lambda^2} \int_0^1 (C-1)^2 dx =: K_0,$$
(3.10)

which implies

$$\|\sqrt{w_q} - 1\|_{\infty} \le K_1,$$

observing that $\frac{(w_q)_x^2}{w_q} = 4[(\sqrt{w_q})_x]^2$ and taking $K_1 = \sqrt{\frac{K_0}{c_2}}$. The L^{∞} bound (3.4) follows by setting $w_M = (1 + K_1)^2$, while the H^2 -bound (3.5) can be easily derived from (3.10), in view of (3.4).

Last step is to show that $w_q \ge \sqrt{\underline{n}}$ for all $x \in \Omega$ and $\underline{n} = \min\{1, C_0\}$.

Let $(w_q - \sqrt{\underline{n}})^- := \min(0, w_q - \sqrt{\underline{n}})$ used as a test function in the weak formulation of the problem (3.1) as follows

$$2\varepsilon^{2} \int_{0}^{1} Q_{q} \frac{((w_{q} - \sqrt{\underline{n}})^{-})_{xx}^{2}}{w_{q}} dx + 2 \int_{0}^{1} \left(T - \frac{J^{2}}{w_{q}^{4}}\right) \frac{((w_{q} - \sqrt{\underline{n}})^{-})_{x}^{2}}{w_{q}} dx$$
$$+ 2\varepsilon^{2} \int_{0}^{1} Q_{q}^{\prime} \frac{((w_{q} - \sqrt{\underline{n}})^{-})_{x}((w_{q} - \sqrt{\underline{n}})^{-})_{xx}}{w_{q}} dx$$
$$= -\frac{1}{\lambda^{2}} \int_{0}^{1} (w_{q}^{2} - \sqrt{\underline{n}}^{2})(w_{q} - \sqrt{\underline{n}})^{-} dx + \frac{1}{\lambda^{2}} \int_{0}^{1} (C - \underline{n})(w_{q} - \sqrt{\underline{n}})^{-} dx$$
$$+ \int_{0}^{1} \frac{J}{\tau w_{q}^{2}} ((w_{q} - \sqrt{\underline{n}})^{-})_{x} dx + \nu \int_{0}^{1} (w_{q} - \sqrt{\underline{n}})^{-} (w_{q})_{xxx} dx =: L_{1} + L_{2} + L_{3} + L_{4}$$

We recall that $w_q|_{\partial\Omega} = 1 > \sqrt{\underline{n}}$, so $(w_q - \sqrt{\underline{n}})^-|_{\partial\Omega} = 0$, and $(w_q - \sqrt{\underline{n}})^- \in H_0^1(\Omega)$. Concerning the first two terms on the right-hand side of the previous equation, one has

$$L_1 + L_2 \le -\frac{1}{\lambda^2} \int_0^1 ((w_q - \sqrt{\underline{n}})^-)^2 (w_q + \sqrt{\underline{n}}) \, dx + \frac{1}{\lambda^2} \int_0^1 (C - \underline{n}) (w_q - \sqrt{\underline{n}})^- \, dx.$$

Mathematics in Engineering

In order to estimate the L_3 term, we observe that the interval Ω can be seen as a disjoint union of the sub-intervals $\Omega^+ = \bigcup_i \Omega_i^+$, $\Omega^- = \bigcup_i \Omega_i^-$ plus isolated points, where

 $\Omega_i^+ = \{ x \in \Omega \text{ such that } w_q \ge \sqrt{\underline{n}} \}, \text{ and } \Omega_j^- = \{ x \in \Omega \text{ such that } w_q < \sqrt{\underline{n}} \}.$

Therefore, L_3 can be rewritten as

$$L_{3} = -\int_{0}^{1} \frac{J}{\tau w_{q}^{2}} ((w_{q} - \sqrt{\underline{n}})^{-})_{x} dx$$

= $-\sum_{i} \int_{\Omega_{i}^{+}} \frac{J}{\tau w_{q}^{2}} ((w_{q} - \sqrt{\underline{n}})^{-})_{x} dx - \sum_{j} \int_{\Omega_{j}^{-}} \frac{J}{\tau w_{q}^{2}} ((w_{q} - \sqrt{\underline{n}})^{-})_{x} dx$

and then

$$L_3 = -\sum_j \int_{\Omega_j^-} \frac{J}{\tau w_q^2} ((w_q - \sqrt{\underline{n}}))_x dx.$$

The integral L_3 must be computed on each interval Ω_j^- . We just consider a single interval $\Omega_j^- = (a_j, b_j)$ contained in the open set (0, 1) (the result can easily be generalized to a greater number of intervals), obtaining

$$L_3 = -\int_{a_j}^{b_j} \frac{J}{\tau w_q^2} (w_q)_x \, dx = \frac{J}{\tau w_q(b_j)} - \frac{J}{\tau w_q(a_j)} = 0.$$
(3.11)

Here we have used (3.5) to show that w_q is a continuous function in $[a_j, b_j]$ and $w_q(a_j) = w_q(b_j) = \sqrt{\underline{n}}$.

Finally, we prove that also $L_4 = 0$, indeed

$$L_4 = -\nu \int_0^1 (w_q - \sqrt{\underline{n}})_x^- (w_q - \sqrt{\underline{n}})_{xx}^- dx = -\frac{1}{2}\nu ((w_q - \sqrt{\underline{n}})_x^-)_x^2 \Big|_0^1 = 0.$$
(3.12)

In view of (2.9), (3.11), and (3.12), arguing as for (3.9), one can find two non negative constants named c_1 , c_2 and c_3 such that

$$\frac{c_1}{2} \int_0^1 ((w_q - \sqrt{\underline{n}})^-)_{xx}^2 dx + \underline{c_2} \int_0^1 ((w_q - \sqrt{\underline{n}})^-)_x^2 dx + \underline{c_3} \int_0^1 ((w_q - \sqrt{\underline{n}})^-)^2 (w_q + \sqrt{\underline{n}}) dx \le \frac{1}{\lambda^2} \int_0^1 (C - \underline{n}) (w_q - \sqrt{\underline{n}})^- dx,$$

therefore $(w_q - \sqrt{\underline{n}})^- = 0$ and then (3.3).

Lemma 3.2. Set $u_q = \ln n_q$ and assume that the hypotheses of Lemma 3.1 hold, then

$$\varepsilon \sqrt{q} \|(u_q)_{xx}\|_{L^2(\Omega)} + \sqrt{T - J^2/\underline{n}^2} \|(u_q)_x\|_{L^2(\Omega)}$$

$$\leq \varepsilon \|\sqrt{Q_q}(u_q)_{xx}\|_{L^2(\Omega)} + \sqrt{T - J^2/\underline{n}^2} \|(u_q)_x\|_{L^2(\Omega)} \leq K_0.$$
(3.13)

Mathematics in Engineering

Volume 6, Issue 5, 705–725.

Proof. We consider the following equation

$$\varepsilon^{2} \left(Q_{q} \left((u_{q})_{xx} + \frac{(u_{q})_{x}^{2}}{2} \right) + Q_{q}'(u_{q})_{x} \right)_{xx} + (J^{2} e^{-2u_{q}}(u_{q})_{x})_{x}$$

$$- T(u_{q})_{xx} + \frac{e^{u_{q}} - C(x)}{\lambda^{2}} - \left(\frac{J}{\tau} e^{-u_{q}} \right)_{x} + \nu (e^{\frac{u_{q}}{2}})_{xxx} = 0,$$
(3.14)

obtained from (2.7) setting $w_q = e^{u_q/2}$ and deriving with respect to x.

Clearly

$$u_q(0) = u_q(1) = 0,$$
 $(u_q)_x(0) = (u_q)_x(1) = 0.$ (3.15)

Let's multiply (3.14) by u_q and integrate by parts. In view of the boundary conditions (3.15), we get

$$\begin{split} \varepsilon^2 & \int_0^1 Q_q(u_q)_{xx}^2 \, dx + \int_0^1 \left(T - \frac{J^2}{e^{2u_q}} \right) (u_q)_x^2 \, dx \\ &= -\frac{1}{\lambda^2} \int_0^1 (e^{u_q} - C) u_q \, dx \\ &+ \frac{J}{\tau} \int_0^1 e^{-u_q} (u_q)_x \, dx + \varepsilon^2 \int_0^1 Q_q' \frac{(u_q)_x^3}{6} \, dx - \varepsilon^2 \int_0^1 Q_q''(x) \frac{(u_q)_x^2}{2} \, dx \\ &- \nu \int_0^1 (e^{\frac{u_q}{2}})_{xx} (u_q)_x \, dx \\ &=: N_1 + N_2 + N_3 + N_4 + N_5. \end{split}$$

According to the results in [22], we get

$$N_1 \leq \frac{1}{\lambda^2} (e^{-1} + \|C \ln C\|_{L^{\infty}}).$$

Moreover $N_2 = 0$, in view of the boundary conditions, and

$$N_{3} + N_{4} \leq \frac{\varepsilon^{2}}{6} ||Q_{q}'||_{\infty} ||(u_{q})_{x}||_{\infty}^{3} + \frac{\varepsilon^{2}}{2} ||Q_{q}''||_{\infty} ||(u_{q})_{x}||_{\infty}^{2}$$
$$\leq \frac{\alpha \varepsilon^{2}}{2} ||(u_{q})_{x}||_{\infty}^{2} \left(\frac{||(u_{q})_{x}||_{\infty}}{3} + 1\right).$$

Concerning N_5 , we have

$$N_{5} = v \int_{0}^{1} (e^{\frac{u_{q}}{2}})_{x}(u_{q})_{xx} dx$$

$$= v \int_{0}^{1} e^{\frac{u_{q}}{2}} \frac{(u_{q})_{x}}{2}(u_{q})_{xx} dx$$

$$= \frac{1}{8} v \int_{0}^{1} e^{\frac{u_{q}}{2}} (u_{q})_{x}^{3} dx$$

$$\leq v \frac{1}{4} e^{\frac{w_{M}}{2}} ||(u_{q})_{x}||_{\infty}^{3}.$$
(3.16)

Mathematics in Engineering

Finally, in view of the estimation above, we obtain the following inequality

$$\varepsilon^{2} q \int_{0}^{1} (u_{q})_{xx}^{2} dx + \left(T - \frac{J^{2}}{\underline{n}^{2}}\right) \int_{0}^{1} (u_{q})_{x}^{2} dx$$

$$\leq \varepsilon \|\sqrt{Q_{q}}(u_{q})_{xx}\|_{L^{2}(\Omega)} + \sqrt{T - J^{2}/\underline{n}^{2}} \|(u_{q})_{x}\|_{L^{2}(\Omega)}$$

$$\leq K_{0}$$
(3.17)

which implies (3.13).

Theorem 3.3. Assume that the hypotheses of Lemma 3.1 and (2.2) hold. Then, the boundary value problem (3.14)-(3.15) admits at least one weak solution $u_q \in H^2(\Omega)$.

Proof. As already noted in [13], Eq (3.14) is equivalent to the standard QHD model because $Q_q \ge q > 0$. Therefore, we can employ the same techniques applied in [22, 26, 27].

For $\sigma \in [0, 1]$ and $\rho \in X = C^{0,1}(\Omega)$, we introduce the equation

$$\varepsilon^{2} \left(Q_{q} \left((u_{q})_{xx} + \frac{\sigma}{2} (\rho)_{x}^{2} \right) + Q_{q}'(u_{q})_{x} \right)_{xx} + \sigma J^{2} \left(e^{-2\rho} \rho_{x} \right)_{x}$$

$$- T(u_{q})_{xx} + \frac{\sigma}{\lambda^{2}} \left(\frac{e^{\rho} - 1}{\rho} u_{q} + 1 - C \right) - \sigma \frac{J}{\tau} (e^{-\rho})_{x} - \sigma \nu (e^{\frac{\rho}{2}})_{xxx} = 0$$
(3.18)

and coupled it to (3.15). It is not difficult to see that for each $u_q, \phi \in H^2(\Omega)$ the following bi-linear form

$$a(u_q,\phi) = \int_0^1 \left(\varepsilon^2 \left(Q_q(u_q)_{xx} + Q'_q(u_q)_x \right) \phi_{xx} + T(u_q)_x \phi_x + \frac{\sigma}{\lambda^2} \frac{e^{\rho} - 1}{\rho} u_q \phi \right) dx$$

is continuous and coercive in $H^2(\Omega)$.

Moreover a linear and continuous functional can be defined as follows:

$$F(\phi) = \int_0^1 \left(-Q_q \frac{\varepsilon^2 \sigma}{2} \rho_x^2 \phi_{xx} + \sigma J^2 e^{-2\rho} \rho_x \phi_x + \frac{\sigma}{\lambda^2} (C-1) \phi \right) dx$$
$$- \int_0^1 \left(\sigma \frac{J}{\tau} e^{-\rho} \phi_x \right) dx - \int_0^1 \left(\frac{1}{2} \sigma \nu e^{\frac{\rho}{2}} \rho_x \phi_{xx} \right) dx.$$

Then the Lax-Milgram Lemma guarantees the existence of a unique solution $u_q \in H^2(\Omega)$ to the boundary value problem (3.15)–(3.18). Then a continuous and compact map *S* on the functional space *X* can be defined as

$$S: X \times [0,1] \to X, \ (\rho,\sigma) \to u_q \tag{3.19}$$

such that

- $S(\rho, 0) = 0$ for all $\rho \in X$,
- there is a constant c > 0 such that

$$||u_q||_X \le c$$
, for all $(u_q, \sigma) \in X \times [0, 1]$ satisfying $S(u_q, \sigma) = u_q$. (3.20)

Mathematics in Engineering

Applying the Leray-Schauder fixed point theorem we can prove that u_q is a fixed point for the map *S* and also a weak solution to the BVP (3.14)-(3.15).

Now we are ready to prove Theorem 2.2.

Proof of Theorem 2.2. We consider Eq (3.14)

$$\varepsilon^{2} \left(Q_{q} \left((u_{q})_{xx} + \frac{(u_{q})_{x}^{2}}{2} \right) + Q_{q}'(u_{q})_{x} \right)_{xx} + (J^{2} e^{-2u_{q}}(u_{q})_{x})_{x}$$
$$- T(u_{q})_{xx} + \frac{e^{u_{q}} - C(x)}{\lambda^{2}} - \left(\frac{J}{\tau} e^{-u_{q}} \right)_{x} + v (e^{\frac{u_{q}}{2}})_{xxx} = 0,$$

from which we have

$$\begin{split} \varepsilon^2 Q_q(u_q)_{xxxx} &= -\varepsilon^2 (Q_q \frac{(u_q)_x^2}{2})_{xx} - \varepsilon^2 (Q_q'(u_q)_{xxx} + Q_q''(u_q)_x) + (J^2 e^{-2u_q}(u_q)_x)_x \\ &- T(u_q)_{xx} + \frac{e^{u_q} - C(x)}{\lambda^2} - \left(\frac{J}{\tau} e^{-u_q}\right)_x + v(e^{\frac{u_q}{2}})_{xxx}. \end{split}$$

Observing that $u_q \in H^2(\Omega)$, by Theorem 3.3, and arguing as in Corollary 2.6 in [22], it is not difficult to prove that $(u_{q_x}^2)_{xx} \in H^{-1}(\Omega)$. Concerning the viscous term $(e^{\frac{u_q}{2}})_{xxx}$ we have

$$(e^{u_q/2})_{xxx} = \frac{e^{u_q/2}}{2} \left(u_{q_{xxx}} + u_{q_x} u_{q_{xx}} + u_{q_x}^3/4 \right).$$

It is easy to see that $u_{q_x}u_{q_{xx}}$ and $u_{q_x}^3$ both belongs to $L^2(\Omega)$ and $u_{q_{xxx}} \in H^{-1}(\Omega)$. Proceeding as in [22] and taking into account the regularity of $Q_q > q > 0$, we can deduce that $(u_q)_{xxxx}$ and then $(w_q)_{xxxx}$ are in $L^2(\Omega)$. Since problem (2.7) is equivalent to (3.14)-(3.15), the existence of a solution $w_q \in H^4$ follows easily. Finally, from the Poisson equation, we deduce $V_q \in H^2$ and that concludes the proof.

4. Hybrid limit

In this section we perform the hybrid limit for Eq (2.7), assuming $q \rightarrow 0$. Unlike the previous works of the authors in this line [13, 15–17], in this paper we consider the quantum effects localized in the central part of the device, where Q > 0, which is more correct from the physical point of view. On the boundaries of the device we set Q = 0, assuming classical behaviour.

Now we present the proof of the main result of the paper.

Proof of Theorem 2.5. Let $0 < \delta^* < \delta^{**} < 1$. Define the function *Q* as follows:

$$Q(x) \begin{cases} = 0 & \text{if } 0, \le x \le \delta^* \text{ and } \delta^{**} \le x \le 1, \\ > 0, & \text{if } \delta^* < x < \delta^{**}, \end{cases}$$
(4.1)

and $\Omega_c := [0, \delta^*] \cup [\delta^{**}, 1].$

Once the function Q has been chosen as in (4.1), we construct the sequence of the approximating functions $\{Q_q\}$ to Q, satisfying (2.6). Let $(w_q, V_q)(x)$ be the solutions to (2.7) corresponding to Q_q . In the sequel, we will denote constants independent from q as \bar{K} or \bar{c}_i .

Mathematics in Engineering

We recall that from (3.4) and (3.5) the following *q*-independent estimate holds:

$$\|w_q\|_{H^1(\Omega)} \le \bar{K} \tag{4.2}$$

and we briefly prove also the following:

$$\|\sqrt{Q_q}w_{q_{xx}}\|_{L^2(\Omega)} \le \bar{K}.\tag{4.3}$$

Proceeding as in Lemma 3.1, we rearrange the first three terms of the left-hand side in (3.8) as

$$2\int_{0}^{1} \left[\frac{\varepsilon^{2}Q_{q}}{w_{q}} w_{q_{xx}}^{2} + \frac{2\varepsilon^{2}Q_{q}'}{w_{q}} w_{q_{x}} w_{q_{xx}} + \left(\frac{T}{w_{q}} - \frac{J^{2}}{w_{q}^{5}}\right) w_{q_{x}}^{2} \right] dx$$

+
$$\int_{0}^{1} \left[\frac{\varepsilon^{2}Q_{q}}{w_{q}} w_{q_{xx}}^{2} + \left(\frac{T}{w_{q}} - \frac{J^{2}}{w_{q}^{5}}\right) w_{q_{x}}^{2} \right] dx$$

=:
$$\int_{0}^{1} (\mathcal{A}_{2}w_{q_{xx}}^{2} + \mathcal{B}_{2}w_{q_{x}}w_{q_{xx}} + C_{2}w_{q_{x}}^{2}) dx + \int_{0}^{1} \left[\frac{\varepsilon^{2}Q_{q}}{w_{q}} w_{q_{xx}}^{2} + \left(\frac{T}{w_{q}} - \frac{J^{2}}{w_{q}^{5}}\right) w_{q_{x}}^{2} \right] dx.$$

The first term on the right-hand side is positive by (2.6), since $\mathcal{B}_2^2 - 4\mathcal{R}_2C_2 < 0$, where

$$\begin{aligned} \mathcal{B}_2^2 - 4\mathcal{A}_2 C_2 &= \frac{4}{w_q^2} \Big[|\varepsilon^2 Q_q'|^2 - 4\varepsilon^2 Q_q \left(T - \frac{J^2}{w_q^4} \right) \Big] \\ &< \frac{4\varepsilon^2}{w_q^2} \Big[\varepsilon^2 |Q_q'|^2 - 4Q_q \left(T - \frac{J^2}{\underline{n}^2} \right) \Big] \\ &< 0, \text{ for } n \ge n. \end{aligned}$$

As in the proof of Lemma 3.1, we obtain

$$\int_{0}^{1} \frac{\varepsilon^{2} Q_{q}}{w_{q}} w_{q_{xx}}^{2} dx + \int_{0}^{1} \left(\frac{T}{w_{q}} - \frac{J^{2}}{w_{q}^{5}} \right) w_{q_{x}}^{2} dx \le \bar{K}.$$
(4.4)

By (2.9), we have $\frac{T}{w_q} - \frac{J^2}{w_q^5} > 0$ and recalling that $w_q \ge \sqrt{n_*}$, we can rewrite (4.4) as

$$\bar{c}_2 \int_0^1 Q_q w_{q_{xx}}^2 dx + \bar{c}_3 \int_0^1 w_{q_x}^2 dx \le \bar{K}$$
(4.5)

and then we get (4.3).

Therefore, $\sqrt{Q_q} w_{q_{xx}}$ is uniformly bounded in $L^2(\Omega)$ and there exists a w(x) as the hybrid limit of the sequence w_q with

$$\sqrt{Q_q} w_{q_{XX}} \rightharpoonup \sqrt{Q} w_{XX}$$
 in $L^2(\Omega)$, for $q \to 0$, (4.6)

while, from (4.2), we have

$$w_q \rightarrow w$$
 in $H^1(\Omega)$, for $q \rightarrow 0$. (4.7)

Mathematics in Engineering

Considering the weak form of (2.7)

$$2\varepsilon^{2} \int_{0}^{1} \left(Q_{q} \frac{w_{q_{xx}}}{w_{q}} + Q_{q}' \frac{w_{q_{x}}}{w_{q}} \right) \phi_{xx} dx + 2 \int_{0}^{1} \left(\left(T - \frac{J^{2}}{w_{q}^{4}} \right) \frac{w_{q_{x}}}{w_{q}} \right) \phi_{x} dx$$

$$+ \int_{0}^{1} \frac{1}{\lambda^{2}} (w_{q}^{2} - C) \phi dx + \int_{0}^{1} \frac{J}{\tau w_{q}^{2}} \phi_{x} dx + \nu \int_{0}^{1} w_{q_{x}} \phi_{xx} dx = 0,$$
(4.8)

we perform the hybrid limit $q \rightarrow 0$.

We just note that since $0 \le \sqrt{\underline{n}} \le w_q \le w_M$ for every q and $w_q \to w$ in $C^0(\Omega)$, for $q \to 0$, we can write $\frac{1}{w_q} \to \frac{1}{w}$ and $w_q^2 \to w^2$ for $q \to 0$, similarly for the other nonlinear terms.

So we obtain as limit

$$2\varepsilon^{2} \int_{0}^{1} \left(Q \frac{w_{xx}}{w} + Q' \frac{w_{x}}{w} \right) \phi_{xx} dx + 2 \int_{0}^{1} \left(\left(T - \frac{J^{2}}{w^{4}} \right) \frac{w_{x}}{w} \right) \phi_{x} dx$$

$$+ \int_{0}^{1} \frac{1}{\lambda^{2}} (w^{2} - C) \phi dx + \int_{0}^{1} \frac{J}{\tau w^{2}} \phi_{x} dx + \nu \int_{0}^{1} w_{x} \phi_{xx} dx = 0,$$

$$(4.9)$$

for any $\phi \in C_0^{\infty}(\Omega)$.

Then $n = w^2$ satisfies $(1.9)_1$ in the weak sense.

In particular, the weak limit Eq (4.9) in Ω_c becomes

$$2\int_{\Omega_c} \left((T - \frac{J^2}{w^4}) \frac{w_x}{w} \right) \phi_x \, dx + \frac{1}{\lambda^2} \int_{\Omega_c} (w^2 - C) \phi_x \, dx + \int_{\Omega_c} \frac{2J^2}{\tau w^3} \phi_x \, dx$$
$$+ \nu \int_{\Omega_c} w_x \phi_{xx} \, dx = 0, \quad \text{for all} \quad \phi \in C_0^\infty(\Omega)$$

thanks to the hypothesis 2.12, in agreement with the previous estimates and $(2.6)_1$.

It follows that the limit solution *w* satisfies

$$2\left((T - \frac{J^2}{w^4})\frac{w_x}{w}\right)_x + \frac{1}{\lambda^2}(w^2 - C) + \left(\frac{2J^2}{\tau w^3}\right)_x + vw_{xxx} = 0$$
(4.10)

in Ω_c .

Concerning the electric potential V_q , by integrating (1.1) with respect to x and using (1.3), we obtain

$$V_q = -2\varepsilon^2 Q_q \frac{w_{q_{xx}}}{w_q} - 2\varepsilon^2 Q'_q \frac{w_{q_x}}{w_q} + \frac{J^2}{2w_q^4} + 2T \ln w_q - \frac{J}{\tau} \int_0^x \frac{1}{w_q^2} dx + v w_{qxx}.$$
 (4.11)

The assumption (2.6) and the uniform estimates (4.3) imply that $||V_q||_{L^2} \leq \overline{K}$. Therefore, there exists *V* such that

$$V_q \rightarrow V$$
 in $L^2(\Omega)$, (4.12)

when $q \rightarrow 0$.

As before, we prove that the limit V is the weak solution of the hybrid problem. To this end, we multiply (4.11) by $\phi \in C_0^{\infty}(\Omega)$ and integrate it in Ω :

Mathematics in Engineering

$$\int_{0}^{1} V_{q} \phi \, dx = -2\varepsilon^{2} \int_{0}^{1} Q_{q} \frac{w_{q_{xx}}}{w_{q}} \phi \, dx - 2\varepsilon^{2} \int_{0}^{1} Q_{q}' \frac{w_{q_{x}}}{w_{q}} \phi \, dx + \int_{0}^{1} \frac{J^{2}}{2w_{q}^{4}} \phi \, dx \qquad (4.13)$$
$$+ 2T \int_{0}^{1} (\ln w_{q}) \phi \, dx - \frac{J}{\tau} \int_{0}^{1} \int_{0}^{x} \frac{1}{w_{q}^{2}} \, ds \, \phi \, dx - \nu \int_{0}^{1} w_{qx} \phi_{xx} dx.$$

The uniform estimate in (4.2)-(4.3) and the properties of $\{Q_q\}$ allow that, for $q \to 0$, we have

$$\int_{0}^{1} V\phi \, dx = -2\varepsilon^{2} \int_{0}^{1} Q \frac{w_{xx}}{w} \phi \, dx - 2\varepsilon^{2} \int_{0}^{1} Q' \frac{w_{x}}{w} \phi \, dx + \int_{0}^{1} \frac{J^{2}}{2w^{4}} \phi \, dx \qquad (4.14)$$
$$+ 2T \int_{0}^{1} (\ln w)\phi \, dx - \frac{J}{\tau} \int_{0}^{1} \int_{0}^{x} \frac{1}{w^{2}} \, ds \, \phi \, dx - \nu \int_{0}^{1} w_{x} \phi_{xx} dx.$$

Thus, the limit potential V verifies the Poisson equation in the weak sense.

In order to conclude the proof, we need to verify the boundary conditions $(w)_x(0) = (w)_x(1) = 0$ for the limit solution. To this end, we have to prove that $(w_q)_{xx}$ is weakly convergent in L^2 on a small region near each of the two extrema 0 and 1 of Ω . We write Eq (2.7) as follows:

$$2\varepsilon^{2}\left(\frac{Q_{q}(w_{q})_{xx}}{w_{q}} + \frac{Q_{q}'(w_{q})_{x}}{w_{q}}\right)_{xx} - \nu(w_{q})_{xxx} = 2\left(\left(T - \frac{J^{2}}{w_{q}^{4}}\right)\frac{(w_{q})_{x}}{w_{q}}\right)_{x} - \frac{(w_{q}^{2} - C)}{\lambda^{2}} - \frac{2J(w_{q})_{x}}{\tau w_{q}^{3}}.$$

By the previous uniform estimates, we can see that the right-hand side of the above equation is in $H^{-1}(\Omega)$. Then there exists a function $f \in L^2(\Omega)$ such that

$$\left(2\varepsilon^{2}\left(Q_{q}\frac{(w_{q})_{xx}}{w_{q}}+Q_{q}'\frac{(w_{q})_{x}}{w_{q}}\right)_{x}-\nu(w_{q})_{xx}-f\right)_{x}=0,$$

which implies that

$$\left(2\varepsilon^2 \left(Q_q \frac{(w_q)_{xx}}{w_q} + Q'_q \frac{(w_q)_x}{w_q}\right)_x - \nu (w_q)_{xx}\right) = f + constant$$

is in $L^2(\Omega)$.

Then $2\varepsilon^2 \left(Q_q \frac{(w_q)_{xx}}{w_q} + Q'_q \frac{(w_q)_x}{w_q}\right)_x - \nu (w_q)_{xx}$ belongs to $L^2(\Omega)$ and, in view of the assumption (2.12), we conclude that, at least in a small region close to the boundaries, the convergence of the sequence w_q to w is weak in H^2 .

By the inclusion $H^2(\Omega_c) \hookrightarrow C^1(\Omega_c)$, we can conclude that

$$\lim_{q \to 0} (w_q)_x(0) = 0 = w_x(0)$$

and

$$\lim_{q \to 0} (w_q)_x(1) = 0 = w_x(1).$$

The proof of Theorem 2.5 is complete.

Mathematics in Engineering

Volume 6, Issue 5, 705–725.

5. Numerical simulations

In the previous sections, we have introduced a new hybrid viscous model (VH-QHD) and we have discussed how the viscous term $v(\sqrt{n})_{xx}$ allows the treatment of the classical boundaries making the problem well-posed.

In this section, we show the regularizing effects of viscosity by means of some numerical simulations on a simple $n^+|n|n^+$ transistor. For this device one usually assumes the following doping profile as in [13]

$$\bar{C}(x) = \begin{cases} C_m, & \forall x \in [x_1, x_2], \\ 1, & \forall x \in [0, x_1) \text{ and } x \in (x_2, 1], \end{cases}$$
(5.1)

with $0 < C_m < 1$ and $0 < x_1 < x_2 < 1$. Within this paper the quantum regions is localized in the central part of the domain whereas the external ones, close to the Ohmic contacts, behave classically.

In this case we have

$$\begin{cases} \text{Quantum Region} & \forall x \in [y_1, y_2], \\ \text{Classical Region} & \forall x \in [0, y_1) \text{ and } x \in (y_2, 1], \end{cases}$$
(5.2)

where $0 < y_1 < y_2 < 1$. To solve numerically the following boundary value problems we use COLNEW, a SCILAB tool (see [6]). To perform our computations, we consider the hybrid model in the following form:

$$\varepsilon^{2} \left(Q \left(u_{xx} + \frac{u_{x}^{2}}{2} \right) + Q' u_{x} \right)_{xx} + (J^{2} e^{-2u} u_{x})_{x} - T u_{xx} + \frac{e^{u} - C(x)}{\lambda^{2}} - \left(\frac{J}{\tau} e^{-u} \right)_{x} = v(e^{\frac{u}{2}})_{xxx},$$

coupled with the boundary conditions

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

where, as usual, $u = \ln n$. Both the doping profile C(x) and the quantum function Q(x) have been approximated by regular functions as follows:

$$C(x) = 1 - (0.5 - C_m/2)(\tanh(1000(x - 1/3)) - \tanh(1000(x - 2/3))),$$

$$Q(x) = Q_{cqc}(x) = (q - 0.5)(\tanh(h(x - (2/3))) - \tanh(h(-(x - 1/3))) + q,$$
(5.3)

where $x \in [0, 1]$, $C_m = 0.2$ and q = 0.01.

For sake of completeness we also consider the quantum boundary case, not included in the theoretical part, but extensively discussed in previous works [14–16]. In this case, the quantum function can be approximated by

$$Q_{aca}(x) = (0.5 - q/2)((\tanh(40(x - 2/3)) - \tanh(40(x - 1/3))) + 1.$$
(5.4)

The two quantum functions are displayed in Figure 1.

Mathematics in Engineering



Figure 1. Quantum function behaviour: Q_{cqc} on the left side and the Q_{qcq} on the right side.

The other parameters, namely the scaled Debye length λ , the scaled temperature T, the scaled Plank constant ε , the current density J, and the relaxation time τ are assigned as follows:

$$\lambda = 0.1, T = 1, \varepsilon = 0.01, J = 0.1, \tau = 0.125.$$

To evaluate the effect of the viscosity, we compare the behavior of the charge density assuming v = 0 and v = 0.001, for both quantum functions Q_{cqc} (Figures 2 and 3) and Q_{qcq} (Figures 4 and 5). Observing Figure 2 we can see small oscillations of the charge density close to the boundaries, while this effect disappears by adding a small viscosity.

In Figure 3 the charge density behavior close to x = 0 is displayed in detail for three different viscosity values, namely v = 0, 0.0001, 0.001.

The behavior in the non-viscous case is the same as that obtained for very low viscosity. As the viscosity increases, the function's trend near the edges appears more regular. These fluctuations could be caused by the fact that the problem is not well-posed at the boundaries. However, it is also possible that these effects are related to the numeric scheme used by COLNEW. To better understand the cause of these fluctuations it is necessary to design an *ad-hoc* numerical scheme, which is beyond the aim of this article. Conversely, using (5.4) as a quantum function, the problem is well-posed on the boundaries and the behaviour of the charge density appears regular over the entire domain, both in the viscous and in the non-viscous cases, as in Figure 4.



Figure 2. Charge density assuming Q_{cqc} as quantum functions, for non-viscous (left) and the viscous problem (right).

Mathematics in Engineering



Figure 3. Detail of the charge density behavior close to the boundary x = 0, assuming Q_{cqc} and different values of the viscosity, namely v = 0, 0.0001, 0.001.



Figure 4. Charge density assuming Q_{qcq} as quantum functions, for non-viscous (left) and the viscous problem (right).



Figure 5. Detail of the charge density behaviour close to the boundary x = 0, assuming Q_{qcq} and different values of the viscosity, namely v = 0,00001 and v = 0.001.

6. Conclusions

In this paper we discuss the existence of solutions for a hybrid classical-quantum hydrodynamic problem, assuming quantum effects localized in the central part of the domain. The existence of a weak solution is obtained as a limit-solution of a fully quantum regularised problem. Numerical simulations show that the viscous term contributes to limiting spurious oscillations on the boundary. However, a stationary one-dimensional model like the one discussed here cannot fully describe the complexity of the phenomenon under analysis. Further studies involving two-dimensional and time-dependent models are still in progress.

Acknowledgments

Bruno Rubino has been partially funded by the European Union - NextGenerationEU under the Italian Ministry of University and Research (MUR) National Centre for HPC, Big Data and Quantum Computing CN 00000013 - CUP: E13C22001000006.

Conflict of interest

The authors declare no conflicts of interest.

References

- 1. M. G. Ancona, G. J. Iafrate, Quantum correction to the equation of state of an electron gas in a semiconductor, *Phys. Rev. B*, **39** (1989), 9536–9540. https://doi.org/10.1103/physrevb.39.9536
- 2. P. Antonelli, P. Marcati, The quantum hydrodynamics system in two space dimensions, *Arch. Rational Mech. Anal.*, **203** (2012), 499–527. https://doi.org/10.1007/s00205-011-0454-7
- N. Ben Abdallah, C. Jourdana, P. Pietra, N. Vauchelet, A hybrid classical-quantum approach for ultra-scaled confined nanostructures: modeling and simulation, *ESAIM: Proc.*, **35** (2012), 239–244. https://doi.org/10.1051/proc/201235021
- 4. N. Ben Abdallah, A hybrid kinetic-quantum model for stationary electron transport, *J. Stat. Phys.*, **90** (1998), 627–662. https://doi.org/10.1023/a:1023216701688
- 5. N. Ben Abdallah, F. Méhats, N. Vauchelet, Diffusive transport of partially quantized particles: existence, uniqueness and long time behaviour, *Proc. Edinb. Math. Soc.*, **49** (2006), 513–549. https://doi.org/10.1017/S0013091504000987
- 6. G. Bader, U. Ascher, A new basis implementation for a mixed order boundary value ODE solver, *SIAM J. Sci. Stat. Comput.*, **8** (1987), 483–500. https://doi.org/10.1137/0908047
- M. Baro, N. Ben Abdallah, P. Degond, A. El Ayyadi, A 1D coupled Schrödinger drift-diffusion model including collisions, *J. Comput. Phys.*, 203 (2005), 129–153. https://doi.org/10.1016/j.jcp.2004.08.009
- 8. F. Brezzi, I. Gasser, P. A. Markowich, C. Schmeiser, Thermal equilibrium states of the quantum hydrodynamic model for semiconductors in one dimension, *Appl. Math. Lett.*, **8** (1995), 47–52. https://doi.org/10.1016/0893-9659(94)00109-p

- 9. S. Chiarelli, F. Di Michele, B. Rubino, A hybrid drift diffusion model: derivation, weak steady state solutions and simulations, *Math. Appl.*, **1** (2012), 37–55. https://doi.org/10.13164/ma.2012.03
- P. Degond, P. A. Markowich, On a one-dimensional steady-state hydrodynamic model for semiconductors, *Appl. Math. Lett.*, **3** (1990), 25–29. https://doi.org/10.1016/0893-9659(90)90130-4
- F. Di Michele, P. Marcati, B. Rubino, Steady states and interface transmission conditions for heterogeneous quantum classical 1-d hydrodynamic model of semiconductor devices, *Phys. D*, 243 (2013), 1–13. https://doi.org/10.1016/j.physd.2012.08.012
- F. Di Michele, P. Marcati, B. Rubino, Stationary solution for transient quantum hydrodynamics with bohmenian-type boundary conditions, *Comp. Appl. Math.*, **36** (2017), 459–479. https://doi.org/10.1007/s40314-015-0235-2
- F. Di Michele, M. Mei, B. Rubino, R. Sampalmieri, Stationary solution to hybrid quantum hydrodynamical model of semiconductors in bounded domain, *Int. J. Numer. Anal. Mod.*, 13 (2016), 898–925.
- 14. F. Di Michele, M. Mei, B. Rubino, R. Sampalmieri, Thermal equilibrium solution to new model of bipolar hybrid quantum hydrodynamics, J. Differ. Equations, 263 (2017), 1843–1873. https://doi.org/10.1016/j.jde.2017.03.032
- 15. F. Di Michele, M. Mei, B. Rubino, R. Sampalmieri, Stationary solutions for a new hybrid quantum model for semiconductors with discontinuous pressure functional and relaxation time, *Math. Mech. Solids*, 24 (2018), 2096–2115. https://doi.org/10.1177/1081286518814289
- F. Di Michele, M. Mei, B. Rubino, R. Sampalmieri, Existence and uniqueness for a stationary hybrid quantum hydrodynamical model with general pressure functional, *Commun. Math. Sci.*, 19 (2021), 2049–2079. https://doi.org/10.4310/cms.2021.v19.n8.a1
- F. Di Michele, M. Mei, B. Rubino, R. Sampalmieri, A steady-state mathematical model for an EOS capacitor: the effect of the size exclusion, *Netw. Heteroge. Media*, **11** (2016), 603–625. https://doi.org/10.3934/nhm.2016011
- F. Di Michele, B. Rubino, R. Sampalmieri, Existence of solutions for a viscous hybrid quantum system for arbitrary large current density, *Math. Mech. Solids*, 27 (2022), 2189–2200. https://doi.org/10.1177/10812865221105812
- I. M. Gamba, A. Jüngel, Positive solutions to singular second and third order differential equations for quantum fluids, *Arch. Rational Mech. Anal.*, **156** (2001), 183–203. https://doi.org/10.1007/s002050000114
- 20. C. L. Gardner, The quantum hydrodynamic model for semiconductor devices, *SIAM J. Appl. Math.*, **54** (1994), 409–427. https://doi.org/10.1137/s0036139992240425
- Y. Guo, W. Strauss, Stability of semiconductor states with insulating and contact boundary conditions, Arch. Rational Mech. Anal., 179 (2006), 1–30. https://doi.org/10.1007/s00205-005-0369-2
- 22. M. T. Gyi, A. Jüngel, A quantum regularization of the one-dimensional hydrodynamic model for semiconductors, *Adv. Differ. Equ.*, **5** (2000), 773–800. https://doi.org/10.57262/ade/1356651347

- 23. F. Huang, M. Mei, Y. Wang, H. Yu, Asymptotic convergence to stationary waves for unipolar hydrodynamic model of semiconductors, *SIAM J. Math. Anal.*, 43 (2011), 411–429. https://doi.org/10.1137/100793025
- F. Huang, M. Mei, Y. Wang, H. Yu, Asymptotic convergence to planar stationary waves for multidimensional unipolar hydrodynamic model of semiconductors, *J. Differ. Equations*, 251 (2011), 1305–1331. https://doi.org/10.1016/j.jde.2011.04.007
- 25. C. Jourdana, P. Pietra, A hybrid classical-quantum transport model for the simulation of carbon nanotube transistors, *SIAM J. Sci. Comput.*, **36** (2014), B486–B507. https://doi.org/10.1137/130926353
- 26. A. Jüngel, H. Li, Quantum Euler-Poisson systems: existence of stationary states, *Arch. Math.* (*Brno*), **40** (2004), 435–456.
- A. Jüngel, H. Li, Quantum Euler-Poisson systems: global existence and exponential decay, *Quart. Appl. Math.*, 62 (2004), 569–600. https://doi.org/10.1090/qam/2086047
- 28. H. Li, P. Markowich, M. Mei, Asymptotic behaviour of solutions of the hydrodynamic model of semiconductors, *Proc. R. Soc. Edinburgh*, **132** (2002), 359–378. https://doi.org/10.1017/s0308210500001670
- 29. P. Marcati, R. Natalini, Weak solutions to a hydrodynamic model for semiconductors and relaxation to the drift-diffusion equation, *Arch. Rational Mech. Anal.*, **129** (1995), 129–145. https://doi.org/10.1007/bf00379918
- 30. P. Natalini, T. Luo, Z. Xin, Large time behavior of the solutions to a hydrodynamic model for semiconductors, *SIAM J. Appl. Math.*, **59** (1998), 810–830. https://doi.org/10.1137/s0036139996312168
- S. Nishibata, M. Suzuki, Initial boundary value problems for a quantum hydrodynamic model of semiconductors: asymptotic behaviors and classical limits, *J. Differ. Equations*, 244 (2008), 836– 874. https://doi.org/10.1016/j.jde.2007.10.035
- 32. O. Salas, P. Lanucara, P. Pietra, S. Rovida, G. Sacchi, Parallelization of a quantumclassic hybrid model for Nanoscale Semiconductor devices, *Rev. Mat.*, **18** (2011), 231–248. https://doi.org/10.15517/rmta.v18i2.2096



© 2024 the Author(s), licensee AIMS Press. This is an open access article distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/4.0)