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Thermal equilibrium solution to new model of bipolar hybrid quantum hydrodynamics

Federica Di Michele [a], Ming Mei [b,c], Bruno Rubino [a,*], Rosella Sampalmieri [a]

[a] *Department of Information Engineering, Computer Sciences and Mathematics, University of L'Aquila, via Vetoio, loc. Coppito, I-67010 L'Aquila, Italy*

[b] *Department of Mathematics, Champlain College Saint-Lambert, Quebec, J4P 3P2, Canada*

[c] *Department of Mathematics and Statistics, McGill University, Montreal, Quebec, H3A 2K6, Canada*

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Abstract

In this paper we study the hybrid quantum hydrodynamic model for nano-sized bipolar semiconductor devices in thermal equilibrium. By introducing a hybrid version of the Bhom potential, we derive a bipolar hybrid quantum hydrodynamic model, which is able to account for quantum effects in a localized region of the device for both electrons and holes. Coupled with Poisson equation for the electric potential, the steady-state system is regionally degenerate in its ellipticity, due to the quantum effect only in part of the device. This regional degeneracy of ellipticity makes the study more challenging. The main purpose of the paper is to investigate the existence and uniqueness of the weak solutions to this new type of equations. We first establish the uniform boundedness of the smooth solutions to the modified bipolar quantum hydrodynamic model by the variational method, then we use the compactness technique to prove the existence of weak solutions to the original hybrid system by taking hybrid limit. In particular, we account for two different kinds of hybrid behaviour. We perform the first hybrid limit when both electrons and holes behave quantum in a given region of the device, and the second one when only one carrier exhibits hybrid behaviour, whereas the other one is presented classically in the whole domain. The semi-classical limit results are also obtained. Finally, the theoretical results are tested numerically on a simple toy model.
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* Corresponding author.
E-mail address: bruno.rubino@univaq.it (B. Rubino).

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Contents

1. Introduction and derivation of the model

Due to recent progresses in semiconductor technology, we are able to project and produce nano-sized devices, operated by means of quantum effects. Quantum hydrodynamic models (QHDs), which describe such devices, give a fairly accurate account of the macroscopic behaviour of ultra small semiconductor devices only in terms of macroscopic quantities such as particle densities, current densities and electric fields (see [1,2,18,21,22,24,23,26,27,30,28] and reference therein). The bipolar QHD, reduced in thermal equilibrium, is the following 3×3 system of stationary equations [30,31]

$$\begin{cases} n\nabla V + T_n \nabla W_n(n) - 2\varepsilon^2 n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0, \\ -p\nabla V + T_p \nabla W_p(p) - 2\varepsilon^2 p\xi \nabla \left(\frac{\Delta \sqrt{p}}{\sqrt{p}} \right) = 0, \\ -\lambda^2 \Delta V = n - p - C, \\ \int_\Omega n(x)dx = N, \quad \int_\Omega p(x)dx = P, \quad \int_\Omega V(x)dx = 0, \end{cases} \tag{1}$$

where the unknown functions $n(x) \geq 0$, $p(x) \geq 0$ and $V(x)$ represent the particle density of electrons in the conduction band, the particle density of holes in the valence band, and the electrostatic potential, respectively. Ω is a bounded domain in $\mathbb{R}^d$, $d = 1, 2, 3$. ε is the scaled Planck's constant, and ξ is the ratio of the effective masses of electrons and holes. Without loss of generality, we assume $\xi = 1$ throughout the paper. T_n and T_p are the temperature constants for the electrons and the holes, respectively, and the constant λ is the minimal Debye length. $W_n(n)$ and $W_p(p)$ are the pressure functions for the electrons and the holes, respectively, and both are positive, continuously differentiable and increasing. $C(x)$ is the doping profile, which is assumed to be equal to $N_D - N_A$, where $N_D = N_D(x) \geq 0$ and $N_A = N_A(x) \geq 0$ are the space densities of donor and acceptor atoms, respectively. N (correspondingly P) is the total numbers of electrons (holes) in the conductivity band (the valence band), given by

$$N = n_i + \int_\Omega N_D(x)dx, \quad P = n_i + \int_\Omega N_A(x)dx,$$

where $n_i > 0$ is an intrinsic constant taking into account that the number of electrons (holes) in the conduction (valence) band is not only determined by doping but also by intrinsic thermal

excitation processes. The relation between N, P and C implies total charge neutrality. Hence, Poisson equation

$$-\lambda^2 \triangle V = n - p - C,$$

which provides a description of the electrostatic potential V, has exactly one solution V satisfying $\int_\Omega V(x)dx = 0$, by assuming $(n - p - C) \in L^2(\Omega)$.

Dividing the first and the second equations of (1) by n and p, respectively, differentiating them with respect to x, and substituting the third equation of (1) to the resulting equations, we get the following uniform 4th order elliptic equations

$$\begin{cases} 2\varepsilon^2 \Delta\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) - T_n \nabla\left(\frac{\nabla W_n(n)}{n}\right) = \frac{1}{\lambda^2}(n - p - C), \\ 2\varepsilon^2 \xi \Delta\left(\frac{\Delta\sqrt{p}}{\sqrt{p}}\right) - T_p \nabla\left(\frac{\nabla W_p(p)}{p}\right) = -\frac{1}{\lambda^2}(n - p - C). \end{cases} \tag{2}$$

The existence and uniqueness of the stationary solutions to (1) were proved by Unterreiter [30] by using the variational method and the semi-classical limit as $\varepsilon \to 0$ as well as the zero space charge limit $\lambda \to 0$ were also carried out by the compactness-by-convexity principle. The time-dependent solutions to the bipolar QHDs and their asymptotic convergence to the corresponding thermal equilibria were further investigated by G. Zhang et al. [31,32].

Regarding quantum phenomenon, the effect for the device is essential, but the related computations can be rather expensive. The above-mentioned system (1) is an ideal model where the quantum effect is presented everywhere in the device. However, the practical case is that the quantum effect is usually localized in a small regions of the device, whereas the other parts of the system can be treated classically. This is called a *hybrid* quantum effect case. Starting from this experimental observation, many theoretical hybrid approaches to model quantum semiconductor devices have been recently introduced. Basically, the idea is to employ a quantum description for the charges distribution in a small and well localized region of the device domain, and to use a simpler classical approach elsewhere, in order to reduce the computational efforts. The study concerning the classical and the quantum equations has recently become popular, see, for example [2,8,11,16–19,21,22,24–27,30,28] and references therein, but, as a new topic, the study related to hybrid systems is very limited, and several problems concerning the existence of solutions as well as their asymptotic behaviour still remain open. Some hybrid models of unipolar quantum hydrodynamics for semiconductors have been recently proposed [5,7,6,12,13,15,20,29]. The main difficulty is to establish a suitable set of interface conditions linking the two regions. In [10] and [14], a different approach was introduced, in order to avoid these difficulties. Inspired by the pioneering study [1], the authors of [10] and [14] physically derived an intrinsic hybrid equation by assuming that the quantum terms in the density of energy is modulated by means of a space dependent function, called $Q(x)$. That is, $Q = 1$ in the quantum domain and $Q = 0$ in the classical region. These two regions are smoothly connected by introducing an artificial semi-classical region. In this paper, we apply the same idea to derive a hybrid quantum hydrodynamic model for bipolar semiconductors device, by introducing a new term in the Bohm potential which depends on the gradient of the function Q. Then we will discuss a hybrid quantum bipolar model (H-QBM) matching classical and quantum hydrodynamical equation, limiting our analysis to isothermal condition. To the best of our knowledge, our work in this paper represents the first attempt to study a bipolar hybrid QHD system. Since the governing steady-state elliptic system is regionally degenerate, this causes us some essential difficulties in the theoretical study.

The main assumption is that the internal energies of the electrons and the holes do not depend on ∇n and ∇p respectively, in the whole domain, but just in a well defined sub-domain. Therefore we introduce a smooth function $Q^w(x) : \Omega \to [0, 1]$, for $w = n, p$, which indicates where the internal energy depends on the gradient of the charge density, i.e. we may regard Q^w as almost 0 in the classical region and almost 1 in the quantum region. We can write the internal energies e_w, for $w = n, p$, by

$$e_n(n, \nabla n) = T_n \ln n - Q^n \frac{\varepsilon^2}{2} \frac{\nabla n \cdot \nabla n}{n^2},$$
$$e_p(p, \nabla p) = T_p \ln p - Q^p \frac{\varepsilon^2}{2} \frac{\nabla p \cdot \nabla p}{p^2}.$$

The associated chemical potentials F_w, for $w = n, p$, can be written in terms of e_w like

$$F_w = \frac{\partial (w e_w)}{\partial w} - \nabla \cdot \left[w \frac{\partial (e_w)}{\partial \nabla w} \right].$$

Following [1], one finally obtains

$$F_w = \ln w - \varepsilon^2 \left(Q^w \left(\frac{\Delta w}{w} - \frac{1}{2} \frac{\nabla w \cdot \nabla w}{w^2} \right) + \frac{\nabla Q^w \cdot \nabla w}{w} \right)$$

or equivalently

$$F_w = \ln w + 2\varepsilon^2 \left(Q^w \left(\frac{\Delta \sqrt{w}}{\sqrt{w}} \right) + \frac{\nabla Q^w \cdot \nabla \sqrt{w}}{\sqrt{w}} \right).$$

The previous formula includes a new intrinsically hybrid expression of the Bhom potential:

$$B[w](x) = 2\varepsilon^2 \left(Q^w \left(\frac{\Delta \sqrt{w}}{\sqrt{w}} \right) + \frac{\nabla Q^w \cdot \nabla \sqrt{w}}{\sqrt{w}} \right).$$

Introducing the above expression in the stationary hydrodynamical equation with partial quantum effect, we obtain

$$\begin{cases} 2\varepsilon^2 w \nabla (Q^w \dfrac{\Delta(\sqrt{w})}{\sqrt{w}}) + \dfrac{\nabla Q^w \cdot \nabla(\sqrt{w})}{\sqrt{w}}) - T_w \nabla w + \nabla \cdot (\dfrac{J \otimes J}{w}) + w \nabla V = \dfrac{J}{\tau}, \\ J = constant, \end{cases} \tag{3}$$

where $w = n, p$, $\tau > 0$ is the relaxation time, J is the current density, and T_w is the electron and hole reference temperature, respectively. Thus, the system (3), coupled with Poisson equation, is referred to hybrid quantum hydrodynamic model (H-QHD). Here, as indicated before, $C(x)$ is the doping profile in $L^2(\Omega)$ and $\lambda > 0$ is the scaled Debye length.

In the sequel, taking $J = 0$ in the stationary hydrodynamic equation, we obtain the following system

$$\begin{cases} n\nabla V + T_n \nabla W_n(n) - 2\varepsilon^2 n\nabla\left(Q^n \frac{\Delta\sqrt{n}}{\sqrt{n}} + \frac{\nabla Q^n\cdot\nabla\sqrt{n}}{\sqrt{n}}\right) = 0, \\ -p\nabla V + T_p \nabla W_p(p) - 2\varepsilon^2 p\nabla\left(Q^p \frac{\Delta\sqrt{p}}{\sqrt{p}} + \frac{\nabla Q^p\cdot\nabla\sqrt{p}}{\sqrt{p}}\right) = 0, \\ -\lambda^2\Delta V = n - p - C, \\ \int_\Omega n(x)dx = N, \quad \int_\Omega p(x)dx = P, \quad \int_\Omega V(x)dx = 0, \end{cases} \tag{4}$$

where $x \in \Omega \subset \mathbf{R}^d$, for $d = 1, 2, 3$.

Dividing the first and second equation of (4) by n and p, respectively, differentiating them in x, and substituting the third equation of (4) to the resultant equations, we have

$$\begin{cases} 2\varepsilon^2\Delta\left(Q^n \frac{\Delta\sqrt{n}}{\sqrt{n}} + \frac{\nabla Q^n\cdot\nabla\sqrt{n}}{\sqrt{n}}\right) - T_n\nabla\cdot\left(\frac{\nabla W_n(n)}{n}\right) = \frac{1}{\lambda^2}(n - p - C), \\ 2\varepsilon^2\Delta\left(Q^p \frac{\Delta\sqrt{p}}{\sqrt{p}} + \frac{\nabla Q^p\cdot\nabla\sqrt{p}}{\sqrt{p}}\right) - T_p\nabla\cdot\left(\frac{\nabla W_p(p)}{p}\right) = -\frac{1}{\lambda^2}(n - p - C). \end{cases} \tag{5}$$

Accounting for the properties of the quantum effect functions Q^w, the typical example of Q^w is the Heaviside function. This leads the above 4th order elliptic equations to be regionally degenerate, and causes the study for the hybrid QHD case to be totally different from the regular QHD case. In fact, if the solutions exist, they are weak and their regularity in the classical sense is lost.

The main purpose in this paper is to investigate the existence of the weak solutions to the hybrid quantum hydrodynamic model (4), and to perform the semi-classical limit as $\varepsilon \to 0$. The adopted approach is the artificial vanishing viscosity method. Since we cannot directly work on the system (4) due to its regional degeneracy of the 4th order ellipticity, we first artificially add some viscosity to the quantum effect terms to modify the system (4) to be uniformly elliptic. Then we define an energy functional, and use the variational method to prove that the corresponding variational problem has a unique minimizer in a suitable space. Such a minimizer is just the solution of the modified 4th order uniformly elliptic equations. After establishing some regularities and uniform boundedness of the solution to the artificial viscosity problem, we further show the existence of the weak solution for the original hybrid QHD (4) by using the vanishing viscosity technique, namely, by taking the hybrid limit.

This paper is organized as follows. In Section 2, we consider the modified hybrid QHD model with $Q^w \geq q > 0$ such that the system (4) is uniformly elliptic, and prove the existence of solutions for a suitably regularized hybrid problem, namely approximating Q_w by a strictly positive sequence smooth functions. In Section 3 we state the main results of this paper. Here we discuss the convergence of the solutions of the approximating problem to two different classes of hybrid models. In the first case we assume that both the electrons and the holes exhibit quantum behaviour in a small region of the device, whereas in the rest of device both the carriers behave classically. In the second case just the electrons exhibit the hybrid behaviour as in the previous case, whereas the holes behave classically on whole domain. In Section 4, we discuss the semi-classical limit of the approximation problem and finally in Section 5 our model and the hybrid limits are validated numerically on a simple toy model.

2. Regularized bipolar H-QHD model

We consider the system (4) derived heuristically in the previous section. We recall that the final purpose of this paper is to introduce and discuss the hybrid limits for the thermal equilibrium solution of the bipolar quantum hydrodynamic model. Therefore we ideally divide the domain Ω into two disjoint subsets: a classical sub-domain Ω_c and a quantum one Ω_q. Since there are

not quantum effects in the classical domain, $Q^n = Q^p = 0$ for all $x \in \Omega_c$, the equations $(4)_1$ and $(4)_2$ degenerate. This makes the problem very difficult to be solved from the theoretical point of view. Therefore, following the approach proposed in [14], we construct a sequence of solutions for a suitable set of regularized problems, then we prove that this sequence converges (weakly) to a weak solution of the correspondent bipolar hybrid problem.

To obtain the approximate problem, we introduce a particular choice for the smooth functions Q^n and Q^p, by setting, for $w = n, p$,

$$Q^w(x) = (H * \eta_{\alpha_w})(x) = \int_\Omega H(x-y)\eta_{\alpha_w}(y)dy + \alpha_w =: H^w_{\alpha_w}(x), \tag{6}$$

where η_{α_w} are the smoothing kernels (or mollifiers) and $\alpha_w \in (0, \delta]$, $\delta \ll 1$. We have that $H^w_{\alpha_w}(x) \to H(x)$ if $\alpha_w \to 0^+$, where $H(x)$ is the usual Heaviside function, namely

$$H(x) = \begin{cases} 1, \ \forall x \in \Omega_q, \\ 0, \ \forall x \in \Omega_c. \end{cases} \tag{7}$$

Integrating $(4)_1$ and $(4)_2$ with respect to x, we obtain the following equivalent form

$$\begin{cases} 2\varepsilon^2 \nabla \cdot \left(H^n_{\alpha_n} \nabla \sqrt{n}\right) = \sqrt{n}(V + g_n(n) - \beta_n), \\ 2\varepsilon^2 \nabla \cdot \left(H^p_{\alpha_p} \nabla \sqrt{p}\right) = \sqrt{p}(-V + g_p(p) - \beta_p), \\ -\lambda^2 \Delta V = n - p - C, \\ \int_\Omega n(x)dx = N, \quad \int_\Omega p(x)dx = P, \quad \int_\Omega V(x)dx = 0, \end{cases} \tag{8}$$

where

$$g'_w(t) := \frac{1}{t}\frac{dW_w(t)}{dt} \quad \text{for } w = n, p,$$

and $\beta_n, \ \beta_p \in \mathbf{R}$, are the Lagrange multipliers associated with the constrains $\int_\Omega n(x)dx = N$ and $\int_\Omega p(x)dx = P$.

The thermal equilibrium solution we are looking for must satisfy (4) (or equivalently (8)), but this provides just a necessary condition. A physically consistent thermal equilibrium solution must also minimize the following energy functional:

$$\begin{aligned} \Xi_{\alpha_n,\alpha_p}(n, p) := {} & 2\varepsilon^2 \int_\Omega H^n_{\alpha_n} |\nabla \sqrt{n}|^2 dx + 2\varepsilon^2 \int_\Omega H^p_{\alpha_p} |\nabla \sqrt{p}|^2 dx \\ & + \int_\Omega G_n(n)dx + \int_\Omega G_p(p)dx \\ & + \frac{\lambda^2}{2} \int_\Omega |\nabla V[n - p - C]|^2 dx, \end{aligned} \tag{9}$$

where $G_w(v) = \int_1^v g(s)_w ds, \ \text{for } w = n, p.$

It is not difficult to show that (8) are the Euler–Lagrange equations of the energy functional $\Xi_{\alpha_n,\alpha_p}(n, p)$ defined above, as done in [14]. All the results presented in this paper refer to the following assumptions, and can be regarded as a generalized hybrid version of those considered in [30].

MAIN ASSUMPTIONS:

(a) $\Omega \subset \mathbb{R}^d$, where $d = 1, 2, 3$, is a bounded domain with $\partial\Omega \in C^{0,1}$.
(b) Let $H^n_{\alpha_n}$ and $H^p_{\alpha_p}$ be the functions defined in (6). Assume that there exist two strictly positive sequences of constants, called H_{m,α_w} and H_{M,α_w}, such that $\lim_{\alpha_w\to 0^+} H_{m,\alpha_w} = 0$, $\lim_{\alpha_w\to 0^+} H_{M,\alpha_w} = 1$ and

$$H_{m,\alpha_w} \le H^w_{\alpha_w}(x) \le H_{M,\alpha_w},\ \forall x \in \Omega,$$

where $w = n, p$.
(c) There exists a constant $K = K(\Omega) > 0$ such that

$$\|V[f]\|_{L^\infty} \le K\|f\|_{L^2}.$$

(d) The doping profile $C \in L^\infty$, moreover $N - P = \int_\Omega C(x)dx$, $N > \int_\Omega C^+(x)dx$ and $P > \int_\Omega C^-(x)dx$.
e) $g_w \in C(0,\infty) \cap L^1_{loc}([0,\infty))$, for $w = n, p$, is a strictly increasing function such that:

$$\lim_{v\to+\infty} g_w(v) = +\infty, \qquad \lim_{v\to 0^+} g_n(v) =: \underline{g_w} \in (-\infty, +\infty).$$

The assumption (e) is verified by the enthalpy functions more widely used in modelling semiconductor devices, namely $g(\kappa) = \ln(\kappa)$ and $g(t) = \frac{\kappa}{\kappa-1}t^{\kappa-1}$, corresponding to the pressure functions $W(t) = t^\kappa$, for $\kappa = 1$ and $\kappa > 1$ respectively.

The main result of this section is the following theorem

Theorem 2.1. *Under the assumptions (a)–(e), the functional Ξ_{α_n,α_p} admits a unique minimizer (n, p) in*

$$\Gamma = \Big\{\rho_n, \rho_p \in L^1(\Omega) :\ \rho_n, \rho_p \ge 0,\ \sqrt{\rho_n}, \sqrt{\rho_n} \in H^1(\Omega),\ \int_\Omega \rho_n dx = N,\ \int_\Omega \rho_p dx = P\Big\}, \tag{10}$$

solving $(8)_1$ and $(8)_2$ (or equivalently $(4)_1$ and $(4)_2$). Consequently, $V \in H^1(\Omega)$ is defined as the unique solution to Poisson equation of $(8)_3$. Therefore the set (n, p, V) is the unique solution of the problem (8).

From now on, without loss of generality, we assume $g_n = g_p = g$, and $G(v) = \int_1^v g(\sigma)d\sigma$, in order to simplify the notation.

First of all, following [30], we introduce a truncated enthalpy function g_i defined in the following way:

Definition 2.2. For $i \in (0, \infty]$ and $\nu \in [0, \infty)$, we define the truncated enthalpy

$$g_i(\nu) = \min\{i\nu, \max(-i, g(\nu))\}, \quad \text{and} \quad G_i(\nu) = \int_0^\nu g_i(\sigma)d\sigma. \tag{11}$$

As shown in [28], one can prove

$$\begin{aligned} &G_i \geq G_m \\ &G_i \leq |G_m| + |G(\nu)| \\ &\nu g_i(\nu) \geq G_m, \end{aligned} \tag{12}$$

where $G_m := \inf_{\nu\in(0,\infty)} G(\nu)$ is a constant independent of i.

Before proving Theorem 2.1, we present some introductory results, starting from the following lemma:

Lemma 2.3. *Under the assumptions (a)–(e) for all $i \in (0, \infty]$, the following functional*

$$\begin{aligned} \Xi^+_{\alpha_n,\alpha_p,i}(r,s) = 2\varepsilon^2 \int_\Omega H^n_{\alpha_n}|\nabla r|^2 dx + 2\varepsilon^2 \int_\Omega H^p_{\alpha_p}|\nabla s|^2 dx + \int_\Omega G_i((r^+)^2)dx \\ + \int_\Omega G_i((s^+)^2) + \frac{\lambda^2}{2}\int_\Omega |\nabla V[(r^+)^2 - (s^+)^2 - C]|^2 dx \end{aligned} \tag{13}$$

has a unique non-negative minimizer (R_i, S_i) in

$$\Gamma^+ = \left\{ (r,s) \in H^1(\Omega)\times H^1(\Omega) : \int_\Omega (r^+)^2(x)dx = N, \int_\Omega (s^+)^2(x)dx = P \right\},$$

where s^+ and r^+ are the positive part of r and s, respectively,

Remark 2.4. This lemma has been already proved in [30] for the standard quantum hydrodynamic problem, that is when $H^n_{\alpha_n}, H^p_{\alpha_p} \equiv 1$ in Ω. Here we basically apply the same arguments by observing that $H^n_{\alpha_n}, H^p_{\alpha_p}$ are strictly positive functions (see the assumption (b)).

Proof. The existence of a minimizer $(R_i, S_i) \in \Gamma^+$ for $\Xi^+_{\alpha_n,\alpha_p,i}$ follows from the standard theory.

To prove that (R_i, S_i) are non-negative functions, we observe that also the positive part (R_i^+, S_i^+) belongs to Γ^+ and $\Xi^+_{\alpha_n,\alpha_p,i}(R_i^+, S_i^+) \leq \Xi^+_{\alpha_n,\alpha_p,i}(R_i, S_i)$, which implies $(R_i^+, S_i^+) = (R_i, S_i)$.

Finally we show that (R_i, S_i) is the unique minimizer of the functional $\Xi^+_{\alpha_n,\alpha_p,i}$, proceeding by contradiction. Let us assume that there exist two couples $(R_i, S_i) \geq 0$ and $(R_i^*, S_i^*) \geq 0$ minimizing $\Xi^+_{\alpha_n,\alpha_p,i}$. Following [30] we introduce $(R_\delta, S_\delta) \geq 0$, defined as follows:

$$R_\delta = \sqrt{\delta(R_i)^2 + (1-\delta)(R_i^*)^2}, \qquad S_\delta = \sqrt{\delta(S_i)^2 + (1-\delta)(S_i^*)^2}. \tag{14}$$

Both R_δ and S_δ belong Γ^+ and it is not difficult to see that

$$\Xi^+_{\alpha_n,\alpha_p,i}(R_\delta, S_\delta) < \delta\,\Xi^+_{\alpha_n,\alpha_p,i}(R_i, S_i) + (1-\delta)\,\Xi_{\alpha_n,\alpha_p,i}(R_i^*, S_i^*), \tag{15}$$

which contradicts the assumption that both (R_i, S_i) and (R_i^*, S_i^*) are minimizers of the energy functional $\Xi^+_{\alpha_n,\alpha_p,i}$ in Γ^+. This concludes the proof. □

From now on, due to the positiveness of the minimizers of $\Xi^+_{\alpha_n,\alpha_p,i}$, stated by the previous lemma, we can omit the index "+" in the energy functional.

Now we show that the minimizer of $\Xi_{\alpha_n,\alpha_p,i}$, is also the solution of a suitable Euler–Lagrange problem, namely:

Lemma 2.5. *Let $i \in (1,\infty)$. The minimizer (R_i, S_i) of $\Xi_{\alpha_n,\alpha_p,i}$ on the set Γ^+ satisfies the Euler–Lagrange equations*

$$\begin{cases} 2\varepsilon^2 \nabla\cdot\left(H^n_{\alpha_n}\nabla R_i\right) = R_i(V_i + g_i(R_i^2) - \beta_{n,i}) \\ 2\varepsilon^2 \nabla\cdot\left(H^p_{\alpha_p}\nabla S_i\right) = S_i(-V_i + g_i(S_i^2) - \beta_{p,i}) \\ -\lambda^2\Delta V_i = R_i^2 - S_i^2 - C \\ \int_\Omega R_i^2(x)dx = N, \quad \int_\Omega S_i^2(x)dx = P, \quad \int_\Omega V_i(x)dx = 0. \end{cases} \tag{16}$$

Moreover (R_i, S_i) verifies homogeneous Neumann boundary conditions.

Remark 2.6. In this lemma we refer to the homogeneous Neumann boundary conditions satisfied by the minimizers since they are necessary in order to perform reasonable numerical simulations.

Proof. We know that $(R_i, S_i) \in \Gamma^+$, take $l \in \mathbb{R}$ and $\varphi \in H^1(\Omega)$, such that $R_i + l\varphi \in \Gamma^+$ and $S_i + l\varphi \in \Gamma^+$. We derive just the first equation in (16), the second one can be derived in the same way.

$$\begin{aligned} &\Xi^+_{\alpha_n,\alpha_p,i}(R_i + l\varphi, S_i) - \Xi^+_{\alpha_n,\alpha_p,i}(R_i, S_i) \\ &= -2\varepsilon^2 \int_\Omega (H^n_{\alpha_n}|\nabla R_i + l\nabla\varphi|^2 - H^n_{\alpha_n}|\nabla R_i|^2)dx \\ &\quad + \int_\Omega \left(G_i\left((R_i + l\varphi)^2\right) - G_i\left(R_i^2\right)\right)dx \\ &\quad + \frac{\lambda^2}{2}\int_\Omega \left(\left|\nabla V_i\left[(R_i + l\varphi))^2 - (S_i)^2 - C\right]\right|^2 - \left|\nabla V_i\left[(R_i)^2 - (S_i)^2 - C\right]\right|^2\right)dx \\ &=: I_1 + I_2 + I_3. \end{aligned}$$

It is easy to see that

$$I_1 = 2\varepsilon^2 \int_\Omega H^n_{\alpha_n} \left(|\nabla R_i|^2 + l^2 |\nabla \varphi|^2 + 2\nabla R_i \cdot l\nabla\varphi \right) dx - 2\varepsilon^2 \int_\Omega H^n_{\alpha_n}(x) |\nabla R_i|^2 dx$$
$$= 2\varepsilon^2 \int_\Omega H^n_{\alpha_n} \nabla R_i \cdot l\nabla\varphi dx + o(l),$$
$$I_2 = \int_\Omega \left(\int_{R_i^2}^{(R_i + l\varphi)^2} g_i(u) du \right) dx = \int_\Omega 2R_i l\varphi g_i(R_i^2) dx + o(l).$$

Then, concerning the term I_3, following [9], one has

$$I_3 = 2 \int_\Omega V_i \left[R_i^2 - S_i^2 - C \right] R_i l\varphi dx + o(l).$$

Finally we obtain

$$\Xi^+_{\alpha_n,\alpha_p,i}(R_i + l\varphi, S_i) - \Xi^+_{\alpha_n,\alpha_p,i}(R_i, S_i) \tag{17}$$
$$= 2 \left(\varepsilon^2 \int_\Omega H^n_{\alpha_n} \nabla R_i \cdot l\nabla\varphi dx + \int_\Omega R_i \left(g_i + V_i - \beta_{n,i} \right) l\varphi dx \right) + o(l).$$

Observing that if (R_i, S_i) is a minimizer of $\Xi_{\alpha_n,\alpha_p,i}$ in Γ^+, then as $l \to 0^\pm$, the difference $\Xi^+_{\alpha_n,\alpha_p,i}(R_i + l\varphi, S_i) - \Xi^+_{\alpha_n,\alpha_p,i}(R_i, S_i)$ computed as in (17) is non-negative. The first equation in (16) can be formally derived dividing by l and considering $l \to 0^\pm$.

To prove that couple R_i, S_i verifies homogeneous Neumann boundary condition on $\partial\Omega$, we use as test function for (16) $\varphi \in H^1(\Omega)$. □

The case $\underline{g} = -\infty$ (see the assumption (e)), which corresponds to $i = \infty$, can not be included in Lemma 2.5 due to the lack of differentiability of $G_i(t)$ for $t = 0$ (see [30]). In the following lemma, we derive a set of a priori estimates needed to perform the limit $i \to \infty$.

Lemma 2.7. *Let (R_i, S_i) be the unique non-negative minimizer to (13) in Γ^+, then R_i and S_i verify the following set of estimates:*

$$\|R_i\|_{L^6}, \|S_i\|_{L^6} \le K, \tag{18}$$
$$\|V_i\|_{L^\infty} \le K, \tag{19}$$
$$\int_\Omega R_i^2 V_i dx \le K, \quad \int_\Omega S_i^2 V_i dx \le K, \tag{20}$$
$$\int_\Omega R_i V_i dx \le K, \quad \int_\Omega S_i V_i dx \le K, \tag{21}$$

$$\int_\Omega R_i^2 g_i(R_i^2)dx \le K, \quad \int_\Omega S_i^2 g_i(S_i^2)dx \le K, \tag{22}$$

$$|\beta_{n,i}|, |\beta_{p,i}| \le K, \tag{23}$$

where K denotes a general i-independent constant.

Proof. We just prove the estimates listed above for R_i, with analogous arguments the same results can be proved for S_i. We basically recall the results given in [28–30] and we adapt them to our problem.

First of all we prove that $\Xi_{\alpha_n,\alpha_p,i}$ is bounded from above, uniformly in i. Following the approach proposed in [28], we introduce $M_n \equiv \sqrt{N/\Omega}$ and $M_p \equiv \sqrt{P/\Omega}$. Clearly M_n and M_p belong to Γ^+ and $\Xi_{\alpha_n,\alpha_p,i}(R_i, S_i) \le \Xi_{\alpha_n,\alpha_p,i}(M_n, M_p)$ indeed (R_i, S_i) is the unique minimizer of the functional $\Xi_{\alpha_n,\alpha_p,i}$. Moreover, due to the assumption (c) and $(12)_2$ we get

$$\begin{aligned}
&\Xi_{\alpha_n,\alpha_p,i}(M_n, M_p)\\
&\le |\Omega|(G_i(M_n^2) + G_i(M_p^2)) + |\Omega|K\int_\Omega (M_n^2 - M_p^2 - C)^2 dx\\
&\le |\Omega|(G(M_n^2) + G(M_p^2)) + 2|G_m| + |\Omega|K\int_\Omega (M_n^2 - M_p^2 - C)^2 dx,
\end{aligned}$$

which implies, in view of the assumptions (d), that

$$\Xi_{\alpha_n,\alpha_p,i}(R_i, S_i) \le K.$$

Finally, by using the relation $(12)_1$ we get

$$\begin{aligned}
&2\varepsilon^2 H_{m,\alpha_n}\int_\Omega |\nabla R_i|^2 dx + 2\varepsilon^2 H_{m,\alpha_p}\int_\Omega |\nabla S_i|^2\, dx + 2G_m|\Omega|\\
&+ \frac{\lambda^2}{2}\int_\Omega |\nabla V_i[R^2 - S^2 - C]|^2 dx \le K.
\end{aligned} \tag{24}$$

The constrains $(8)_4$ together to (24) and to the assumption (b), imply

$$\|R_i\|_{H^1}, \|S_i\|_{H^1} \le K$$

and then (18).

Inequality (19) follows from the assumption (c), taking into account that $C \in L^\infty$ (see the assumption (d)). Moreover, the inequalities (20) and (21) can be easily proved in view of (19), recalling that $\|R_i\|_{L^2}^2 = N$.

Finally, using the approach detailed in [28] we prove (22) and (23). First of all we introduce m_i as

$$m_i = \frac{\int_\Omega R_i^2 dx}{\int_\Omega R_i dx}.$$

We show by contradiction that this quantity is well defined, that is $\int_\Omega R_i dx > 0$. We have $R_i \geq 0$ for all $x \in \Omega \subset \mathbb{R}^d$, with $d = 1, 2, 3$. Assume $\int_\Omega R_i dx = 0$, then $R_i = 0$ a.e, which contradicts $(8)_4$. Therefore there exists $K_i > 0$, such that $\int_\Omega R_i \geq K_i$.

Let us multiply $(8)_1$ by $(R_i - m_i)$ and integrate it by parts. After some calculations, in view of (20)–(21), we get

$$\begin{aligned} &\int_\Omega R_i^2 g_i(R_i^2) dx - m_i \int_\Omega R_i g_i(R_i^2) dx \\ &= -2\varepsilon^2 \int_\Omega H_{\alpha_n}^n |\nabla R_i|^2 dx + \int_\Omega R_i^2 V_i dx - m_i \int_\Omega R_i V_i dx \leq K. \end{aligned} \tag{25}$$

Then the inequality (22) follows from (25) as showed in [28].

Finally we show (23). We multiply $(8)_1$ by R_i and we integrate by part, after some simple calculations we get

$$\begin{aligned} \int_\Omega R_i^2 \beta_{n,i} dx &= N\beta_{n,i}|\Omega| \\ &= 2\varepsilon^2 \int_\Omega H_{\alpha_n}^n |\nabla R_i|^2 dx + \int_\Omega R_i^2 V_i dx + \int_\Omega R_i^2 g_i(R_i^2) dx \\ &\leq K. \end{aligned} \tag{26}$$

Therefore, we obtain $N\beta_{n,i}|\Omega| \leq K$ and then (23). □

In the following lemma, we prove that both R_i and S_i are bounded from above by a given constant K_M.

Lemma 2.8. *Assume (a)–(e), then there exists a constant K_M, independent of i, such that $R_i, S_i \leq K_M$.*

Proof. Given $K_M > 1$ we multiply the first equation in (16) by $[R_i - K_M]^+ / R_i$. After an integration by parts we get

$$\begin{aligned} &2\varepsilon^2 K_M \int_\Omega H_{\alpha_n}^n \frac{|\nabla [R_i - K_M]^+|^2}{R_i^2} dx \\ &= \int_\Omega [R_i - K_M]^+ (-V_i - g_i(R_i^2) + \beta_{n,i}) dx. \end{aligned} \tag{27}$$

Using the results summarized in the Lemma 2.7 and the monotonicity of the enthalpy function $g(\sigma)$, we estimate the right hand side term in (27) as:

$$\int_\Omega [R_i - K_M]^+(-V_i - g_i(R_i^2) + \beta_{n,i})dx \le (K - g_i(K_M^2)) \int_\Omega [R_i - K_M]^+ dx, \tag{28}$$

where K is a suitable constant independent of i.

Combining (27) and (28), we obtain

$$\begin{aligned}&(K - g_i(K_M^2)) \int_\Omega [R_i - K_M]^+ dx \\ &\ge 2\varepsilon^2 K_M \int_\Omega H_{\alpha_n}^n \frac{|\nabla [R_i - K_M]^+|^2}{R_i^2} dx \ge 0.\end{aligned} \tag{29}$$

Fixing K_M large enough, the left hand side in (29) becomes negative, which implies $R_i \le K_M$. An analogous result holds for S_i. □

In the following lemma, we will prove that R_i and S_i are strictly positive.

Lemma 2.9. *Assume (a)–(e) hold, then R_i, S_i are strictly positive.*

Proof. The proof is given in the line of [28]. As usual, we show the result for R_i, the same holds for S_i. We consider $(16)_1$

$$-2\varepsilon^2 \nabla \cdot (H_{\alpha_n}^n \nabla R_i) + R_i(V_i + g_i(R_i^2) - \beta_{n,i}) = 0 \tag{30}$$

that we rewrite as

$$-2\varepsilon^2 \nabla \cdot (a \nabla R_i) + b_i R_i = 0, \tag{31}$$

where $a = H_{\alpha_n}^n$ and $b_i = V_i + g_i(R_i^2) - \beta_{n,i}$. As $a \in C^\infty$, $b_i \in L^\infty$ and $R_i \ge 0$, we have enough regularity for the solution R_i to apply the Harnack's inequality:

$$\sup_{B_\rho(y)} R_i \le c \inf_{B_\rho(y)} R_i,$$

for $c = c(\Omega, \rho)$ and for all $y \in \Omega$, $\rho > 0$, with $B_{4\rho}(y) \subset \Omega$. By contradiction if R_i was zero for some y in Ω, then one would have $R_i \equiv 0$ in Ω, which contradicts the assumption $\|R_i^2\|_{L^2} = N$. □

Now we are able to prove Theorem 2.1.

Proof. In order to pass the limit as $i \to +\infty$ in the weak formulation of (16), we have to distinguish two cases. If $\underline{g_n} = -\infty$, since b_i in (30) is in L^∞, it is always possible to choose $K_m > 0$, independent of i, such that

$$\lim_{i \to +\infty} g_i(K_m^2) < -\|V_i - \beta_{n,i}\|_{L^\infty} \tag{32}$$

As in [28], we introduce, for i large enough, the set $\Omega_i = \{x \in \Omega : R_i \leq K_m\}$. Proceeding by contradiction, if Ω_i was not empty, $\nabla \cdot (H^n_{\alpha_n} \nabla R_i) \leq 0$ in Ω_i, then by the maximum principle R_i would be constant on Ω_i. Therefore $R_i \geq K_m > 0$ on Ω.

In the second case, corresponding to $\underline{g_n} > -\infty$, there are no problems in the limit due to the continuity of $R_i g_i(R_i^2)$ and to the boundedness of R_i $(0 < R_i \leq K_m)$. Accounting for the estimates listed above and for preparatory lemmas, there exist a sequence $(R_i, S_i)_{i \in \mathbf{N}}$ such that, for $i \to \infty$, $R_i \to R$ and $S_i \to S$ weakly in $H^1(\Omega)$ and weak* in $L^\infty(\Omega)$. Proceeding as in [28] and [30], one can prove that (R, S) are the unique minimizers of the functional E^+_∞ in Γ^+ and solve the correspondent Euler–Lagrange problem. □

3. Main results: hybrid limits

In this section we discuss the so called *hybrid limits*. As explained in the introduction, in the contest of the semiconductor models, the word *hybrid* indicates the coupling between a classic model and a quantum model, describing the behaviour of the charged carriers in different regions of the device domain. Here the assumptions (b) and (e) must be modified. In particular, in order to simplify the notation

For readability, the assumptions we are using in this section are listed below. We assume the case in which both $H^n_{\alpha_n}(x)$ and $H^p_{\alpha_p}(x)$ converge to an appropriate step function. In this way the device is ideally divided into two sub-domains: a classic sub-domain where $H^n_{\alpha_n}, H^p_{\alpha_p} \to 0$ and a quantum one where $H^n_{\alpha_n}, H^p_{\alpha_p} \to 1$.

In order to simplify the notation we set $\alpha_n = \alpha_p = \alpha$, therefore $H^n_{\alpha_n}(x) = H^p_{\alpha_p}(x) = H_\alpha(x)$, where

$$H_\alpha(x) = \int_\Omega H(x-y)\eta_\alpha(y)dy + \alpha. \tag{33}$$

As usual η_α is the smoothing kernel (or mollifier), $\alpha \in (0, \delta]$, $\delta > 0$ and $H_\alpha \to H$ if $\alpha \to 0^+$. Then the assumption (b) becomes

(b_h) Let H_α be the functions defined in (33). Assume that there exist two strictly positive sequences of constants, called $H_{m,\alpha}$ and $H_{M,\alpha}$, such that

$$\lim_{\alpha \to 0^+} H_{m,\alpha} = 0, \qquad \lim_{\alpha \to 0^+} H_{M,\alpha} = 1$$

and

$$H_{m,\alpha} \leq H_\alpha x \leq H_{M,\alpha} \leq 1, \ \forall x \in \Omega.$$

Moreover, the assumption (e) must be also modified. In fact, it is not possible to obtain an α-independent lower bound for n_α as p_α if $\underline{g} = -\infty$, due to the degeneracy of the ellipticity for $\alpha \to 0^+$. Therefore (e) becomes

(e_h) $g_\omega \in C(0, \infty) \cap L^1_{loc}([0, \infty))$, for $w = n, p$, is a strictly increasing function such that:

$$\lim_{\nu \to +\infty} g_\omega(\nu) = +\infty, \qquad \lim_{\nu \to 0^+} g_n(\nu) := \underline{g_\omega} \in [0, +\infty).$$

3.1. First hybrid limit: fully hybrid limit

Introducing the new notation for α as listed above, (8) becomes

$$\begin{cases} 2\varepsilon^2\nabla\cdot\left(H_\alpha\nabla\sqrt{n_\alpha}\right)=\sqrt{n_\alpha}(V_\alpha+g(n_\alpha)-\beta_{n\alpha}),\\ 2\varepsilon^2\nabla\cdot\left(H_\alpha\nabla\sqrt{p_\alpha}\right)=\sqrt{p_\alpha}(-V_\alpha+g(p_\alpha)-\beta_{p_\alpha}),\\ -\lambda^2\Delta V_\alpha=n-p-C,\\ \int_\Omega n_\alpha(x)dx=N,\quad \int_\Omega p_\alpha(x)dx=P,\quad \int_\Omega V_\alpha(x)dx=0, \end{cases} \tag{34}$$

where the subscript α indicates that the solutions of the problem above depend on the parameter α, introduced in (33).

The relevant energy is

$$\begin{aligned} \Xi_\alpha=&\,2\varepsilon^2\int_\Omega H_\alpha|\nabla\sqrt{n_\alpha}|^2dx+2\varepsilon^2\int_\Omega H_\alpha|\nabla\sqrt{p_\alpha}|^2dx\\ &+\int_\Omega G(n_\alpha)dx+\int_\Omega G(p_\alpha)dx\\ &+\frac{\lambda^2}{2}\int_\Omega|\nabla V[n_\alpha-p_\alpha-C]|^2dx. \end{aligned} \tag{35}$$

Our aim is to prove that for $\alpha\to 0$ the sequence of solutions $(n_\alpha, p_\alpha, V_\alpha)$ of the problem (34) converges in some suitable space to the weak solution of the following *hybrid model*

$$\begin{cases} 2\varepsilon^2\nabla\cdot\left(H\nabla\sqrt{n}\right)=\sqrt{n}(V+g(n)-\beta_n),\\ 2\varepsilon^2\nabla\cdot\left(H\nabla\sqrt{p}\right)=\sqrt{p}(-V+g(p)-\beta_p),\\ -\lambda^2\Delta V=n-p-C,\\ \int_\Omega n(x)dx=N,\quad \int_\Omega p(x)dx=P,\quad \int_\Omega V(x)dx=0. \end{cases} \tag{36}$$

Definition 3.1. A set of functions $(n, p, V)(x)$ is said to be a weak solution of (36), if it holds

$$2\varepsilon^2\int_\Omega H\nabla\sqrt{n}\cdot\nabla\phi dx+\int_\Omega\sqrt{n}(V+g(n)-\beta_n)\phi dx=0, \tag{37}$$

$$2\varepsilon^2\int_\Omega H\nabla\sqrt{p}\cdot\nabla\phi dx+\int_\Omega\sqrt{p}(-V+g(p)-\beta_p)\phi dx=0, \tag{38}$$

$$\lambda^2\int_\Omega\nabla V\cdot\nabla\phi dx=\int_\Omega(n-p-C)\phi dx, \tag{39}$$

$$\int_\Omega n(x)dx=N,\quad \int_\Omega p(x)dx=P,\quad \int_\Omega V(x)dx=0, \tag{40}$$

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

The convergence result, namely, the existence of the weak solution to (36), is summarized as follows.

Theorem 3.2. *Assume (a), (b_h), (c), (d), (e_h). Let $(n_\alpha, p_\alpha, V_\alpha) \in L^\infty(\Omega) \cap H^1(\Omega)$ be the sequence of solutions of the problem (34). Then there exist (n, p, V) such that*

$$\begin{cases} n_\alpha \rightharpoonup n \ \ in\ L^2(\Omega), \\ p_\alpha \rightharpoonup p \ \ in\ L^2(\Omega), \\ V_\alpha \rightharpoonup V \ \ in\ H^1(\Omega), \end{cases} \qquad as\ \alpha \to 0 \tag{41}$$

and the limit functions $(n, p, V)(x)$ are the weak solutions to hybrid problem (36).

Proof. Within this section $\bar{K}$ is a general α-independent constant. Due to the conservation of the total number of particles, $\|n_\alpha\|_{L^1(\Omega)} = N$ and $\|p_\alpha\|_{L^1(\Omega)} = P$. Arguing as in Lemma 2.7 we can prove the following relations

$$\|V_\alpha\|_{L^\infty} \le \bar{K}, \tag{42}$$

$$\int_\Omega n_\alpha V_\alpha dx \le \bar{K}, \quad \int_\Omega p_\alpha V_\alpha dx \le \bar{K}, \tag{43}$$

$$\int_\Omega \sqrt{n_\alpha} V_\alpha dx \le \bar{K}, \quad \int_\Omega \sqrt{p}\alpha V_\alpha dx \le \bar{K}, \tag{44}$$

$$\int_\Omega n_\alpha g_\alpha(n_\alpha) dx \le \bar{K}, \quad \int_\Omega p_\alpha g_\alpha(p_\alpha) dx \le \bar{K}, \tag{45}$$

$$|\beta_{n,\alpha}|, |\beta_{p,\alpha}| \le \bar{K}. \tag{46}$$

As shown in Lemma 2.8, we can find a positive constant $\bar{K}_M$ such that

$$n_\alpha,\ p_\alpha \le \bar{K}_M, \tag{47}$$

and then

$$\int_\Omega n_\alpha^2 dx \le \bar{K}_M N \le \bar{K}, \qquad \int_\Omega p_\alpha^2 dx \le \bar{K}_M P \le \bar{K}.$$

Therefore there exists $(n, p)(x)$ such that

$$(n_\alpha, p_\alpha) \rightharpoonup (n, p) \ \text{ weakly in } \ L^2(\Omega). \tag{48}$$

We multiply the Poisson equation $(34)_3$ by V and integrate by parts

$$\int_\Omega |\nabla V|^2 dx = \frac{1}{\lambda^2} \int_\Omega V(n - p - C) dx$$

Then, using the Young's inequality, in view of the Poincarè inequality and of the assumption (d), we get $\|V_\alpha\|_{H^1} \le \bar{K}$, and therefore

$$V_\alpha \to V \ \text{ strongly in } \ L^2(\Omega) \quad \text{and} \quad V_\alpha \rightharpoonup V \ \text{ weakly in } \ H^1(\Omega). \tag{49}$$

By $n_\alpha,\ p_\alpha \le \bar{K}_M$, in view of the assumption (e_h) one can show that

$$\int_\Omega n_\alpha g(n_\alpha)^2 dx \le \bar{K}, \qquad \int_\Omega p_\alpha g(p_\alpha)^2 dx \le \bar{K}. \tag{50}$$

Again, as shown in Lemma 2.7, it is not difficult to show that

$$2\varepsilon^2 H_{m,\alpha} \int_\Omega |\nabla\sqrt{n_\alpha}|^2 dx + 2\varepsilon^2 H_{m,\alpha} \int_\Omega |\nabla\sqrt{p_\alpha}|^2\, dx + 2G_m|\Omega| \tag{51}$$
$$+ \frac{\lambda^2}{2} \int_\Omega |\nabla V[n_\alpha - p_\alpha - C]|^2 dx \le \bar{K},$$

which implies, by the assumption (b_h), that

$$\int_\Omega H_\alpha^2 |\nabla n|^2 dx \le \int_\Omega H_\alpha |\nabla n|^2 dx \le \bar{K}, \tag{52}$$

$$\int_\Omega H_\alpha^2 |\nabla p|^2 dx \le \int_\Omega H_\alpha |\nabla p|^2 dx \le \bar{K}. \tag{53}$$

Finally (45), (47) and (e_h) implies

$$\int_\Omega n_\alpha g_\alpha(n_\alpha)^2 \le \bar{K}, \quad \int_\Omega p_\alpha g_\alpha(p_\alpha)^2 \le \bar{K}. \tag{54}$$

It remains to prove that (n, p, V) is the weak solution of (36). First of all we multiplying $(34)_1$ by ϕ, where $\phi \in C_0^\infty(\Omega)$ is any given test function. After integration by parts we get

$$\int_\Omega H_\alpha \nabla n_\alpha \cdot \nabla\phi\, dx + \int_\Omega \sqrt{n_\alpha}(V_\alpha + g(n_\alpha) - \beta_n)\phi\, dx = 0. \tag{55}$$

In view of the estimates derived above, (55) converges weakly in L^2 to the weak form of the limit problem, namely

$$\int_\Omega H \nabla n \cdot \nabla\phi\, dx + \int_\Omega \sqrt{n}(V + g(n) - \beta_n)\phi\, dx = 0, \tag{56}$$

therefore (n, V) is a weak solution of $(8)_1$.

In the same way, we can show that (p, V) is a weak solution of $(36)_2$. Let us consider $(34)_3$, multiply it by ϕ and integrate it by parts, then we have

$$\lambda^2 \int_\Omega \nabla V_\alpha \cdot \nabla \phi \, dx + \int_\Omega (n_\alpha - p_\alpha - C)\phi \, dx = 0, \tag{57}$$

which, in view of (49) and (48), converges in L^2 to the weak formulation of $(36)_3$. □

3.2. Second hybrid limit: classical-hybrid limit

In some experimental situations the quantum effects correspond to a high concentration of just one carrier, electrons, for example. In this case the holes can be described by using the classical model in the whole domain, whereas the electrons by using the hybrid model. Therefore, in this section, we assume that H^n_α converges to an appropriate step function, whereas H^p_α converges to zero, as $\alpha \to 0$.

In this way the device is again divided into two sub-domains: a classic sub-domain where $H^n_{\alpha_n} = H^p_{\alpha_p} \to 0$ and a quantum one where only the electrons exhibit a quantum behaviour, therefore $H^n_{\alpha_n} \to 1$ and $H^p_{\alpha_p} \to 0$. One possible choice is to set

$$H^n_\alpha(x) = H_\alpha, \quad H^p_\alpha(x) = \alpha^2, \tag{58}$$

where H_α has been already defined in (33). Under these assumptions, (8) becomes

$$\begin{cases} 2\varepsilon^2 \nabla \cdot \left(H_\alpha \nabla \sqrt{n_\alpha}\right) = \sqrt{n_\alpha}(V_\alpha + g(n_\alpha) - \beta_{n\alpha}), \\ 2(\varepsilon\alpha)^2 \Delta \sqrt{p_\alpha} = \sqrt{p_\alpha}(-V_\alpha + g(p_\alpha) - \beta_{p_\alpha}), \\ -\lambda^2 \Delta V_\alpha = n_\alpha - p_\alpha - C, \\ \int_\Omega n_\alpha(x)dx = N, \quad \int_\Omega p_\alpha(x)dx = P, \quad \int_\Omega V_\alpha(x)dx = 0. \end{cases} \tag{59}$$

The relevant energy is

$$\Xi_\alpha = 2\varepsilon^2 \int_\Omega H_\alpha |\nabla \sqrt{n_\alpha}|^2 dx + 2(\varepsilon\alpha)^2 \int_\Omega |\nabla \sqrt{p_\alpha}|^2 dx + \int_\Omega G(n_\alpha)dx$$
$$+ \int_\Omega G(p_\alpha)dx + \frac{\lambda^2}{2} \int_\Omega |\nabla V[n_\alpha - p_\alpha - C]|^2 dx. \tag{60}$$

Our aim is to prove that for $\alpha \to 0$ the sequence of solutions $(n_\alpha, p_\alpha, V_\alpha)$ of the problem (59) converges in some suitable space to the solution of the following *hybrid model*

$$\begin{cases} 2\varepsilon^2 \nabla \cdot \left(H(x) \nabla \sqrt{n}\right) = \sqrt{n}(V + g(n) - \beta_n), \\ \sqrt{p}(-V + g(p) - \beta_p) = 0, \\ -\lambda^2 \Delta V = n - p - C, \\ \int_\Omega n(x)dx = N, \quad \int_\Omega p(x)dx = P, \quad \int_\Omega V(x)dx = 0. \end{cases} \tag{61}$$

Definition 3.3. A pair of functions $(n, p, V)(x)$ is said to be a weak solution of (61), if it holds

$$2\varepsilon^2 \int_\Omega H\nabla\sqrt{n}\cdot\nabla\phi dx + \int_\Omega \sqrt{n}(V + g(n) - \beta_n)\phi dx = 0, \tag{62}$$

$$\int_\Omega \sqrt{p}(-V + g(p) - \beta_p)\phi dx = 0, \tag{63}$$

$$\lambda^2 \int_\Omega \nabla V\cdot\nabla\phi dx = \int_\Omega (n - p - C)\phi dx, \tag{64}$$

$$\int_\Omega n(x)dx = N, \quad \int_\Omega p(x)dx = P, \quad \int_\Omega V(x)dx = 0, \tag{65}$$

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

The convergence result is summarized in the following theorem.

Theorem 3.4. *Assume (a), (b_h) (c), (d), (e_h) hold and the function $H_\alpha(x)$ is given in (58). Let $(n_\alpha, p_\alpha, V_\alpha) \in L^\infty(\Omega)\cap H^1(\Omega)$ be the sequence of solutions of the problem (59). Then there exists (n, p, V) such that*

$$\begin{cases} n_\alpha \rightharpoonup n \ \text{ in } L^2(\Omega), \\ p_\alpha \rightharpoonup p \ \text{ in } L^2(\Omega), \\ V_\alpha \rightharpoonup V \ \text{ in } H^1(\Omega), \end{cases} \qquad \text{as } \alpha \to 0, \tag{66}$$

where the limit function $(n, p, V)(x)$ is the weak solution to the hybrid problem (61).

Proof. The proof follows by using the same calculation detailed in Theorem 3.2. □

4. The semi-classical limit

In this section, we discuss the semi-classical limit ($\varepsilon \to 0$) for the hybrid QHD model presented in Section 2. By carrying out such a limit, we expect to recover the minimizer of the limiting functional. To verify these properties for the problem (4) is important to validate the model. For such a purpose, let us consider the energy functional (35) by fixing the index α, say $\bar\alpha$, as follows

$$\Xi_\varepsilon = 2\varepsilon^2 \int_\Omega H_{\bar\alpha}|\nabla\sqrt{n}|^2 dx + 2\varepsilon^2 \int_\Omega H_{\bar\alpha}|\nabla\sqrt{p}|^2 dx + \int_\Omega G(n)dx$$
$$+ \int_\Omega G(p)dx + \frac{\lambda^2}{2}\int_\Omega |\nabla V[n - p - C]|^2 dx. \tag{67}$$

The limiting problem coincides with the following classical problem

$$\begin{cases} \sqrt{n}(V+g(n)-\beta_n)=0, \quad \text{for,} \quad \text{if} \quad n>0 \quad x\in\Omega, \\ \sqrt{p}(-V+g(p)-\beta_p)=0, \quad \text{for,} \quad \text{if} \quad p>0 \quad x\in\Omega, \\ \sqrt{n}(V+g(n)-\beta_n)\geq 0, \quad \text{for,} \quad \text{if} \quad n=0 \quad x\in\Omega, \\ \sqrt{p}(-V+g(p)-\beta_p)\geq 0, \quad \text{for,} \quad \text{if} \quad p=0 \quad x\in\Omega, \\ -\lambda^2\Delta V=n-p-C, \quad \text{for} \quad x\in\Omega \\ \int_\Omega n(x)dx=N, \quad \int_\Omega p(x)dx=P, \quad \int_\Omega V(x)dx=0, \end{cases} \tag{68}$$

where

$$\Xi^c=\int\limits_{\Omega_q} G(n)dx+\int\limits_{\Omega_q} G(p)dx+\frac{\lambda^2}{2}\int\limits_{\Omega_q}|\nabla V[n-p-C]|^2dx \tag{69}$$

is the limiting energy functional. We just recall that the problem (68), related to the energy functional (69), admits a unique regular solution (n_0, p_0, V_0) which is the unique minimizer of (69), as proved in Lemma 1 in [30].

Theorem 4.1. *Assume (a)–(e) hold. Let $(n_\varepsilon, p_\varepsilon, V_\varepsilon)\in L^\infty(\Omega)\cap H^1(\Omega)$ be the sequence of solutions of the problem (34) for $\alpha=\bar{\alpha}$, and $(n_0, p_0, V_0)\in L^\infty(\Omega)\cap H^1(\Omega)$ be the unique solution to the classical problem (68). Then there exists a subsequence $(n_\varepsilon, p_\varepsilon, V_\varepsilon)$ (not relabeled) such that $(n_\varepsilon, p_\varepsilon, V_\varepsilon)\to(n_0, p_0, V_0)$, weakly in $H^1(\Omega)$ and strongly in $L^2(\Omega)$.*

Proof. Our aim is to prove $\Xi^c(n_0, p_0)=\lim_{\varepsilon\to 0}\Xi_\varepsilon(n_\varepsilon, p_\varepsilon)$. We observe that, for all $\varepsilon>0$,

$$\Xi_\varepsilon(n_\varepsilon, p_\varepsilon)-\Xi^c(n_\varepsilon, p_\varepsilon)=2\varepsilon^2\int\limits_\Omega H_{\bar{\alpha}}(x)|\nabla\sqrt{n_\varepsilon}|^2dx+2\varepsilon^2\int\limits_\Omega H_{\bar{\alpha}}(x)|\nabla\sqrt{p_\varepsilon}|^2dx.$$

According to the assumption $\sqrt{n_0}, \sqrt{p_0}\in H^1(\Omega)$, one can write

$$\Xi_\varepsilon(n_0, p_0)=\Xi^c(n_0, p_0)+2\varepsilon^2\int\limits_\Omega H_{\bar{\alpha}}|\nabla\sqrt{n_0}|^2dx+2\varepsilon^2\int\limits_\Omega H_{\bar{\alpha}}|\nabla\sqrt{p_0}|^2dx.$$

As $\Xi^c(n_0, p_0)\leq\Xi^c(n_\varepsilon, p_\varepsilon)$ one can deduce

$$\int\limits_\Omega|\nabla\sqrt{n_\varepsilon}|^2dx+\int\limits_\Omega|\nabla\sqrt{p_\varepsilon}|^2dx\leq\int\limits_\Omega|\nabla\sqrt{n_0}|^2dx+\int\limits_\Omega|\nabla\sqrt{p_0}|^2dx, \tag{70}$$

that along with the hypotheses $\|n_\varepsilon\|_{L^2}=N$ and $\|p_\varepsilon\|_{L^2}=P$, implies

$$\|n_\varepsilon\|_{H^1}, \|p_\varepsilon\|_{H^1}\leq K,$$

where K is, within this section, an ε-independent constant.

Thus, the previous uniform bound gives us the existence of a weakly $H^1(\Omega)$ convergent subsequence $(n_\varepsilon, p_\varepsilon)$. Let's call its limit as (n^*, p^*). Consequently, from the assumption (c), we also have

$$V_\varepsilon\to V^* \quad \text{as} \quad \varepsilon\to 0 \quad \text{strongly in} \quad L^3(\Omega),$$

where $V^*=V[n^*-p^*-C]$.

In order to prove $n^* = n_0$ and $p^* = p_0$, we observe that

$$\begin{aligned}\Xi^c(n_0, p_0) &\le \liminf_{\varepsilon\to 0} \Xi^c(n_\varepsilon, p_\varepsilon) \le \liminf_{\varepsilon\to 0} \Xi_\varepsilon(n_\varepsilon, p_\varepsilon)\\ &\le \limsup_{\varepsilon\to 0} \Xi_\varepsilon(n_\varepsilon, p_\varepsilon) \le \liminf_{\varepsilon\to 0} \Xi_\varepsilon(n_0, p_0)\\ &= \Xi^c(n_0, p_0),\end{aligned}$$

then $\Xi^c(n_0, p_0) = \lim_{\varepsilon\to 0} \Xi_\varepsilon(n_\varepsilon, p_\varepsilon)$.

From the weakly-L^2 sequential continuity of the functional Ξ^c, we can write

$$\Xi^c(n^*, p^*) = \liminf_{\varepsilon\to 0} \Xi^c(n_\varepsilon, p_\varepsilon) \le \liminf_{\varepsilon\to 0} \Xi_\varepsilon(n_\varepsilon, p_\varepsilon) = \Xi^c(n_0, p_0), \tag{71}$$

then we can conclude that (n^*, p^*) is a minimizer of (68) on Γ_c. The uniqueness of the minimizer in Γ_c implies $n^* = n_0$ and $p^* = p_0$. □

5. Numerical simulations

In the previous part of this paper, we have introduced a bipolar hybrid model, which is able to account for localized quantum effects by means of a modified expression of the Bohm potential. Compared to the previous results, obtained using a similar approach (see [14]), here we get, as a limit, a fully hybrid solution. In fact no semiclassical region linking classical and quantum domain has to be introduced. In other words the hybrid function H_α converges to the Heavisade function for $\alpha \to 0^+$ (see Section 3).

In this section we would like to analyze, from the numerical point of view, the behaviour of the solution at the interface between classical and quantum system. Therefore we consider, as a test device, a simple $p|n|$ junction, modelled by the following doping profile

$$\bar{C}(x) = \begin{cases} 1, & \forall x \in [0, 1/2], \\ -1, & \forall x \in (1/2, 1], \end{cases} \tag{72}$$

approximated as follows

$$C(x) = -(1 - q_C)\tanh(h_C(x - (1/2))) \quad x \in [0, 1],$$

where $q_C = 10^{-4}$ and $h_C = 10^3$. The behaviour of the doping profile is plotted in Fig. 1.

The quantum function for the electrons is

$$\begin{cases} \text{Quantum Region} & \forall x \le (1/2 + \delta), \\ \text{Classical Region} & \forall x > (1/2 + \delta), \end{cases} \tag{73}$$

whereas for the holes

$$\begin{cases} \text{Quantum Region} & \forall x \ge (1/2 - \delta), \\ \text{Classical Region} & \forall x < (1/2 - \delta), \end{cases} \tag{74}$$

where $0 < \delta < 1/2$.

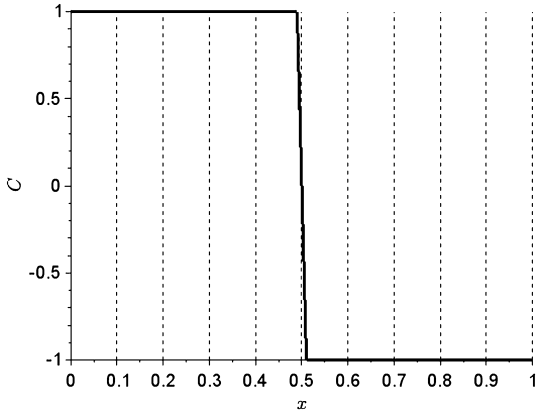

Fig. 1. Behaviour of the doping profile, assuming $q_C = 10^{-4}$ and $h_C = 10^3$.

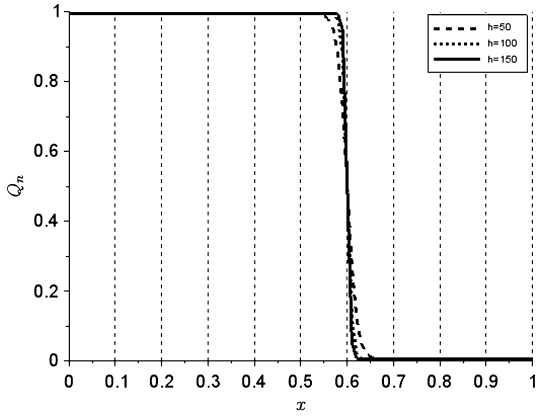

Fig. 2. Behaviour of the quantum function Q_n for $\delta = 0.1$, $q = 0.01$ and different values of h.

The functions $Q^n(x)$, $Q^p(x)$ are approximated as follows

$$Q_n(x) = -\frac{1-q}{2}\tanh(h(x-(1/2+\delta))) + \frac{1}{2}, \quad x \in [0,1]$$
$$Q_p(x) = \frac{1-q}{2}\tanh(h(x-(1/2-\delta))) + \frac{1}{2}, \quad x \in [0,1].$$

Here $\delta = 0.1$, $q = 0.01$ and different value of h are considered. Three examples of Q_n and Q_p, obtained setting $h = 50, 100, 150$, are plotted in Fig. 2 and in Fig. 3, respectively. The parameter h assigns how well the functions Q_n and Q_p approximate the step function.

We consider system (4) in the one-dimensional and isothermal case

$$\begin{cases} \bar{V}_x + \frac{\kappa}{\kappa-1}(n^{\kappa-1})_x - 2\varepsilon^2\left(Q^n\frac{\sqrt{\bar{n}}_{xx}}{\sqrt{\bar{n}}} + \frac{Q^n_x\sqrt{\bar{n}}_x}{\sqrt{\bar{n}}}\right)_x = 0, \\ -\bar{V}_x + \frac{\kappa}{\kappa-1}(p^{\kappa-1})_x - 2\varepsilon^2\left(Q^p\frac{\sqrt{\bar{p}}xx}{\sqrt{\bar{p}}} + \frac{Q^p_x\sqrt{\bar{p}}_x}{\sqrt{\bar{p}}}\right)_x = 0, \\ -\lambda^2\bar{V}_{xx} = \bar{n} - \bar{p} - C, \end{cases} \tag{75}$$

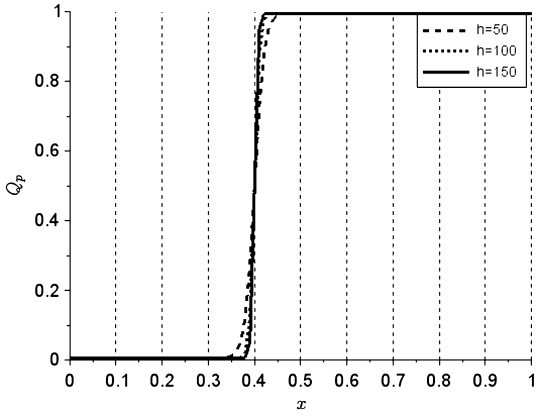

Fig. 3. Behaviour of the quantum function Q_n for $\delta = 0.1$, $q = 0.01$ and different values of h.

coupled with the following set of mixed boundary conditions

$$\begin{aligned} &\bar{n}(0) = 1 \qquad \bar{n}_x(0) = \bar{n}_x(1) = 0, \\ &\bar{p}(0) = 1 \qquad \bar{p}_x(0) = \bar{p}_x(1) = 0, \\ &\bar{V}(0) = 1 \qquad \bar{V}_x(1) = 0. \end{aligned} \tag{76}$$

The obtained solution, namely $(\bar{n}, \bar{p}, \bar{V})$, must be renormalized as to satisfy

$$\int_\Omega n(x)dx = N, \quad \int_\Omega p(x)dx = P, \quad \int_\Omega V(x)dx = 0. \tag{77}$$

The conditions listed above can be simply achieved by setting

$$n = N + \bar{n} - \int_0^1 \bar{n}dx, \quad p = P + \bar{p} - \int_0^1 \bar{p}dx, \quad V = \bar{V} - \int_0^1 V dx, \tag{78}$$

where (n, p, V) is the solution of system (4) (or equivalently (8)).

To solve system (75), we use COLNEW, a SCILAB function for boundary value problems (see [3] and [4] for more details about the code and the integration method).

The parameters of the problem are the scaled Debye length λ, the scaled Plank constant ε and the exponent of the pressure function κ. Within this section we assume

$$\lambda = 0.8, \quad \kappa = 2, \quad \varepsilon = 0.01, \quad N = 1, \quad P = 1.$$

We consider the behaviour of V, n and p together with their first derivatives, for different values of the parameter h. In particular, n_x and p_x could play an important role in our hybrid model, due to the presence of the new terms, $\nabla Q^n \cdot \nabla n$ and $\nabla Q^p \cdot \nabla p$, in the Bohm potentials. Clearly, if Q^n becomes the Heavisade functions we have, in the Bohm potential, a singular term $\delta(x) \cdot \nabla n$, and the same holds for the holes p.

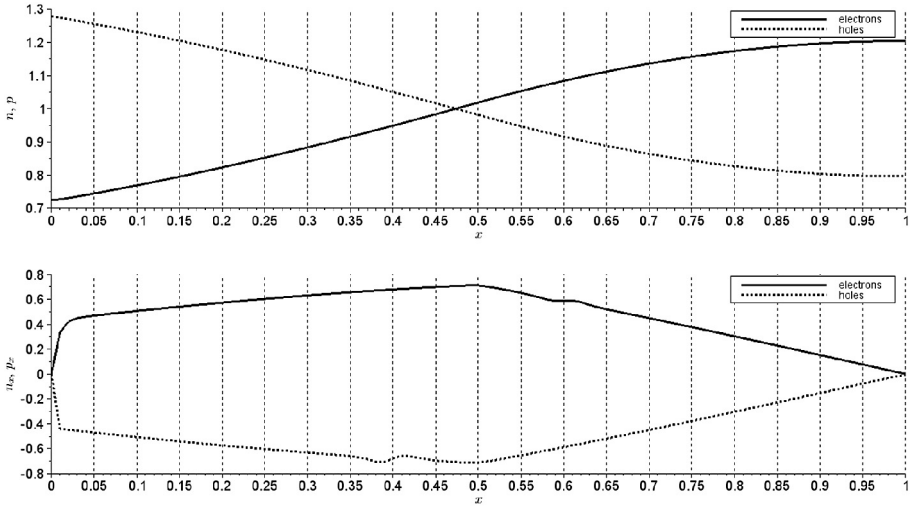

Fig. 4. Behaviour of the charge densities n and p and their first derivatives, n_x and p_x, assuming $h = 50$. We observe a small oscillation in the values of n_x and p_x around $x + \delta$ and $x - \delta$, respectively.

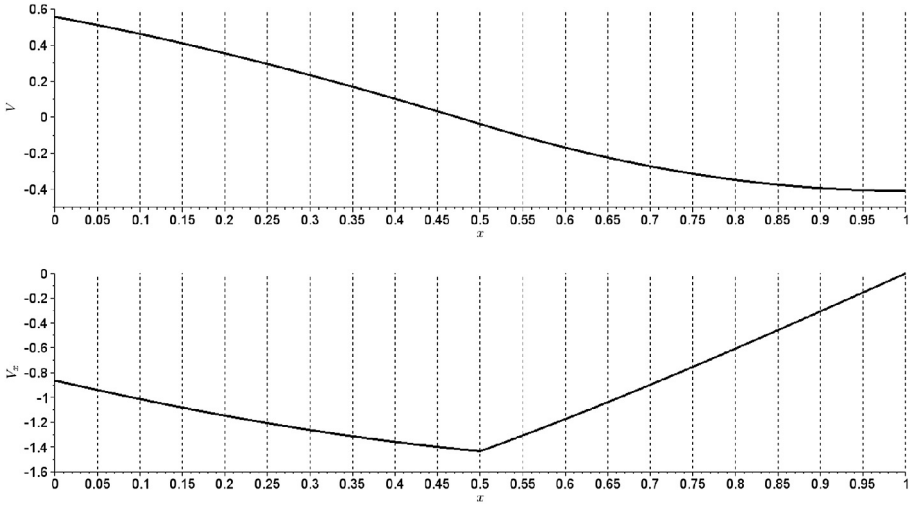

Fig. 5. Behaviour of the electrical potential V and its first derivative V_x, assuming $h = 50$.

According to our theoretical results (see Theorem 3.2), in the hybrid case we just have $n, p \in L^2(\Omega)$. As a consequence $\nabla Q^n \cdot \nabla n$ and $\nabla Q^p \cdot \nabla p$ could be not well defined at the interfaces. Therefore it is very important, in our opinion, to understand, at least numerically and in the one-dimensional regularized case, what happens to n_x and p_x at the interfaces. Roughly speaking, one could aspect that, when Q^n and/ or Q^p approach the Heavisade function (for large h), n and/or p are not continuous and n_x and p_x could be something like the Dirac function.

Three cases are considered: $h = 50$ (Fig. 4–Fig. 5), $h = 100$ (Fig. 6–Fig. 7) and $h = 150$ (Fig. 8–Fig. 9).

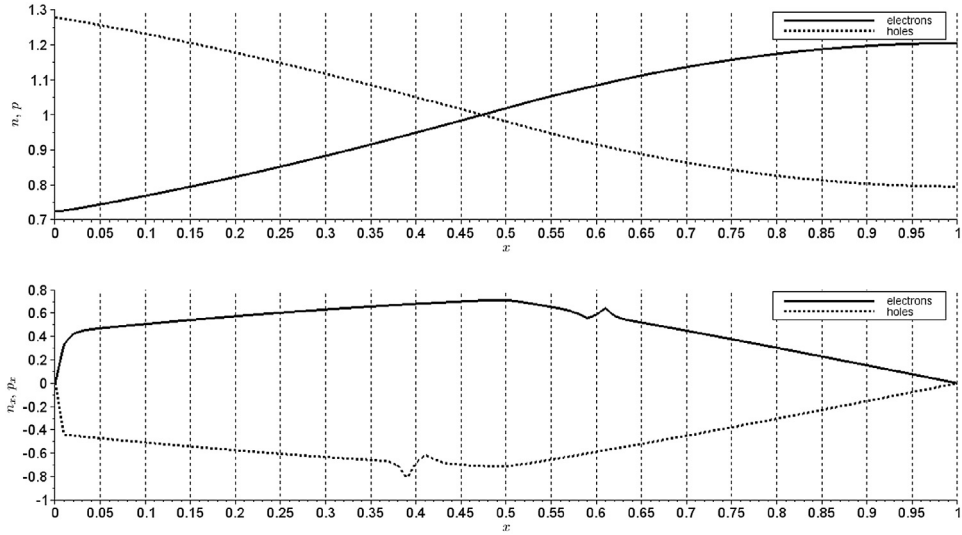

Fig. 6. Behaviour of the charge densities n and p and their first derivatives, n_x and p_x, assuming $h = 100$. The amplitude of the oscillations of n_x and p_x around $x + \delta$ and $x - \delta$, respectively, has increased compared to the previous case.

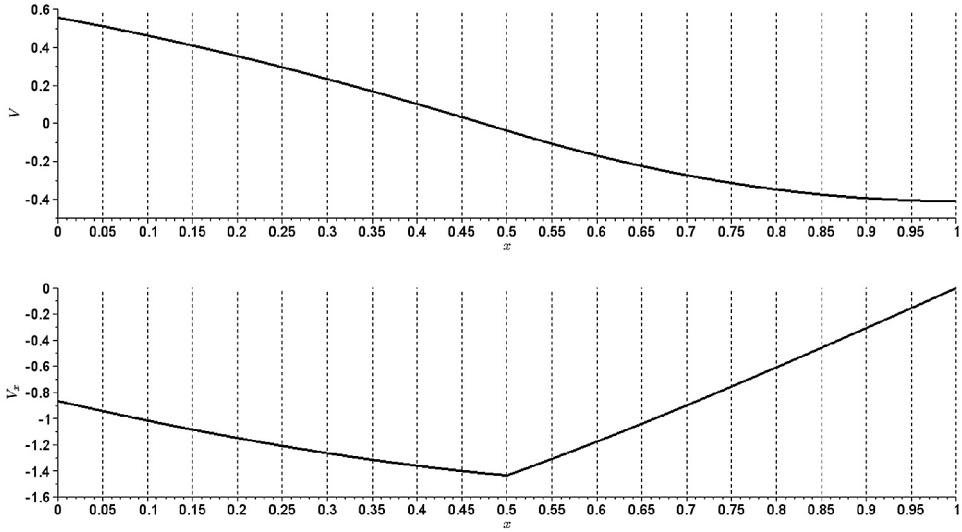

Fig. 7. Behaviour of the electrical potential V and its first derivative V_x, assuming $h = 100$.

We can observe an oscillation in the values of n_x and p_x around $x + \delta$ and $x - \delta$, respectively. This effect is a consequence of the modified Bohm potential that we have introduced. The amplitude of these oscillations increases with h, whereas their period appears to decrease. One could conjecture that, for $h \to +\infty$, the amplitude of these oscillations increases until to infinity and the correspondent period goes to zero. Therefore the effect of the modified Bohm potential on n_x and p_x would be no visible at all. To verify this hypothesis a more complex numerical code should be used. This will be the subject of a forthcoming, paper still in preparation.

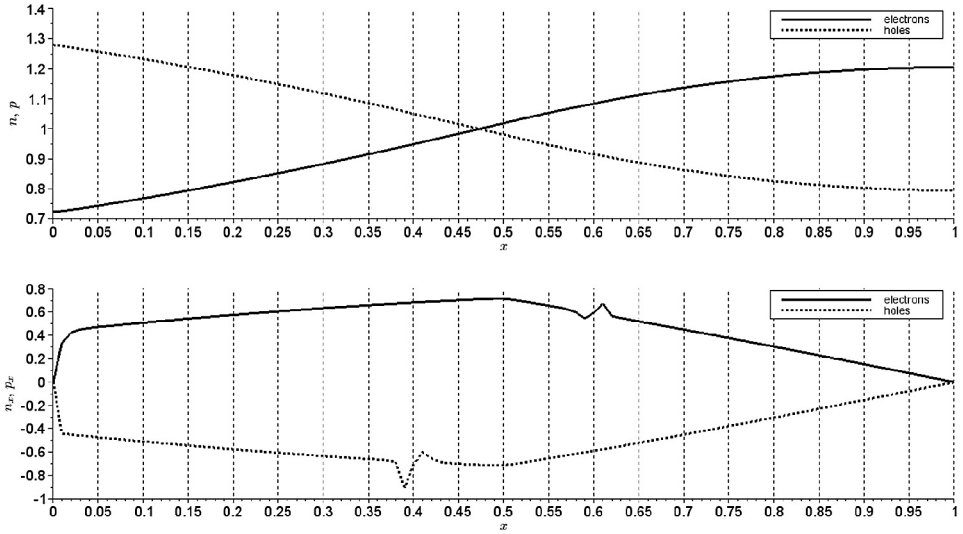

Fig. 8. Behaviour of the charge densities n and p and their first derivatives, n_x and p_x, assuming $h = 150$. The amplitude of the oscillations of n_x and p_x around $x + \delta$ and $x - \delta$, respectively is still increasing.

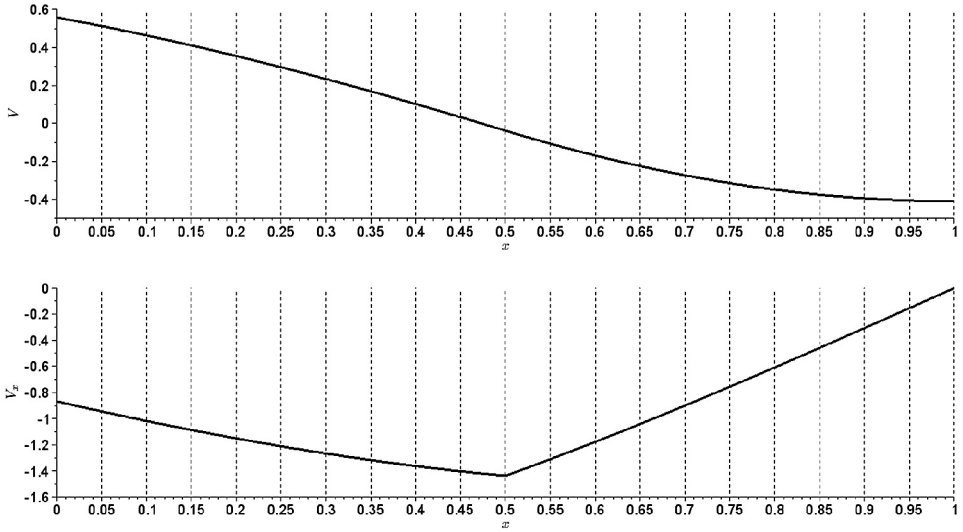

Fig. 9. Behaviour of the electrical potential V and its first derivative V_x, assuming $h = 150$.

Finally we compare the H-QBM presented in this paper and the QHD model, often used to describe quantum devices. Two cases are considered, namely $h = 50$ and $h = 150$. As shown Fig. 10, the behaviour of V and V_x obtained using the H-QBM and the QHD are in very good agreement. The same holds for n and p (see Fig. 11 and Fig. 12). Indeed, as expected, the behaviour of n_x and p_x obtained using the H-QBM and the QHD differs due to presence of the oscillations discussed above around the interface region, that is $x + \delta$ for the electrons and $x - \delta$ for the holes, whereas no remarkable differences are visible elsewhere.

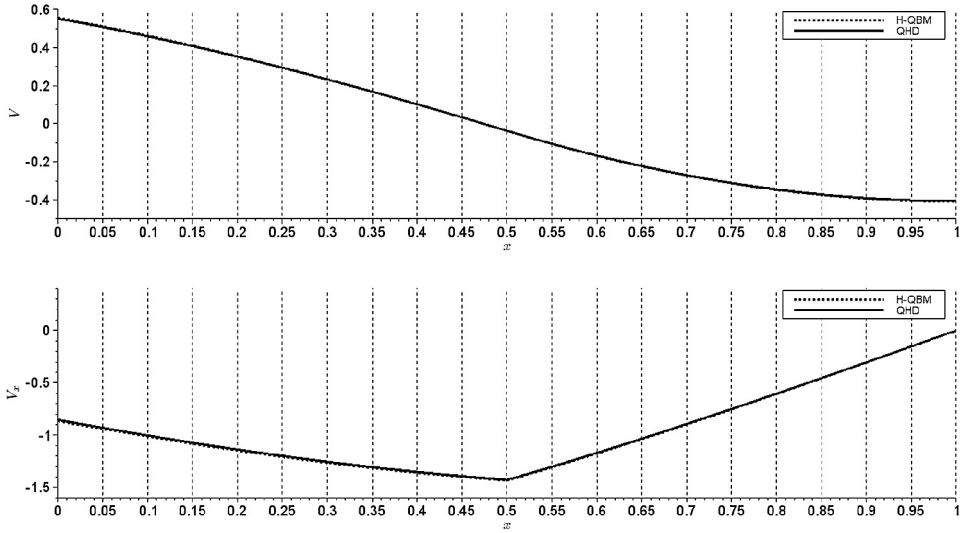

Fig. 10. Behaviour of the charge densities V and V_x computed using the H-QBM ($h = 50$) and the QHD. The behaviour of V and V_x are exactly overlapping.

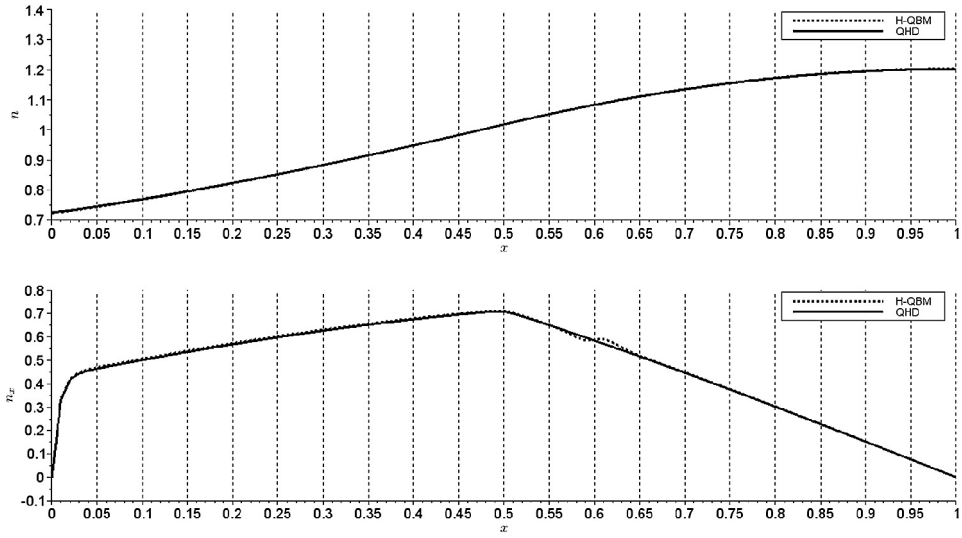

Fig. 11. Behaviour of the charge densities n and n_x computed using the H-QBM ($h = 50$) and the QHD. An oscillation of n_x around $x + \delta$ is visible only for the H-QBM. This effect at the interface is a consequence of the modified Bohm potential.

Similar results are obtained for $h = 150$ as shown in Fig. 13, Fig. 14, and Fig. 15.

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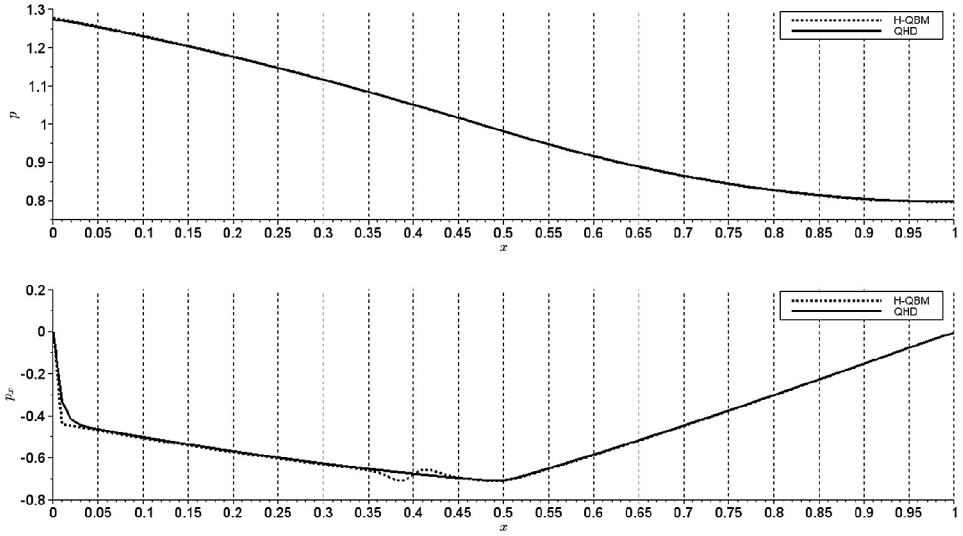

Fig. 12. Behaviour of the charge densities p and p_X computed using the H-QBM ($h = 50$) and the QHD. An oscillation of p_X around $x - \delta$ is visible only for the H-QBM. This effect at the interface is a consequence of the modified Bohm potential.

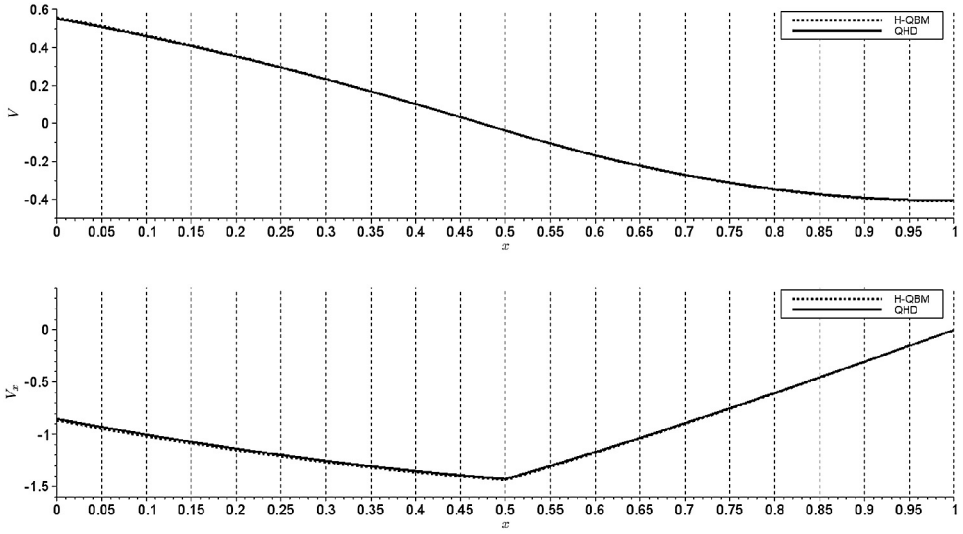

Fig. 13. Behaviour of the charge densities V and V_x computed using the H-QBM ($h = 150$) and the QHD. The behaviour of V and V_X are exactly overlapping.

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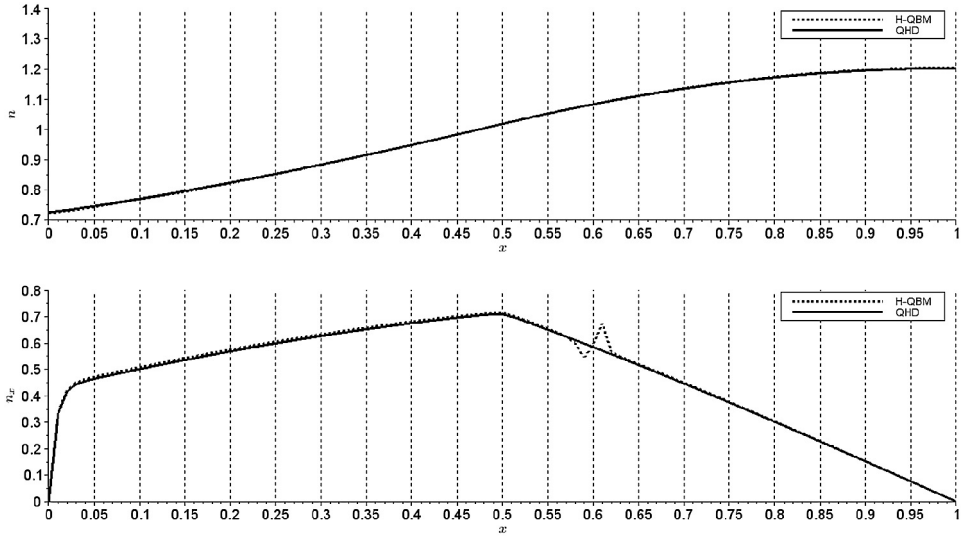

Fig. 14. Behaviour of the charge densities n and n_x computed using the H-QBM ($h = 150$) and the QHD. An oscillation of n_x around $x + \delta$ is visible only for the H-QBM. This effect at the interface is a consequence of the modified Bohm potential.

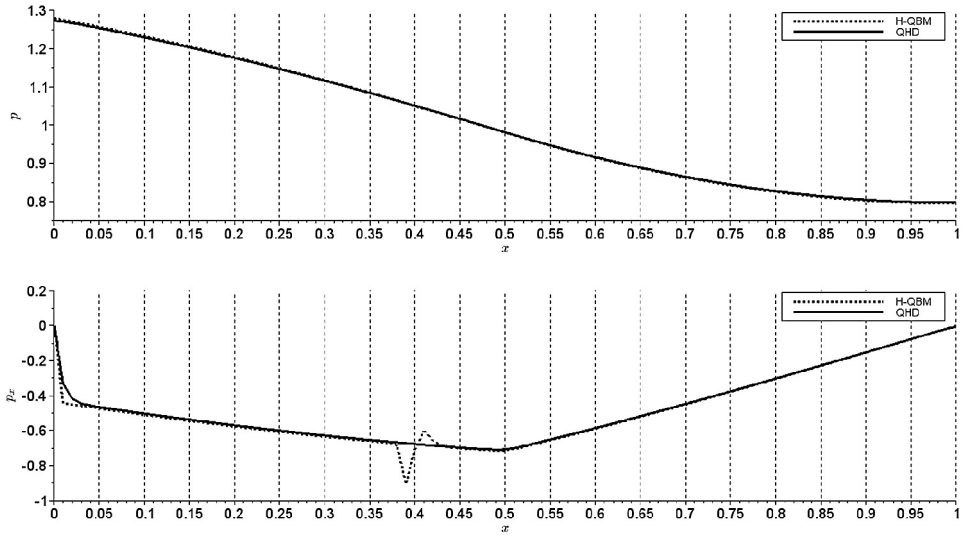

Fig. 15. Behaviour of the charge densities p and p_x computed using the H-QBM ($h = 150$) and the QHD. An oscillation of p_x around $x - \delta$ is visible only for the H-QBM. This effect at the interface is a consequence of the modified Bohm potential.

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