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Large Data Solutions to the Viscous Quantum Hydrodynamic Model with Barrier Potential

Michael Dreher^{a*}, Johannes Schnur^b

We discuss analytically the stationary viscous quantum hydrodynamic model including a barrier potential, which is a nonlinear system of partial differential equations of mixed order in the sense of Douglis–Nirenberg. Combining a reformulation by means of an adjusted Fermi level, a variational functional, and a fixed point problem, we prove the existence of a weak solutions. There are no assumptions on the size of the given data or their variation. We also provide various estimates of the solution that are independent of the quantum parameters.

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1. Introduction and Main Results

Nowadays, modern microelectronic devices are getting ever smaller, and quantum mechanical effects have to be incorporated into the mathematical studies of their behaviour. This can be seen in the viscous quantum hydrodynamic model with barrier potential, which is a parabolic-elliptic system for three unknowns (n, J, V) ,

$$\left\{ \begin{array}{l} \partial_t n - \operatorname{div} J = \nu \Delta n, \\ \partial_t J - \operatorname{div} \left(\frac{J \otimes J}{n} \right) - T_0 \nabla n + n \nabla (V + V_B) + 2\varepsilon_0^2 n \nabla \frac{\Delta \sqrt{n}}{\sqrt{n}} = \nu \Delta J - \frac{1}{\tau_0} J, \\ \lambda_0^2 \Delta V = n - \mathcal{C}. \end{array} \right. \quad (1.1)$$

Here t and x are the usual variables for time and space, $n = n(t, x)$ is the scalar density of electrons in the electronic device, $J = J(t, x)$ the vectorial density of the electric current, and $V = V(t, x)$ the scalar elliptic potential. The physical constants

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are T_0 (temperature), ε_0 (related to the Planck constant \hbar), ν (coming from a description of the collision effects between electrons and the phonons of the crystal lattice via a Fokker–Planck operator), a relaxation time τ_0 , and the Debye length λ_0 . The functions $V_B = V_B(x)$ and $\mathcal{C} = \mathcal{C}(x)$ are called barrier potential and doping profile. They are known and typically piecewise constant. The quantum effects enter the mathematical model via the terms with coefficients ε_0 and ν (which is proportional to \hbar^2).

The quantum hydrodynamical model for the particle transport in a semiconductor was proposed in [1], first without the viscosity terms. We emphasise that the viscosity terms in our model are not an *ad hoc* regularisation; instead they can be physically justified, see [2], and [3], [4] for overviews.

Proving analytical results for (1.1) is quite challenging, and one reason for that is the third order term $2\varepsilon_0^2 n \nabla B(n)$ in the second equation, where we have introduced the abbreviation

$$B(n) = \frac{\Delta \sqrt{n}}{\sqrt{n}}$$

for the so-called Bohm potential. We mention results on local or global existence or various asymptotics (proved using energy methods) in [5], [6], [7], [8], [9], [10]. All these results omit the barrier potential V_B .

However, the system (1.1) is interesting also from another point of view of so-called pure analysis[†]: If we introduce the vector $U := (n, J)^\top$ of main unknowns, then we can bring (1.1) into the form

$$\partial_t U - \begin{pmatrix} \nu \Delta & \operatorname{div} \\ -\varepsilon_0^2 \nabla \Delta & \nu \Delta I_d \end{pmatrix} U = (\text{lower order terms}),$$

with I_d as the $d \times d$ identity matrix in \mathbb{R}^d . The matrix operator turns out to be a parameter-elliptic differential operator of mixed order in the sense of Douglis–Nirenberg, and the idea emerges to tackle (1.1) using semigroup methods. Indeed, the first author succeeded in proving that this matrix differential operator (augmented by appropriate boundary conditions) does generate an analytic semigroup in certain L^p based Sobolev spaces, and then the local well-posedness of (1.1) can be shown in a short and elegant way, see [11], [12], [13], [14].

The key novelty of this paper is to include the barrier potential V_B into the considerations, with the goal of rigorously proven analytical results. We focus our attention to the one-dimensional domain $(0, 1)$ and the time-independent case:

$$J_x + \nu n_{xx} = 0, \tag{1.2}$$

$$-\left(\frac{J^2}{n}\right)_x - T_0 n_x + n(V + V_B)_x + 2\varepsilon_0^2 n B_x - \nu J_{xx} + \frac{1}{\tau_0} J = 0, \tag{1.3}$$

$$\lambda_0^2 V_{xx} = n - \mathcal{C}. \tag{1.4}$$

Since the barrier potential V_B appearing in the applications typically is a function with jumps, (1.3) has to be understood in the sense of distributions. This complication seems to be one reason why analytical results for such a system have not been obtained so far (another reason is that the flow is partly subsonic, partly supersonic). We refer to elaborate numerical simulations in [15], [16], [17].

The remainder of the introduction unfolds as follows: first we discuss boundary conditions to be imposed at the boundary points $x = 0$ and $x = 1$, which we will often call *contacts*. These boundary conditions have to be analytically correct as well as physically relevant. Then we introduce the concept of a weak solution (Definition 1.1).

Next comes our first main result, Theorem 1.2 on the existence of weak solutions, which is the first analytical result at all on the model with barrier potential. We emphasise that we have no assumptions on the positive physical constants (T_0 , ε_0 , ν , τ_0 , λ_0) or the applied voltage $V(1) - V(0)$, and we have very little assumption on the given functions V_B and \mathcal{C} : these functions can be basically any function from L^∞ or L^2 , respectively — we can always guarantee the existence of a weak solution (the only conditions are that V_B has slightly higher regularity near the contacts, and that the doping profile \mathcal{C} has positive total

[†]We wrote *so-called* because, in our opinion, the distinction between pure and applied analysis is misleading, since they belong together.

mass). This is what is meant by *large data solutions* in the title. We also recall that numerical simulations in [18], [17], [19] tell us that multiple solutions (related to hysteresis effects) indeed happen, and therefore the uniqueness of a solution can not be expected. As a side-remark, we mention that the term $T_0 n_x$ in (1.3) could be replaced by a more general term $\partial_x p(n)$ with a pressure $p(n) \sim n^\gamma$, $\gamma \geq 1$. However, in the isothermal case discussed here, our proofs allow for an amazing connection to the nice Csiszár–Kullback inequality, and therefore we restrict our studies to the isothermal case, for reasons of beauty and brevity.

The second main result (Theorem 1.3) shall characterise the shape of the solutions more in detail. Here we put particular emphasis in obtaining various bounds that are uniform in the quantum parameters ε_0 and ν . The motivation for such estimates is to better understand whether the solutions to the viscous model (where $\nu > 0$) do converge (for $\nu \rightarrow 0$) to the solutions of the inviscid model (where $\nu = 0$) as it was introduced by Gardner. This is a hard question which has remained open for many years, and Theorem 1.3 gives partial answers in that direction. More answers (for the equilibrium case) are presented in [20] and [21].

Let us think about boundary conditions for (1.2)–(1.4). From numerical simulations [1], [15], [16], [17], [22] and physical intuition we expect that $n \approx \mathcal{C}$ near the contacts, and n is observed to be basically constant there. Results from numerical simulations by the authors are in Figure 1 in the appendix. Therefore, the boundary conditions ($n = \mathcal{C}$, $n_x = 0$, $n_{xx} = 0$) together with Dirichlet conditions for V are physically reasonable for $x = 0$ and $x = 1$, and the electron density being a flat function near the contacts also matches the numerical observations; but the system becomes formidably overdetermined with these conditions. Note that typically $\mathcal{C}(0) = \mathcal{C}(1)$. As a compromise between the necessity of having an analytically well-posed system and compatibility to numerical simulations, we choose the following boundary conditions:

$$n(0) = n(1), \quad n_x(0) = n_x(1), \quad (1.5)$$

$$n_{xx}(0) = n_{xx}(1), \quad (1.6)$$

$$V(0) = V_l, \quad V(1) = V_r, \quad (1.7)$$

and we additionally prescribe charge neutrality of the device:

$$\int_0^1 n(x) dx = \int_0^1 \mathcal{C}(x) dx =: \mathcal{C}_*, \quad (1.8)$$

and \mathcal{C}_* is supposed as positive. We assume $\mathcal{C} \in L^2((0, 1))$.

Concerning the barrier potential V_B , we suppose

$$V_B \in L^\infty((0, 1)), \quad V_B|_{[0,c]} \in H^1((0, c)), \quad V_B|_{[1-c,1]} \in H^1((1-c, 1)), \quad V_B(0) = V_B(1), \quad (1.9)$$

for some small constant c . The barrier potential may have jump discontinuities, and there the term $nV_{B,x}$ in (1.3) will then only exist as a distribution, which motivates the concept of a weak solution, defined as follows. Observe that (1.3) can be re-arranged into

$$-\left(\frac{J^2}{n}\right)_x + \frac{1}{\tau_0} J - n(h_0(n) - V - V_B - 2\varepsilon_0^2 B(n))_x - \nu J_{xx} = 0, \quad (1.10)$$

with $h_0(n) := T_0 \ln n$ being the enthalpy function.

Definition 1.1 (Weak solution) We say that $(n, J, V) \in H^2((0, 1)) \times H^1((0, 1)) \times H^2((0, 1))$ is a weak solution to (1.2)–(1.8) if $\min_{x \in [0,1]} n(x) > 0$, for each $\varphi \in H^1((0, 1))$ with $\varphi(0) = \varphi(1)$ the identity

$$\int_0^1 \left(-\left(\frac{J^2}{n}\right)_x + \frac{1}{\tau_0} J\right) \varphi dx + \int_0^1 (h_0(n) - V - V_B - 2\varepsilon_0^2 B(n)) (n\varphi)_x dx + \nu \int_0^1 J_x \varphi_x dx + (Vn\varphi) \Big|_{x=0}^1 = 0$$

holds, and the equations (1.2), (1.4), (1.5), (1.7), (1.8) are satisfied.

Theorem 1.2 (Existence of a weak solution) Let the physical constants \mathcal{C}_* , T_0 , τ_0 , λ_0 , ν , ε_0 be positive, the voltage values V_r , V_l be given, and suppose $\mathcal{C} \in L^2((0, 1))$ as well as (1.9).

Then the problem (1.2)–(1.8) possesses at least one weak solution (n_*, J_*, V_*) .

Without loss of generality, we will suppose $V_r \leq V_l$ in both theorems from now on.

Theorem 1.3 (Properties of the weak solution) *Under the assumptions of Theorem 1.2, there is a positive constant C_6 (which depends on $C, \lambda_0, T_0, \tau_0, V_B, V_l - V_r$, but not on the quantum parameters ν and ε_0), such that the first component n_* of the weak solution constructed in Theorem 1.2 has the lower bound*

$$n_*(x) \geq \exp(-C_6(1 + \nu^{-1})), \quad x \in [0, 1]. \quad (1.11)$$

Additionally to the assumptions of Theorem 1.2, suppose that $C \in L^\infty((0, 1))$ is bounded with $\inf_{(0,1)} C(x) > 0$. Put $C_+ := 10 \sup_{(0,1)} C(x)$ and $C_- := \frac{1}{10} \inf_{(0,1)} C(x)$. Define $\varrho_* := \sqrt{n_*}$. Assume that a point $\tilde{x} \in (0, 1)$ exists with the following properties: ϱ_* has C^2 regularity in a neighbourhood of \tilde{x} , and $C_- \leq \varrho_*^2(\tilde{x}) \leq C_+$, and the derivatives of ϱ_* at \tilde{x} are bounded as follows:

$$|\varrho_{*,x}(\tilde{x})| \leq \frac{1}{\sqrt{\varepsilon_0^2 + \nu^2}}, \quad |\varrho_{*,xx}(\tilde{x})| \leq \frac{1}{\varepsilon_0^2 + \nu^2}. \quad (1.12)$$

Then a constant C exists (also being independent of the quantum parameters ν and ε_0) with

$$n_*(x) \leq C, \quad x \in [0, 1]. \quad (1.13)$$

If we additionally suppose that the doping profile C and the barrier potential V_B are piecewise C^1 functions with finitely many jumps of finite height (and \tilde{x} is not one of these jump points), then the function n_* enjoys a uniform pointwise bound of the kinetic energy that is independent of the quantum parameters ν, ε_0 :

$$\frac{(J_*(x))^2}{n_*(x)} \leq C, \quad x \in [0, 1]. \quad (1.14)$$

Here we may replace $J_*(x)$ by the averaged current $\bar{J}_* := \int_0^1 J_*(x) dx$.

And we have a slope bound on the particle density, with a constant C independent of the quantum parameters:

$$|\varrho_{*,x}(x)| \leq \frac{C}{\sqrt{\varepsilon_0^2 + \nu^2}}, \quad x \in [0, 1]. \quad (1.15)$$

And, ultimately, if no voltage is applied (meaning $V_l - V_r = 0$), then n_* possesses uniform in the quantum parameters positive lower and upper bounds.

Let us discuss the physical relevance of the results and assumptions in Theorem 1.3. The lower bound (1.11) indicates that viscosity effects are capable to exclude vacuum, and we remark that this is the first analytically proven lower bound of the particle density at all.

The auxiliary assumption on the existence of at least one point \tilde{x} with the mentioned properties is physically reasonable, because otherwise the particle density n_* would oscillate heavily over the whole interval $[0, 1]$, which seems unrealistic. We refer to numerical simulations as in [1], [15], [16], [17] and [22] for various graphs of n_* , which typically look like in Figure 1 in the appendix. There we find, near the contacts $x = 0$ and $x = 1$ of the device, whole intervals with candidates of the desired point \tilde{x} , and we also observe that (1.5), (1.6) are physically reasonable.

The purpose of (1.14) is to have a uniform lower bound of the particle density $n_*(x)$, assuming that a lower bound of the averaged current \bar{J}_* were given. The expectation is that this lower bound would improve (1.11) quite a bit.

Finally, the uniform bound (1.15) suggests that interfacial layers of the particle density near the jumps of V_B are to be expected to have a width of order $\mathcal{O}(\sqrt{\varepsilon_0^2 + \nu^2})$. This expectation is confirmed in [20] and [21], where asymptotic expansions of the layer profile functions and associated remainder estimates are proved rigorously, with considerable effort.

The structure of the paper is as follows. We will conclude the proof of Theorem 1.2 directly from Theorem 5.7, building upon auxiliary results presented in the sections 2–4. Theorem 1.3 is then proved in Section 6. An appendix provides typical graphs of V_B, C , and a numerically obtained n_* .

2. A Reformulation of the Problem

Lemma 2.1 *Let (n, J, V) be a weak solution to (1.2)–(1.8), and define a number \bar{J} by $\bar{J} := \int_0^1 J(x) dx$. Then the variational identity*

$$\int_0^1 \left(- \left(\frac{\bar{J}^2}{n} \right)_x + 2\nu\bar{J} \left(\frac{n_x}{n} \right)_x + \frac{\bar{J}}{\tau_0} \right) \varphi dx + \int_0^1 \left(\left(1 + \frac{\nu}{T_0\tau_0} \right) h_0(n) - V - V_B - 2(\varepsilon_0^2 + \nu^2)B(n) \right) (n\varphi)_x dx + (Vn\varphi) \Big|_{x=0}^1 = 0 \quad (2.1)$$

holds for each $\varphi \in H^1((0, 1))$ with $\varphi(0) = \varphi(1)$, and the equations (1.2), (1.4), (1.5), (1.7), (1.8) are satisfied.

Conversely, let us be given functions $(n, V) \in H^2((0, 1)) \times H^2((0, 1))$ and a real number \bar{J} , such that $\min_{x \in [0, 1]} n(x) > 0$ and the equations (1.4), (1.5), (1.7), (1.8) as well as the identity (2.1) are satisfied for each $\varphi \in H^1((0, 1))$ with $\varphi(0) = \varphi(1)$. Then (n, J, V) with $J := \bar{J} - \nu n_x$ is a weak solution to (1.2)–(1.8).

Proof It suffices to recall (1.10) and to remark that $B(n) = \frac{1}{2n} n_{xx} - \frac{1}{4} \left(\frac{n_x}{n} \right)^2$, as well as

$$\int_0^1 B(n) \cdot (n\varphi)_x dx = \frac{1}{2} \int_0^1 \left(n_{xx} - \frac{(n_x)^2}{n} \right) \varphi_x dx,$$

for all mentioned φ . □

We define a viscosity-adjusted quantum quasi Fermi level

$$F := \left(1 + \frac{\nu}{T_0\tau_0} \right) h_0(n) - V - V_B - 2(\varepsilon_0^2 + \nu^2)B(n) \pmod{\mathbb{R}}, \quad (2.2)$$

which we regard as a function of x that has been uniquely defined up to an additive constant.

Recall that the traditional quantum quasi Fermi level $F_0 = h_0(n) - (V + V_B + 2\varepsilon_0^2 B(n))$ has been used in the investigations of quantum drift diffusion models, see [23], [24], [25]. On the other hand, this paper discusses the viscous quantum hydrodynamic model, which motivates the viscosity-adjustments. To simplify notations, we define

$$T := T_0 + \frac{\nu}{\tau_0}, \quad \varepsilon := \sqrt{\varepsilon_0^2 + \nu^2}, \quad h(n) := T \ln n = \left(1 + \frac{\nu}{T_0\tau_0} \right) h_0(n),$$

and then the quantum quasi Fermi level of (2.2) turns into $F \equiv h(n) - (V + V_B + 2\varepsilon^2 B(n)) \pmod{\mathbb{R}}$. The rule is that the original physical quantities and constants have a subscript zero, which is omitted for their viscosity-adjusted counterparts.

Lemma 2.2 *Let (n, J, V) be a weak solution to (1.2)–(1.8). Then the Fermi level $F \in L^2((0, 1))$, defined in (2.2), has the distributional derivative*

$$F_x = - \left(\frac{\bar{J}^2}{2n^2} \right)_x + 2\nu\bar{J} \frac{(\ln n)_{xx}}{n} + \frac{\bar{J}}{\tau_0 n} = - \left(\frac{\bar{J}^2 - 4\nu\bar{J}n_x}{2n^2} \right)_x + \bar{J} \left(\frac{1}{\tau_0 n} + 2\nu \frac{(n_x)^2}{n^3} \right), \quad (2.3)$$

where the constant \bar{J} is defined via $\bar{J} := \int_0^1 J(x) dx$.

Moreover, $F \in H^1((0, 1))$, and we have the identity

$$F(1) - F(0) = \bar{J} \int_0^1 \left(\frac{1}{\tau_0 n} + 2\nu \frac{(n_x)^2}{n^3} \right) dx = V_l - V_r. \quad (2.4)$$

Proof Observe that we can exploit

$$\int_0^1 \left(- \left(\frac{\bar{J}^2}{n} \right)_x + 2\nu\bar{J} \left(\frac{n_x}{n} \right)_x + \frac{\bar{J}}{\tau_0} \right) \varphi dx = \int_0^1 \left(- \left(\frac{\bar{J}^2}{2n^2} \right)_x + 2\nu\bar{J} \frac{(\ln n)_{xx}}{n} + \frac{\bar{J}}{\tau_0 n} \right) (n\varphi) dx$$

to rewrite (2.1), and now it suffices to choose $\varphi \in H^1((0, 1))$ in such a way that $n\varphi$ runs through $C_0^\infty((0, 1))$ to get the first claim. The first part of (2.4) follows from integrating (2.3) over $(0, 1)$, and the second part follows from choosing $\varphi = \frac{1}{n}$ in (2.1). \square

Lemma 2.3 *Let (n, J, V) be a weak solution to (1.2)–(1.8), and suppose (1.9). Then n has H^3 regularity on the intervals $(0, c)$ and $(1 - c, 1)$, and it satisfies the boundary condition (1.6).*

Proof The equation (2.2) implies that $B(n)$ has H^1 regularity on $(0, c)$ and $(1 - c, 1)$. In particular, $B(n)$ has traces at $x = 0$ and $x = 1$. From (2.4) we learn that $F(1) + V_r = F(0) + V_l$ which implies $B(n)|_{x=1} = B(n)|_{x=0}$. \square

In view of (2.4), we may introduce

$$F_\Delta := V_l - V_r$$

as the known (nonnegative) difference of the Fermi level F at both ends of the device.

Lemma 2.4 *Let $n \in H^2((0, 1))$ with (1.5), (1.8) and $\min_{x \in [0, 1]} n(x) > 0$ be a given function. Define a function $V \in H^2((0, 1))$ as the unique solution to (1.4) with boundary conditions (1.7), and then define a function $F \in L^2((0, 1))$ via (2.2). Next define a number \bar{J} via*

$$\bar{J} := \frac{F_\Delta}{\int_0^1 \left(\frac{1}{\tau_0 n} + 2\nu \frac{(n_x)^2}{n^3} \right) dx}, \quad (2.5)$$

and suppose that the function F possesses the distributional derivative F_x given in (2.3).

Then (n, J, V) with $J := \bar{J} - \nu n_x$ is a weak solution to (1.2)–(1.8).

Proof We know that

$$\int_0^1 \left(- \left(\frac{\bar{J}^2}{n} \right)_x + 2\nu \bar{J} \left(\frac{n_x}{n} \right)_x + \frac{\bar{J}}{\tau_0} \right) \frac{\psi}{n} dx + \int_0^1 F \psi_x dx + (V\psi)|_{x=0}^1 = 0 \quad (2.6)$$

holds for all functions $\psi \in C_0^\infty((0, 1))$; and by density arguments, also for all functions $\psi \in H_0^1((0, 1))$. Integrating (2.3) over $(0, 1)$, we find that (2.6) remains true for the function $\psi \equiv 1$. By linearity, we then deduce that (2.1) holds for all $\varphi \in H^1((0, 1))$ with $\varphi(0) = \varphi(1)$. It remains to apply the converse part of Lemma 2.1. \square

Remark 2.5 *For completeness, we compare some of our results obtained so far to the (quantum) drift-diffusion system, which is formally obtained from the viscous quantum hydrodynamic system (1.1) by neglecting the acceleration terms $\partial_t J - \operatorname{div}(J \otimes J/n)$ and setting the viscosity constant ν to zero. Then it is well-known [26] that the Fermi level F as defined in (2.2) connects to the vectorial current density J via the relation $J = \mu n \nabla F$, with μ denoting a mobility constant. On the other hand, our relation (2.3) can be written as $\bar{J} = \tau_0 n F_x + (\text{acceleration terms}) + (\text{viscous terms})$. In that sense, Lemma 2.2 is natural.*

Moreover, from the identity (2.5), we conclude that \bar{J} has the same sign as F_Δ . And if $F_\Delta = 0$, then $\bar{J} = 0$, and (2.3) forces the function F to be a constant, which turns the stationary viscous quantum hydrodynamic model into a system of two second order elliptic equations (1.4) and (2.2). Then the approach of [24], [23], [25] becomes directly applicable. A formula similar to (2.5), connecting the averaged current \bar{J} , the applied voltage F_Δ , and the particle density n , can also be found in [27] (e.g., in Lemma 3.1 there), for a classical hydrodynamical semiconductor model.

Now we have two different representations for the viscosity-adjusted quantum quasi Fermi level F , and the following strategy towards a weak solution of (1.2)–(1.8) seems reasonable: Take an initial approximation n_{init} for the electron density; compute \bar{J} via (2.5); construct F modulo constants by (2.3); and then compute (n, V) as solutions to the elliptic system (1.4), (2.2) (for instance, as minimisers of appropriate functionals). This will give us a mapping $n_{\text{init}} \mapsto n$ for which the existence of fixed points can be proved using the Schauder fixed point theorem.

However, it turns out that certain regularisations are advisable in order to handle singularities in the Fermi level F and in the enthalpy h which occur when n reaches zero.

3. First a priori Estimates on the Average Current and Velocity

The relation (2.5) and the charge neutrality condition (1.8) together enable us to find estimates on the average current $\bar{J} := \int_0^1 J(x) dx$ and the “average velocity” $\frac{\bar{J}}{n}$ in various norms.

Through the rest of the paper, we suppose that

$$\tau_0 \leq \nu^{-1}, \quad (3.1)$$

which holds in all physically relevant situations with a wide margin and simplifies some formulae.

Lemma 3.1 *Let $n \in H^1((0, 1))$ be a function with $\min_{x \in [0,1]} n(x) > 0$, and put*

$$K := \int_0^1 \left(\frac{1}{\tau_0 n} + 2\nu \frac{(n_x)^2}{n^3} \right) dx.$$

Under the assumption (3.1), then there is a universal constant C such that

$$\|n^{-1}\|_{L^p(0,1)} \leq CK\tau_0^{1/2+1/(2p)}\nu^{-(1-1/p)/2}, \quad 1 \leq p \leq \infty. \quad (3.2)$$

Proof We have the estimates

$$\|n^{-1/2}\|_{L^2(0,1)} \leq (\tau_0 K)^{1/2}, \quad \|(n^{-1/2})_x\|_{L^2(0,1)} \leq (2K/\nu)^{1/2}, \quad \|n^{-1/2}\|_{H^1(0,1)} \leq CK^{1/2}(\tau_0 + \nu^{-1})^{1/2} \leq CK^{1/2}\nu^{-1/2},$$

and then interpolation gives us

$$\|n^{-1/2}\|_{L^\infty(0,1)} \leq CK^{1/2}\tau_0^{1/4}\nu^{-1/4},$$

which directly implies (3.2) in case of $p = \infty$. The general case follows from interpolation with $\|n^{-1}\|_{L^1(0,1)} \leq K\tau_0$. \square

Now we bring the charge neutrality (1.8) into play and obtain the announced *a priori* estimates. The first one (3.3) relates the averaged current \bar{J} to the applied voltage F_Δ , hence it can be understood as an inequality version of Ohm’s Law. The velocity estimates (3.4) and (3.5) have the following interpretation: If the density n_{init} of mobile electrons is small over a non-small region, then only a little current can flow, hence \bar{J} must also be small. Compare Theorem 3.1 of [16] for a similar estimate with a weaker exponent of ν .

Lemma 3.2 *Let $n_{\text{init}} \in H^1(0, 1)$ be a function with $\min_{x \in [0,1]} n_{\text{init}}(x) > 0$ satisfying the charge neutrality condition (1.8), and let \bar{J}, F_Δ be nonnegative numbers such that (2.5) holds (with n_{init} at the place of n).*

Then the following estimates are valid:

$$\bar{J} \leq \tau_0 F_\Delta C_*, \quad (3.3)$$

$$\left\| \frac{\bar{J}}{n_{\text{init}}} \right\|_{L^\infty(0,1)} \leq CF_\Delta \tau_0^{1/2} \nu^{-1/2}, \quad (3.4)$$

$$\left\| \frac{\bar{J}}{n_{\text{init}}} \right\|_{L^2(0,1)} \leq CF_\Delta \tau_0^{3/4} \nu^{-1/4}. \quad (3.5)$$

Proof Only the case of positive \bar{J}, F_Δ is relevant. By the Cauchy–Schwarz inequality, we have

$$1 = \left(\int_0^1 1 dx \right)^2 \leq \|n_{\text{init}}\|_{L^1(0,1)} \int_0^1 \frac{1}{n_{\text{init}}} dx,$$

and therefore, by (2.5),

$$F_\Delta \geq \frac{\bar{J}}{\tau_0} \int_0^1 \frac{1}{n_{\text{init}}} dx \geq \frac{\bar{J}}{\tau_0 C_*}.$$

The remaining estimates follow from (3.2) with $K := F_\Delta/\bar{J}$. \square

4. A Variational Problem

Now our refined approach is: We take an initial approximation n_{init} with

$$n_{\text{init}} \in H_{\text{per}}^1((0, 1)), \quad \min_{x \in [0,1]} n_{\text{init}}(x) > 0, \quad \int_0^1 n_{\text{init}} dx = \mathcal{C}_*,$$

where $H_{\text{per}}^1(0, 1)$ consists of those functions u of $H^1(0, 1)$ with $u(0) = u(1)$, by definition. Then we calculate \bar{J} via (2.5) (with n_{init} instead of n). According to (2.3), the Fermi level F would satisfy

$$F(x) = \bar{J} \int_0^x \left(\frac{1}{\tau_0 n_{\text{init}}} + 2\nu \frac{(n_{\text{init},x})^2}{n_{\text{init}}^3} \right) (y) dy - \frac{\bar{J}^2 - 4\nu \bar{J} n_{\text{init},x}(x)}{2n_{\text{init}}^2(x)} \quad \text{mod } \mathbb{R}, \quad (4.1)$$

in case that n_{init} were already a component of a weak solution $(n_{\text{init}}, \bar{J} - \nu n_{\text{init},x}, V)$.

Hence, we define a function G by

$$G(x) := \bar{J} \int_0^x \left(\frac{1}{\tau_0 n_{\text{init}}} + 2\nu \frac{(n_{\text{init},x})^2}{n_{\text{init}}^3} \right) (y) dy,$$

which is the part of the Fermi level F in (4.1), for which we have the nice pointwise bounds $0 \leq G(x) \leq F_{\Delta}$. To bound the other terms in F , a regularisation becomes necessary. To this end, for $\delta > 0$, choose $\psi_{\delta} \in C^{\infty}(\mathbb{R})$ with $|\psi'_{\delta}| \leq 2$, and $\psi_{\delta}(s) \geq |s|/2$ and

$$\psi_{\delta}(s) = \begin{cases} |s| & : |s| \geq 2\delta, \\ \delta & : 0 \leq |s| \leq \delta. \end{cases}$$

We also define, for a large constant K , a truncation function

$$\xi_K(s) := \begin{cases} -K & : s \leq -K, \\ s & : -K < s < K, \\ K & : K \leq s, \end{cases}$$

and then we specify a regularised Fermi level

$$F_{(\delta,K)} := G - \frac{\bar{J}^2}{2n_{\text{init}}^2} + \frac{4\nu \bar{J} \sqrt{n_{\text{init}}} \cdot \xi_K((\sqrt{n_{\text{init}}})_x)}{\psi_{\delta}^2(n_{\text{init}})}, \quad (4.2)$$

which clearly allows for pointwise bounds $|F_{(\delta,K)}(x)| \leq C_{\delta,K}$. Because of (3.4), a regularisation of the term $\frac{\bar{J}^2}{2n_{\text{init}}^2}$ is not needed.

Then we intend to find (n, V) as solutions to the coupled elliptic system

$$\begin{cases} F_{(\delta,K)} = h(n) - (V + V_B) - 2\varepsilon^2 B(n) - \beta, \\ \lambda_0^2 V_{xx} = n - \mathcal{C}, \\ n(0) = n(1), \quad n_x(0) = n_x(1), \quad \int_0^1 n dx = \mathcal{C}_*, \\ V(0) = V_l, \quad V(1) = V_r, \end{cases} \quad (4.3)$$

and the unknown (n, V) will turn out to be minimisers of certain functionals, and the parameter $\beta \in \mathbb{R}$ then will be the Lagrange multiplier associated to the constraint (1.8). Recall that (2.2) characterizes the Fermi level F only modulo additive constants, and β can be seen as such a constant. It remains to show that the mapping $n_{\text{init}} \mapsto n$ possesses a fixed point.

To construct the functional of which the desired function n will be a minimiser, we proceed in several steps. Define the inhomogeneous part V_{inh} of V by

$$\lambda_0^2 V_{\text{inh},xx} = -\mathcal{C}, \quad V(0) = V_l, \quad V(1) = V_r.$$

The unique solution V to the boundary value problem

$$\lambda_0^2 V_{xx} = g, \quad V(0) = 0, \quad V(1) = 0$$

will be written as $V = \Phi\{g\}$, with $\Phi: L^2(0, 1) \rightarrow L^2(0, 1)$ as a compact self-adjoint linear operator. By direct computation, we then find:

Lemma 4.1 *The norm of the (extended) operator $\Phi: L^1(0, 1) \rightarrow L^\infty(0, 1)$ is bounded by $C_\Phi \lambda_0^{-2}$ for some uniform constant C_Φ , and Φ has the properties*

$$-\int_0^1 \Phi\{g\} \cdot g \, dx = \lambda_0^2 \int_0^1 |\Phi\{g\}_x|^2 \, dx, \tag{4.4}$$

$$\frac{\lambda_0^2}{2} \int_0^1 |\Phi\{(\varrho_* + t\varphi)^2\}_x|^2 \, dx = \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho_*^2\}_x|^2 \, dx - 2t \int_0^1 \Phi\{\varrho_*^2\} \varrho_* \varphi \, dx + \mathcal{O}(t^2), \tag{4.5}$$

for $t \rightarrow 0$, where $\varrho_* \in L^4((0, 1))$, and $\varphi \in H_{\text{per}}^2((0, 1))$. And for $g, g_* \in L^2((0, 1))$, we have

$$\frac{\lambda_0^2}{2} \int_0^1 |\Phi\{g\}_x|^2 \, dx - \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{g_*\}_x|^2 \, dx = -\int_0^1 \Phi\{g_*\} \cdot (g - g_*) \, dx + \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{g - g_*\}_x|^2 \, dx. \tag{4.6}$$

Next, we select primitive functions to the enthalpy h :

$$H(s) := T(s \ln s - s + 1), \quad H_*(s) := T(s \ln s - s + \mathcal{C}_*), \quad s > 0.$$

We recall the celebrated Csiszár–Kullback inequality [28], [29], [30], see also the survey [31]:

Lemma 4.2 *Let (Ω, Σ, μ) be a probability space, and let $f \in L^1(\Omega, d\mu)$ be real-valued and nonnegative with $\int_\Omega f \, d\mu = 1$. Then*

$$\int_\Omega f \ln f \, d\mu \geq \frac{1}{2} \|f - 1\|_{L^1(\Omega, d\mu)}^2.$$

This inequality will be our main device in the next estimates of the entropy terms:

Lemma 4.3 *For $\varrho \in L^2(0, 1)$ with*

$$\int_0^1 \varrho^2 \, dx = \mathcal{C}_*, \tag{4.7}$$

there holds

$$\int_0^1 H_*(\varrho^2) \, dx = \int_0^1 h(\varrho^2) \varrho^2 \, dx \geq T \mathcal{C}_* \ln \mathcal{C}_* + \frac{T}{2\mathcal{C}_*} \|\varrho^2 - \mathcal{C}_*\|_{L^1(0,1)}^2. \tag{4.8}$$

If $\varrho_\diamond \in L^2(0, 1)$ is an arbitrary function with $\varrho_\diamond \geq c > 0$ on $[0, 1]$ for some constant c , then

$$\int_0^1 H_*(\varrho_\diamond + t\varphi)^2 \, dx = \int_0^1 H_*(\varrho_\diamond^2) \, dx + 2t \int_0^1 h(\varrho_\diamond^2) \varrho_\diamond \varphi \, dx + \mathcal{O}_c(t^2), \quad t \rightarrow 0, \tag{4.9}$$

with $\varphi \in L^2(0, 1)$. And if also $\varrho_* \in L^2(0, 1)$ with $\int_0^1 \varrho_*^2 \, dx = \mathcal{C}_*$, then

$$\int_0^1 H_*(\varrho^2) - H_*(\varrho_*^2) - h(\varrho_*^2)(\varrho^2 - \varrho_*^2) \, dx \geq \frac{T}{2\mathcal{C}_*} \|\varrho^2 - \varrho_*^2\|_{L^1(0,1)}^2. \tag{4.10}$$

Proof We begin with (4.8). Put $f := \varrho^2/C_*$. Then $\int_0^1 f \, dx = 1$, and Lemma 4.2 gives us

$$\begin{aligned} \int_0^1 h(\varrho^2)\varrho^2 \, dx &= T \int_0^1 \ln(f C_*)f C_* \, dx = T C_* \ln C_* + T C_* \int_0^1 f \ln f \, dx \\ &\geq T C_* \ln C_* + \frac{T C_*}{2} \|f - 1\|_{L^1(0,1)}^2 = T C_* \ln C_* + \frac{T}{2 C_*} \|\varrho^2 - C_*\|_{L^1(0,1)}^2. \end{aligned}$$

And to show (4.10), we first calculate

$$\int_0^1 H_*(\varrho^2) - H_*(\varrho_*^2) - h(\varrho_*^2)(\varrho^2 - \varrho_*^2) \, dx = \int_0^1 H\left(\frac{\varrho^2(x)}{\varrho_*^2(x)}\right) \varrho_*^2(x) \, dx.$$

Now we put $f := \varrho^2/\varrho_*^2$ and define a measure

$$d\mu(x) := \frac{\varrho_*^2(x)}{C_*} \, dx,$$

with $\int_0^1 d\mu = 1$ and $\int_0^1 f \, d\mu = 1$, and then from the Csiszár–Kullback inequality we get

$$\int_0^1 H\left(\frac{\varrho^2(x)}{\varrho_*^2(x)}\right) \varrho_*^2(x) \, dx = C_* T \int_0^1 f \ln f \, d\mu \geq \frac{T}{2 C_*} \left(\int_0^1 |\varrho^2(x) - \varrho_*^2(x)| \, dx \right)^2,$$

which completes the proof. \square

Now, with the substitution $n = \varrho^2$, our intention is to minimise the functional

$$\mathcal{F}_{\delta,K}(\varrho^2) := \int_0^1 - (F_{(\delta,K)} + V_B + V_{\text{inh}}) \varrho^2 + H_*(\varrho^2) + \frac{\lambda_0^2}{2} |\Phi\{\varrho^2\}_x|^2 \, dx + \int_0^1 2\varepsilon^2(\varrho_x)^2 \, dx, \quad (4.11)$$

with respect to the function $\varrho \in H_{\text{per}}^1(0, 1)$ over the set

$$X = \{\varrho \in H_{\text{per}}^1(0, 1) : \varrho \text{ satisfies (4.7)}\}. \quad (4.12)$$

Note that we have, by (4.5) and (4.9),

$$\mathcal{F}_{\delta,K}((\varrho_* + t\varphi)^2) = \mathcal{F}_{\delta,K}(\varrho_*^2) + 2t \int_0^1 \left(-(F_{(\delta,K)} + V_B + V_{\text{inh}}) + h(\varrho_*^2) - \Phi\{\varrho_*^2\}_x - 2\varepsilon^2 \frac{\varrho_{*,xx}}{\varrho_*} \right) \varrho_* \varphi \, dx + \mathcal{O}(t^2),$$

for functions $\varrho_* \in H_{\text{per}}^2(0, 1)$ taking only positive values, and $\varphi \in H_{\text{per}}^1(0, 1)$. Therefore, the Euler–Lagrange equation to $\mathcal{F}_{\delta,K}$ with respect to variations of ϱ is indeed the first equation of (4.3) if we set $V = V_{\text{inh}} + \Phi\{\varrho_*^2\}$.

Lemma 4.4 *Let $F_{(\delta,K)} \in L^\infty(0, 1)$ be arbitrary. Then the functional $\mathcal{F}_{\delta,K}$ from (4.11) possesses a unique positive minimiser $\varrho_{\delta,K} \in X \cap H_{\text{per}}^2(0, 1)$, which solves the Euler–Lagrange equation*

$$0 = -(F_{(\delta,K)} + V_B + V)\varrho_{\delta,K} + h(\varrho_{\delta,K}^2)\varrho_{\delta,K} - 2\varepsilon^2 \varrho_{\delta,K,xx} - \beta_{\delta,K} \varrho_{\delta,K}, \quad (4.13)$$

where we have set $V := V_{\text{inh}} + \Phi\{\varrho_{\delta,K}^2\}$, and $\beta_{\delta,K}$ is a Lagrange multiplier.

The minimiser $\varrho_{\delta,K}$ obeys a pointwise lower bound $\varrho_{\delta,K}(x) \geq c_{\delta,K} > 0$, and $c_{\delta,K}$ depends continuously on $\|F_{(\delta,K)}\|_{L^\infty(0,1)}$.

The Lagrange parameter $\beta_{\delta,K}$ can be computed from the identity

$$\beta_{\delta,K} C_* = \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) + \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho_{\delta,K}^2\}_x|^2 \, dx. \quad (4.14)$$

Proof For a proof of the existence of the positive minimiser $\varrho_{\delta,K}$, we refer to [23] and [25], where also the positive lower bound of $\varrho_{\delta,K}$ is determined, and the Euler–Lagrange equation is shown.

It remains to prove (4.14). Multiplying (4.13) by $\varrho_{\delta,K}$ and integrating over $[0, 1]$ give

$$0 = \int_0^1 -(F_{(\delta,K)} + V_B + V)\varrho_{\delta,K}^2 + h(\varrho_{\delta,K}^2)\varrho_{\delta,K}^2 dx - \int_0^1 2\varepsilon^2 \varrho_{\delta,K,xx} \varrho_{\delta,K} dx - \beta_{\delta,K} \int_0^1 \varrho_{\delta,K}^2 dx,$$

which can be recast as

$$\begin{aligned} \beta_{\delta,K} C_* &= \int_0^1 -(F_{(\delta,K)} + V_B + V_{inh})\varrho_{\delta,K}^2 + H_*(\varrho_{\delta,K}^2) + \lambda_0^2 |\Phi\{\varrho_{\delta,K}^2\}_x|^2 + 2\varepsilon^2 (\varrho_{\delta,K,x})^2 dx \\ &= \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) + \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho_{\delta,K}^2\}_x|^2 dx, \end{aligned}$$

see (4.4). □

5. A Fixed Point Problem, and the Proof of Theorem 1.2

In this section, we show that the mapping $\sqrt{n_{init}} \mapsto \varrho_{\delta,K}$ possesses a fixed point for each pair $(\delta, K) \in (0, 1) \times (1, \infty)$. We also prove that this fixed point does not depend on (δ, K) for large enough K and small enough δ , which then makes it possible to drop the regularisation of the functional $\mathcal{F}_{(\delta,K)}$. We begin with some estimates.

Lemma 5.1 *Let $F_{(\delta,K)} \in L^\infty(0, 1)$ be arbitrary. There is a constant C_1 (depending on $V_B, V_{inh}, C_*, \lambda_0$, but not on $F_{(\delta,K)}$) such that for all $\varrho \in X$ with $\min_{x \in [0,1]} \varrho(x) > 0$ we have*

$$\begin{aligned} \mathcal{F}_{\delta,K}(\varrho^2) &\geq - \int_0^1 F_{(\delta,K)}(x)\varrho^2(x) dx - C_1 + T C_* \ln C_* + 2\varepsilon^2 \|\varrho_x\|_{L^2(0,1)}^2, \\ \mathcal{F}_{\delta,K}(C_*) &\leq - \int_0^1 F_{(\delta,K)}(x) C_* dx + C_1 + T C_* \ln C_*. \end{aligned}$$

However, if $F_{(\delta,K)}$ is constructed via (4.2), then we have, for all functions $\varrho \in X$ from (4.12), that

$$\int_0^1 |F_{(\delta,K)}\varrho^2| dx \leq C F_\Delta C_* \left(1 + F_\Delta \tau_0 \nu^{-1} + (\tau_0 \nu / C_*)^{1/4} \|\varrho\|_{W_2^1(0,1)}^{1/2}\right). \quad (5.1)$$

And if $\varrho_{\delta,K}$ is the unique positive minimiser from Lemma 4.4, then

$$\begin{aligned} \mathcal{F}_{\delta,K}(\varrho^2) - \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) &= \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho^2 - \varrho_{\delta,K}^2\}_x|^2 dx + \int_0^1 H\left(\frac{\varrho^2}{\varrho_{\delta,K}^2}\right) \varrho_{\delta,K}^2 dx + 2\varepsilon^2 \int_0^1 \frac{1}{\varrho_{\delta,K}^2} |\varrho_{\delta,K} \varrho_x - \varrho \varrho_{\delta,K,x}|^2 dx \\ &\geq \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho^2 - \varrho_{\delta,K}^2\}_x|^2 dx + \frac{T}{2C_*} \|\varrho^2 - \varrho_{\delta,K}^2\|_{L^1(0,1)}^2 + 2\varepsilon^2 \int_0^1 \varrho^2 \left| \left(\ln \frac{\varrho}{\varrho_{\delta,K}}\right)_x \right|^2 dx. \end{aligned} \quad (5.2)$$

Proof Using (4.8), we directly get

$$\mathcal{F}_{\delta,K}(\varrho^2) \geq - \int_0^1 F_{(\delta,K)} \varrho^2 dx - \|V_B + V_{inh}\|_{L^\infty(0,1)} C_* + T C_* \ln C_* + 2\varepsilon^2 \|\varrho_x\|_{L^2(0,1)}^2,$$

and the estimate on $\mathcal{F}_{\delta,K}(C_*)$ is obvious. To prove (5.1), we write

$$\begin{aligned} \int_0^1 |F_{(\delta,K)}\varrho^2| dx &\leq \int_0^1 G \varrho^2 dx + \int_0^1 \frac{\bar{J}}{n_{init}^2} \frac{\varrho^2}{2} dx + \int_0^1 \frac{4\nu \bar{J} \sqrt{n_{init}} |\xi_K((\sqrt{n_{init}})_x)|}{\psi_\delta^2(n_{init})} \varrho^2 dx \\ &\leq F_\Delta C_* + \left\| \frac{\bar{J}}{n_{init}} \right\|_{L^\infty(0,1)}^2 \frac{C_*}{2} + C \int_0^1 \sqrt{J\nu} \frac{|(\sqrt{n_{init}})_x|}{n_{init}} \cdot \nu^{1/4} \left(\frac{\bar{J}}{n_{init}}\right)^{1/2} \cdot \nu^{1/4} \varrho^2 dx \\ &\leq F_\Delta C_* + C C_* F_\Delta^2 \tau_0 \nu^{-1} + C \left\| \sqrt{J\nu} \frac{(\sqrt{n_{init}})_x}{n_{init}} \right\|_{L^2(0,1)} \cdot \nu^{1/4} \left\| \frac{\bar{J}}{n_{init}} \right\|_{L^\infty(0,1)}^{1/2} \cdot \nu^{1/4} \|\varrho^2\|_{L^2(0,1)}, \end{aligned}$$

where we have used (3.4). To discuss the last item of the sum, we note that (2.5) implies

$$F_{\Delta} \geq \int_0^1 \bar{J}\nu \frac{(n_{\text{init},x})^2}{n_{\text{init}}^3} dx \geq C \int_0^1 \bar{J}\nu \frac{((\sqrt{n_{\text{init}}})_x)^2}{n_{\text{init}}^2} dx \geq C \left\| \sqrt{\bar{J}\nu} \frac{(\sqrt{n_{\text{init}}})_x}{n_{\text{init}}} \right\|_{L^2(0,1)}^2.$$

The second factor is handled by (3.4), and concerning the third factor, we interpolate

$$\|u\|_{L^4(0,1)} \leq C \|u\|_{W_2^1(0,1)}^{1/4} \|u\|_{L^2(0,1)}^{3/4},$$

valid for $u \in W_2^1(0,1)$, from which we deduce that

$$\|\varrho^2\|_{L^2(0,1)} = \|\varrho\|_{L^4(0,1)}^2 \leq C \|\varrho\|_{W_2^1(0,1)}^{1/2} \cdot \|\varrho\|_{L^2(0,1)}^{3/2} = C(C^*)^{3/4} \|\varrho\|_{W_2^1(0,1)}^{1/2},$$

giving us (5.1). And the final claim (5.2) is proved as follows:

$$\begin{aligned} \mathcal{F}_{\delta,K}(\varrho^2) - \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) &= \int_0^1 -(F_{(\delta,K)} + V_B + V_{\text{inh}})(\varrho^2 - \varrho_{\delta,K}^2) + (H_*(\varrho^2) - H_*(\varrho_{\delta,K}^2)) dx \\ &\quad + \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho^2\}_x|^2 - |\Phi\{\varrho_{\delta,K}^2\}_x|^2 dx + 2\varepsilon^2 \int_0^1 (\varrho_x)^2 - (\varrho_{\delta,K,x})^2 dx \\ &= \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho^2 - \varrho_{\delta,K}^2\}_x|^2 dx + \int_0^1 -(F_{(\delta,K)} + V_B + V)(\varrho^2 - \varrho_{\delta,K}^2) dx \\ &\quad + \int_0^1 (H_*(\varrho^2) - H_*(\varrho_{\delta,K}^2)) dx + 2\varepsilon^2 \int_0^1 (\varrho_x)^2 - (\varrho_{\delta,K,x})^2 dx, \end{aligned}$$

where $V := V_{\text{inh}} + \Phi\{\varrho_{\delta,K}^2\}$, using (4.6). Now the Euler–Lagrange (4.13) equation becomes

$$-(F_{(\delta,K)} + V_B + V) = -h(\varrho_{\delta,K}^2) + 2\varepsilon^2 \frac{\varrho_{\delta,K,xx}}{\varrho_{\delta,K}} + \beta_{\delta,K},$$

and then $\int_0^1 \varrho^2 - \varrho_{\delta,K}^2 dx = 0$ brings us to

$$\begin{aligned} \mathcal{F}_{\delta,K}(\varrho^2) - \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) &= \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho^2 - \varrho_{\delta,K}^2\}_x|^2 dx + \int_0^1 (H_*(\varrho^2) - H_*(\varrho_{\delta,K}^2)) - h(\varrho_{\delta,K}^2)(\varrho^2 - \varrho_{\delta,K}^2) dx \\ &\quad + 2\varepsilon^2 \int_0^1 \frac{\varrho_{\delta,K,xx}}{\varrho_{\delta,K}} (\varrho^2 - \varrho_{\delta,K}^2) + (\varrho_x)^2 - (\varrho_{\delta,K,x})^2 dx \\ &= \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho^2 - \varrho_{\delta,K}^2\}_x|^2 dx + \int_0^1 H\left(\frac{\varrho^2}{\varrho_{\delta,K}^2}\right) \varrho_{\delta,K}^2 dx + 2\varepsilon^2 \int_0^1 \frac{1}{\varrho_{\delta,K}^2} |\varrho_{\delta,K} \varrho_x - \varrho \varrho_{\delta,K,x}|^2 dx. \end{aligned}$$

Now it remains to apply (4.10). □

Lemma 5.2 *There is a constant C_2 , depending only on C_1 and the physical parameters (except the quantum parameters ν, ε), but independent of the regularisation parameters δ, K , such that:*

If the function $F_{(\delta,K)}$ is constructed from a function $\sqrt{n_{\text{init}}} \in X$ via (4.2), then the unique minimiser $\varrho_{\delta,K}$ to the functional $\mathcal{F}_{\delta,K}$, as it has been constructed in Lemma 4.4, satisfies the upper bounds

$$\varepsilon^2 \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^2 \leq C_2 (1 + \nu^{-1}), \tag{5.3}$$

$$\|\varrho_{\delta,K}\|_{L^\infty(0,1)}^2 \leq C_2 (1 + \nu^{-1})^{1/2} \varepsilon^{-1}, \tag{5.4}$$

and it also satisfies a lower bound

$$\min_{x \in [0,1]} \varrho_{\delta,K}(x) \geq C_3^{-1}, \tag{5.5}$$

with a constant C_3 depending only on C_2, ε, ν , but not on $(\delta, K) \in (0, 1) \times (1, \infty)$.

The Lagrange multiplier $\beta_{\delta,K}$ is uniformly in (δ, K) bounded by

$$|\beta_{\delta,K}| \leq C_2(1 + \nu^{-1}). \tag{5.6}$$

Proof We clearly have $\mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) \leq \mathcal{F}_{\delta,K}(C_*)$, and then Lemma 5.1 yields

$$\begin{aligned} 2\varepsilon^2 \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^2 &\leq 2C_1 + \left| \int_0^1 F_{(\delta,K)} \varrho_{\delta,K}^2 dx \right| + \left| \int_0^1 F_{(\delta,K)} C_* dx \right| \\ &\leq 2C_1 + CF_{\Delta} C_* \left(1 + F_{\Delta} \tau_0 \nu^{-1} + (\tau_0 \nu / C_*)^{1/4} \|\varrho_{\delta,K}\|_{W_2^1(0,1)}^{1/2} + (\tau_0 \nu / C_*)^{1/4} \|\sqrt{C_*}\|_{W_2^1(0,1)}^{1/2} \right) \\ &\leq 2C_1 + CF_{\Delta} C_* \left(1 + F_{\Delta} \tau_0 \nu^{-1} + (\tau_0 \nu / C_*)^{1/4} \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^{1/2} + (\tau_0 \nu)^{1/4} \right). \end{aligned} \tag{5.7}$$

Now we exploit Young's inequality along the lines of

$$\begin{aligned} \nu^{1/4} \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^{1/2} &= \left(\varepsilon^2 \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^2 \right)^{1/4} \cdot \left(\frac{\nu}{\varepsilon^2} \right)^{1/4} \\ &\leq \varepsilon^2 \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^2 + C \left(\frac{\nu}{\varepsilon^2} \right)^{1/3} \\ &\leq \varepsilon^2 \|\varrho_{\delta,K,x}\|_{L^2(0,1)}^2 + C\nu^{-1}, \end{aligned}$$

which completes the proof of (5.3). The estimate of $\|\varrho_{\delta,K}\|_{L^\infty(0,1)}$ follows from interpolation with $\|\varrho_{\delta,K}\|_{L^2(0,1)}^2 = C_*$. Concerning the lower bound (5.5), we utilise (5.2) with $\varrho^2 = C_*$ and find:

$$\begin{aligned} 2\varepsilon^2 \int_0^1 C_* |(\ln \varrho_{\delta,K})_x|^2 dx &\leq \mathcal{F}_{\delta,K}(C_*) - \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) \\ &\leq 2C_1 + \left| \int_0^1 F_{(\delta,K)} \varrho_{\delta,K}^2 dx \right| + \left| \int_0^1 F_{(\delta,K)} C_* dx \right|, \end{aligned}$$

and this is the right-hand side of (5.7) again. The result then is

$$\int_0^1 |(\ln \varrho_{\delta,K})_x|^2 dx \leq C_2 \varepsilon^{-2} (1 + \nu^{-1}),$$

with possibly new C_2 . Now let $x_0 < x_1$ be arbitrary points of the interval $[0, 1]$. Since $\varrho_{\delta,K}$ is continuous, we have

$$\begin{aligned} |\ln \varrho_{\delta,K}(x_1) - \ln \varrho_{\delta,K}(x_0)| &\leq \|(\ln \varrho_{\delta,K})_x\|_{L^1(x_0,x_1)} \leq \|(\ln \varrho_{\delta,K})_x\|_{L^2(0,1)} \\ &\leq (C_2 \varepsilon^{-2} (1 + \nu^{-1}))^{1/2}, \end{aligned}$$

hence $\max_{x \in [0,1]} \ln \varrho_{\delta,K}(x) - \min_{x \in [0,1]} \ln \varrho_{\delta,K}(x)$ is bounded from above. Due to $\|\varrho_{\delta,K}\|_{L^2(0,1)}^2 = C_*$, we have $\max_{x \in [0,1]} \ln \varrho_{\delta,K}(x) \geq (\ln C_*)/2$, and then (5.5) follows. \square

Lemma 5.3 *The minimiser $\varrho_{\delta,K}$ constructed in Lemma 4.4 depends continuously on the regularised quantum quasi Fermi level $F_{(\delta,K)}$ in the following sense: let $F_{(\delta,K)}$ and $\tilde{F}_{(\delta,K)}$ be given functions from $L^\infty(0, 1)$ (not necessarily constructed via (4.2)), and let $\varrho_{\delta,K}, \tilde{\varrho}_{\delta,K}$ be the unique positive minimizers to the functionals $\mathcal{F}_{\delta,K}$ and $\tilde{\mathcal{F}}_{\delta,K}$. Then it holds*

$$\|\varrho_{\delta,K}^2 - \tilde{\varrho}_{\delta,K}^2\|_{L^1(0,1)} \leq \frac{\sqrt{2}}{\sqrt{T}} C_* \|F_{(\delta,K)} - \tilde{F}_{(\delta,K)}\|_{L^\infty(0,1)}^{1/2}.$$

Proof Without losing generality, we may assume $\mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) \geq \tilde{\mathcal{F}}_{\delta,K}(\tilde{\varrho}_{\delta,K}^2)$. Then we have the chain of inequalities

$$\begin{aligned} \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) &\geq \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2) \geq \tilde{\mathcal{F}}_{\delta,K}(\tilde{\varrho}_{\delta,K}^2) \\ &= \mathcal{F}_{\delta,K}(\tilde{\varrho}_{\delta,K}^2) - \int_0^1 (\tilde{F}_{(\delta,K)} - F_{(\delta,K)}) \tilde{\varrho}_{\delta,K}^2 dx \\ &\geq \mathcal{F}_{\delta,K}(\tilde{\varrho}_{\delta,K}^2) - \|\tilde{F}_{(\delta,K)} - F_{(\delta,K)}\|_{L^\infty(0,1)} C_*, \end{aligned}$$

hence we find that

$$\|\tilde{F}_{(\delta,K)} - F_{(\delta,K)}\|_{L^\infty(0,1)} C_* \geq \mathcal{F}_{\delta,K}(\tilde{\varrho}_{\delta,K}^2) - \mathcal{F}_{\delta,K}(\varrho_{\delta,K}^2).$$

Now it suffices to apply (5.2) with $\varrho := \tilde{\varrho}_{\delta,K}$. □

Now we discuss the mapping

$$n_{\text{init}} \mapsto (\bar{J}, n_{\text{init}}) \mapsto F_{(\delta,K)} \mapsto \varrho_{\delta,K}^2 =: \mathcal{T}_{\delta,K}(n_{\text{init}}),$$

where \bar{J} is computed from n_{init} via (2.5); then $F_{(\delta,K)}$ is constructed from $(\bar{J}, n_{\text{init}})$ using (4.2); and finally $\varrho_{\delta,K}$ is determined as the unique minimiser of $\mathcal{F}_{\delta,K}$ as per Lemma 4.4.

Lemma 5.4 Let $(\delta, K) \in (0, 1) \times (1, \infty)$. For $R \in (1, \infty)$, define a set

$$M_R := \left\{ n \in C_{\text{per}}^1([0, 1]): \min_{x \in [0, 1]} n(x) \geq \frac{1}{2} C_3^{-2}, \int_0^1 n dx = C_*, \quad \|n\|_{C^1([0, 1])} \leq R \right\}.$$

Then a constant \hat{R} exists, depending on all the physical parameters and (δ, K) , such that $\mathcal{T}_{\delta,K}$ sends the non-empty set $M_{\hat{R}}$ into

$$M_{\hat{R}} \cap \left\{ n \in W_\infty^2(0, 1): \|n_{xx}\|_{L^\infty(0, 1)} \leq \hat{R} \right\}.$$

Proof Take $n_{\text{init}} \in \bigcup_{R \geq 1} M_R$, and construct $\bar{J}, F_{(\delta,K)} \in L^\infty((0, 1))$ by (2.5) and (4.2). By Lemma 4.4, a unique minimiser $\varrho_{\delta,K}$ of $\mathcal{F}_{\delta,K}$ exists, with the regularity

$$\varrho_{\delta,K}^2 \in H_{\text{per}}^2(0, 1), \quad \int_0^1 \varrho_{\delta,K}^2 dx = C_*.$$

and $\varrho_{\delta,K}$ solves the Euler–Lagrange equation (4.13). We have the upper bound (5.4) and the lower bound (5.5) on $\varrho_{\delta,K}$, and then the equation (4.13) together with (5.6) gives us a (uniform in R) estimate of $\|\varrho_{\delta,K,xx}\|_{L^\infty(0, 1)}$. Here we exploit that $\|\tilde{F}_{(\delta,K)}\|_{L^\infty(0, 1)}$ can be estimated from above using only δ and K . Selecting \hat{R} sufficiently large will complete the proof. □

Proposition 5.5 With \hat{R} from in Lemma 5.4, the mapping $\mathcal{T}_{\delta,K}$ possesses a fixed point $\varrho_{\delta,K} \in M_{\hat{R}}$.

Proof Clearly, $M_{\hat{R}}$ is a convex, closed, non-empty subset of $C^1([0, 1])$. We will be able to apply Schauder’s fixed point theorem when we have shown that $\mathcal{T}_{\delta,K}$ is continuous as a mapping from $M_{\hat{R}} \subset C^1([0, 1])$ into $C^1([0, 1])$. To do so, we first note that the mapping $n_{\text{init}} \mapsto \bar{J}$ given by (2.5) is continuous from $M_R \subset C^1([0, 1])$ into \mathbb{R} . And (4.2) induces a map $(\bar{J}, n_{\text{init}}) \mapsto F_{(\delta,K)}$ that is continuous in the sense of $\mathbb{R} \times C^1([0, 1]) \rightarrow C^0([0, 1])$.

Now let n_{init} and \tilde{n}_0 be functions from $M_{\hat{R}}$, to which we construct $F_{(\delta,K)}$ and $\tilde{F}_{(\delta,K)}$. By Lemma 5.3,

$$\|\mathcal{T}_{\delta,K}(n_{\text{init}}) - \mathcal{T}_{\delta,K}(\tilde{n}_0)\|_{L^1(0, 1)} \leq \text{const} \|F_{(\delta,K)} - \tilde{F}_{(\delta,K)}\|_{L^\infty(0, 1)}^{1/2}.$$

However, we also know $\|\mathcal{T}_{\delta,K}(n_{\text{init}})\|_{W_\infty^2(0, 1)} \leq 2\hat{R}$ and $\|\mathcal{T}_{\delta,K}(\tilde{n}_0)\|_{W_\infty^2(0, 1)} \leq 2\hat{R}$. By interpolation, we find an exponent $\theta \in (0, 1)$ such that

$$\|\mathcal{T}_{\delta,K}(n_{\text{init}}) - \mathcal{T}_{\delta,K}(\tilde{n}_0)\|_{C^1([0, 1])} \leq \text{const} \|F_{(\delta,K)} - \tilde{F}_{(\delta,K)}\|_{L^\infty(0, 1)}^\theta,$$

giving us the desired continuity. □

We need one more estimate before we can drop the regularisation parameters (δ, K) .

Lemma 5.6 *There is a constant C_4 , depending on all the physical parameters, but not on (δ, K) , such that the fixed points $\varrho_{\delta,K}$ of the mappings $\mathcal{T}_{\delta,K}$ satisfy*

$$\|\varrho_{\delta,K}\|_{C^1([0,1])} \leq C_4,$$

for all $(\delta, K) \in (0, 1) \times (1, \infty)$.

Proof In the Euler–Lagrange equation (4.13), to which the fixed point $\varrho_{\delta,K}$ is a solution, we find the product $F_{(\delta,K)}\varrho_{\delta,K}$, whose L^1 -norm we estimate using a variant of (5.1). This results in an estimate of $\|\varrho_{\delta,K,xx}\|_{L^1(0,1)}$ that does not depend on (δ, K) . Now it remains to apply Sobolev’s embedding theorem. \square

Now we may assume that the cut-off parameter K has been chosen right from the beginning so large that $\xi_K(\varrho_{\delta,K,x}) = \varrho_{\delta,K,x}$ everywhere on $[0, 1]$; and the parameter δ has been selected so small that $\psi_\delta^2(\varrho_{\delta,K}^2) \equiv \varrho_{\delta,K}^4$.

Then the following key result is obtained, which completes the proof of Theorem 1.2:

Theorem 5.7 *There is a function $\varrho_* \in H_{\text{per}}^2(0, 1)$ satisfying (4.7) and $\min_{x \in [0,1]} \varrho_*(x) \geq C_3$ such that the following holds: If*

$$\begin{aligned} \bar{J}_* &:= F_\Delta \left(\int_0^1 \frac{1}{\tau_0 \varrho_*^2} + 8\nu \frac{(\varrho_{*,x})^2}{\varrho_*^4} dx \right)^{-1}, \\ F_*(x) &:= G_*(x) - \frac{\bar{J}_*^2 - 8\nu \bar{J}_* \varrho_*(x) \varrho_{*,x}(x)}{2\varrho_*^4(x)} \\ &:= \bar{J}_* \int_0^x \left(\frac{1}{\tau_0 \varrho_*^2} + 8\nu \frac{(\varrho_{*,x})^2}{\varrho_*^4} \right) (y) dy - \frac{\bar{J}_*^2 - 8\nu \bar{J}_* \varrho_*(x) \varrho_{*,x}(x)}{2\varrho_*^4(x)} \\ &= F_\Delta \frac{\int_0^x \left(\frac{1}{\tau_0 \varrho_*^2} + 8\nu \frac{(\varrho_{*,x})^2}{\varrho_*^4} \right) (y) dy}{\int_0^1 \left(\frac{1}{\tau_0 \varrho_*^2} + 8\nu \frac{(\varrho_{*,x})^2}{\varrho_*^4} \right) (y) dy} - \frac{\bar{J}_*^2 - 8\nu \bar{J}_* \varrho_*(x) \varrho_{*,x}(x)}{2\varrho_*^4(x)}, \end{aligned}$$

then ϱ_* minimises the functional

$$\mathcal{F}_*(\varrho^2) := \int_0^1 - (F_* + V_B + V_{\text{inh}}) \varrho^2 + H_*(\varrho^2) + \frac{\lambda_0^2}{2} |\Phi\{\varrho^2\}_x|^2 + 2\varepsilon^2 (\varrho_x)^2 dx$$

over the set $\{\varrho \in H_{\text{per}}^1(0, 1) : \min_{x \in [0,1]} \varrho(x) \geq C_3/2\}$ under the constraint (4.7). The function ϱ_* solves the Euler–Lagrange equation

$$0 = -(F_* + V_B + V_*)\varrho_* + h(\varrho_*^2)\varrho_* - 2\varepsilon^2 \varrho_{*,xx} - \beta_* \varrho_*, \tag{5.8}$$

where $V_* = V_{\text{inh}} + \Phi\{\varrho_*^2\}$ is the unique solution to

$$\lambda_0^2 V_{*,xx} = \varrho_*^2 - C, \quad V_*(0) = V_l, \quad V_*(1) = V_r,$$

and the Lagrange multiplier β_* is given by

$$\beta_* C_* = \mathcal{F}_*(\varrho_*^2) + \frac{\lambda_0^2}{2} \int_0^1 |\Phi\{\varrho_*^2\}_x|^2 dx. \tag{5.9}$$

The “averaged” kinetic energy is bounded via

$$\int_0^1 \frac{\bar{J}_*^2}{\varrho_*^2} dx \leq \tau_0 \bar{J}_* F_\Delta. \tag{5.10}$$

6. The Proof of Theorem 1.3

Now the existence of ϱ_* is established, and our next task is to improve several of its estimates.

Lemma 6.1 *If ϱ_* , \mathcal{F}_* and β_* are as in Theorem 5.7, then the following inequalities hold:*

$$\begin{aligned}\mathcal{F}_*(\varrho_*^2) &\geq -CF_\Delta C_* (1 + F_\Delta \tau_0^2) - C_1 + T C_* \ln C_* + 2\varepsilon^2 \|\varrho_{*,x}\|_{L^2(0,1)}^2, \\ \mathcal{F}_*(C_*) &\leq CF_\Delta C_* (1 + F_\Delta \tau_0^2 \nu^{-1/2}) + C_1 + T C_* \ln C_*, \\ -C_5 &\leq \beta_* \leq C_5(1 + \nu^{-1/2}),\end{aligned}\tag{6.1}$$

with some constant C_5 depending on all the physical constant except the quantum parameters ν, ε_0 . We have the estimate

$$\varepsilon^2 \|\varrho_{*,x}\|_{L^2(0,1)}^2 \leq C + \beta_* C_*.\tag{6.2}$$

If no voltage is applied ($F_\Delta = 0$), then $\beta_* \leq C_5$.

Proof The two estimates on \mathcal{F}_* follow from Lemma 5.1, (5.10), and

$$\begin{aligned}\left| \int_0^1 F_* \varrho_*^2 dx \right| &\leq \int_0^1 G_* \varrho_*^2 dx + \int_0^1 \frac{J_*^2}{2\varrho_*^2} dx + 4 \left| \int_0^1 \frac{J_* \varrho_*^3}{\varrho_*^4} \cdot \nu \varrho_{*,x} dx \right| \\ &\leq F_\Delta C_* + CF_\Delta^2 \tau_0^2 C_*, \\ \left| \int_0^1 F_* C_* dx \right| &\leq \int_0^1 G_* C_* dx + \int_0^1 \frac{J_*^2}{2\varrho_*^4} C_* dx + 4 \left| \int_0^1 \frac{J_* C_*}{\varrho_*^3} \cdot \nu \varrho_{*,x} dx \right| \\ &\leq F_\Delta C_* + CF_\Delta^2 \tau_0^{3/2} \nu^{-1/2} C_*.\end{aligned}$$

The inequalities on β_* then are consequences of (5.9), $\mathcal{F}_*(\varrho_*^2) \leq \mathcal{F}_*(C_*)$, (6.1), and Lemma 4.1. \square

Now we determine lower and upper bounds of ϱ_* via maximum principles. The next result tells us that good upper bounds on β_* will give upper bounds of ϱ_* .

Lemma 6.2 *There is a constant C_6 , depending on all the physical data (but not on the quantum parameters ε_0 and ν) such that all the solutions ϱ_* constructed in Theorem 5.7 fulfill*

$$\min_{x \in [0,1]} \varrho_*^2(x) \geq \exp(-C_6 - C_6 \nu^{-1}),\tag{6.3}$$

$$\max_{x \in [0,1]} \varrho_*^2(x) \leq \exp(C_6 + T^{-1} \beta_*).\tag{6.4}$$

If no voltage is applied ($F_\Delta = 0$), then $\min_{x \in [0,1]} \varrho_*^2(x) \geq \exp(-C_6)$.

Proof First, we re-arrange the Euler–Lagrange equation (5.8) to

$$\left(G_* + V_B + V_* + \beta_* - \frac{J_*^2}{2\varrho_*^4} - T \ln(\varrho_*^2) \right) \varrho_* = -2\varepsilon^2 \varrho_{*,xx} - \frac{4\nu J_* \varrho_{*,x}}{\varrho_*^2}.\tag{6.5}$$

Then there is a constant C_6 , such that we have the inequalities

$$\operatorname{ess-inf}_{(0,1)} (G_* + V_B + V_* + \beta_*) \geq -C_6 T, \quad \left\| \frac{J_*^2}{2\varrho_*^4} \right\|_{L^\infty(0,1)} \leq C_6 T \nu^{-1}, \quad \operatorname{ess-sup}_{(0,1)} (G_* + V_B + V_*) \leq C_6 T,$$

and we can find positive numbers c_1 and c_2 such that the left-hand side of (6.5) must be positive for all those $x \in [0, 1]$ with $\varrho_*^2(x) < c_1$, and must be negative for all $x \in [0, 1]$ with $\varrho_*^2(x) > c_2$. The conditions determining c_1 and c_2 are

$$0 = -C_6 - C_6 \nu^{-1} - \ln c_1, \quad 0 = C_6 + \beta_* T^{-1} - \ln c_2.$$

Now we show the proof of (6.3). Let $[x_0, x_1] \subset [0, 1]$ be an interval such that $\varrho_*^2(x) \leq c_1$ on $[x_0, x_1]$ with $\varrho_*^2(x_0) = \varrho_*^2(x_1) = c_1$. We multiply (6.5) by $\varrho_* - c_1^{1/2}$ and integrate over $[x_0, x_1]$:

$$\begin{aligned} & \int_{x_0}^{x_1} (\varrho_* - c_1^{1/2}) \left(G_* + V_B + V_* + \beta_* - \frac{\bar{J}_*^2}{2\varrho_*^4} - h(\varrho_*^2) \right) \varrho_* \, dx \\ &= -2\varepsilon^2 \int_{x_0}^{x_1} (\varrho_* - c_1^{1/2}) \varrho_{*,xx} \, dx - 4\nu \bar{J}_* \int_{x_0}^{x_1} (\varrho_* - c_1^{1/2}) \frac{1}{\varrho_*^2} \cdot \varrho_{*,x} \, dx \\ &= 2\varepsilon^2 \int_{x_0}^{x_1} |\varrho_{*,x}|^2 \, dx. \end{aligned}$$

Now the left-hand side is nonpositive, but the right-hand side is nonnegative. This can be resolved only if $\varrho_* \equiv c_1^{1/2}$ on the interval $[x_0, x_1]$, resulting in the uniform lower bound (6.3). The upper bound is shown similarly. Finally, we remark that $F_\Delta = 0$ enforces $\bar{J}_* = 0$. \square

Definition 6.3 Let ϱ_* be the solution as constructed in Theorem 5.7. We define a function

$$A(\varrho_*^2, x) := \varrho_*^2 \left(G_*(x) + V_B(x) + V_*(x) + \beta_* + \frac{\bar{J}_*^2}{2\varrho_*^4} + T(1 - \ln \varrho_*^2) \right),$$

where we consider V_* as a function of x alone; in particular, we forget about the nonlocal dependence of V_* on ϱ_*^2 via the operator Φ .

Lemma 6.4 Let ϱ_* be the solution as constructed in Theorem 5.7, and A be given as in Definition 6.3. Then ϱ_* solves the ordinary differential equation

$$\frac{\partial A(\varrho_*^2(x), x)}{\partial(\varrho_*^2)} \cdot \varrho_*(x) = -2\varepsilon^2 \varrho_{*,xx}(x) - 4\nu \bar{J}_* \frac{\varrho_{*,x}(x)}{\varrho_*^2(x)}, \quad (6.6)$$

and it holds

$$A - \frac{\partial A}{\partial(\varrho_*^2)} \cdot \varrho_*^2 = \frac{\bar{J}_*^2}{\varrho_*^2} + T \varrho_*^2, \quad (6.7)$$

$$\int_0^1 A(\varrho_*^2(x), x) \, dx = \int_0^1 \frac{\bar{J}_*^2}{\varrho_*^2(x)} \, dx + T C_* + 2\varepsilon^2 \int_0^1 (\varrho_{*,x}(x))^2 \, dx. \quad (6.8)$$

Moreover, we have the distributional identity

$$\frac{d}{dx} \left(A(\varrho_*^2(x), x) + 2\varepsilon^2 \varrho_{*,x}(x)^2 - \frac{\bar{J}_*}{\tau_0} x - V_*(x) \mathcal{C}(x) - \frac{\lambda_0^2}{2} V_{*,x}(x)^2 \right) = \varrho_*(x)^2 V_{B,x}(x) - V_*(x) \mathcal{C}_x(x). \quad (6.9)$$

Proof First we note that

$$\frac{\partial A}{\partial(\varrho_*^2)} = G_* + V_B + V_* + \beta_* - \frac{\bar{J}_*^2}{2\varrho_*^4} - T \ln \varrho_*^2,$$

and then (6.6) is just a reformulation of (6.5). The relation (6.7) is easily verified, and for the proof of (6.8) we only remark that a multiplication of (6.6) by ϱ_* and integration over $[0, 1]$ gives

$$\int_0^1 \frac{\partial A(\varrho_*^2(x), x)}{\partial(\varrho_*^2)} \varrho_*^2(x) \, dx = 2\varepsilon^2 \int_0^1 \varrho_{*,x}(x)^2 \, dx.$$

To show (6.9), we multiply (6.6) by $2\varrho_{*,x}$:

$$\frac{d}{dx} A(\varrho_*^2(x), x) - \frac{\partial A(\varrho_*^2, x)}{\partial x} = \frac{\partial A}{\partial(\varrho_*^2)} \cdot \frac{\partial \varrho_*^2}{\partial x} = -2\varepsilon^2 (\varrho_{*,x}(x)^2)_x - 8\nu \bar{J}_* \left(\frac{\varrho_{*,x}(x)}{\varrho_*(x)} \right)^2.$$

The last item on the right seems nasty, but it can be cancelled, since we have

$$\begin{aligned} -\frac{\partial A(\varrho_*^2, x)}{\partial x} &= -\varrho_*^2 (G_{*,x}(x) + V_{B,x}(x) + V_{*,x}(x)) \\ &= -\frac{\bar{J}_*}{\tau_0} - 8\nu\bar{J}_* \left(\frac{\varrho_{*,x}(x)}{\varrho_*(x)} \right)^2 - \varrho_*(x)^2 (V_{B,x}(x) + V_{*,x}(x)), \end{aligned}$$

in the sense of distributions, hence we conclude that

$$\begin{aligned} \frac{d}{dx} \left(A(\varrho_*^2(x), x) + 2\varepsilon^2 \varrho_{*,x}(x)^2 - \frac{\bar{J}_* x}{\tau_0} \right) &= \varrho_*(x)^2 (V_{B,x}(x) + V_{*,x}(x)) \\ &= \varrho_*(x)^2 V_{B,x}(x) + \mathcal{C}(x) V_{*,x}(x) + \lambda_0^2 V_{*,xx}(x) V_{*,x}(x), \end{aligned}$$

which brings us to (6.9). □

Proof [Proof of Theorem 1.3] The estimate (1.11) was shown in Lemma 6.2. From (6.6) and the assumption (1.12) we get, using (3.3),

$$\left| \frac{\partial A(\varrho_*^2(\tilde{x}), \tilde{x})}{\partial(\varrho_*^2)} \varrho_*(\tilde{x}) \right| \leq 2\varepsilon^2 |\varrho_{*,xx}(\tilde{x})| + 4\nu \frac{\bar{J}_*}{\varrho_*^2(\tilde{x})} \cdot |\varrho_{*,x}(\tilde{x})| \leq 2 + \frac{4\tau_0 F_\Delta \mathcal{C}_*}{\mathcal{C}_-} \frac{\nu}{\sqrt{\varepsilon_0^2 + \nu^2}} \leq C.$$

Due to (6.7) and $\mathcal{C}_- \leq \varrho_*^2(\tilde{x}) \leq \mathcal{C}_+$, it follows that

$$A(\varrho_*^2(\tilde{x}), \tilde{x}) \leq C \mathcal{C}_+^{1/2} + \frac{\bar{J}_*^2}{\varrho_*^2(\tilde{x})} + T \varrho_*^2(\tilde{x}).$$

Observe that Definition 6.3 has the direct consequence

$$\beta_* \varrho_*^2(\tilde{x}) = A(\varrho_*^2(\tilde{x}), \tilde{x}) - \varrho_*^2(\tilde{x}) (G_*(\tilde{x}) + V_B(\tilde{x}) + V_*(\tilde{x})) + T \varrho_*^2(\tilde{x}) (\ln \varrho_*^2(\tilde{x}) - 1) - \frac{\bar{J}_*^2}{2\varrho_*^2(\tilde{x})},$$

which allows for an upper estimate of β_* that does not depend on ν and ε_0 . Here we have used $\mathcal{C}_- \leq \varrho_*^2(\tilde{x}) \leq \mathcal{C}_+$, $0 \leq G_* \leq F_\Delta$, $V_B \in L^\infty$, $V_* \in L^\infty$ via Lemma 4.1, and (3.3). Applying (6.4) then shows (1.13). And the estimates (1.14), (1.15) are shown by integrating (6.9) over the interval from \tilde{x} to x . □

We conclude the paper with a final result. Lemma 6.6 allows to reduce the third-order system (1.2)–(1.4) to a first-order differential equation that follows from (6.10) if we assume that \mathcal{C} and V_B are piecewise constant, which is the standard case in applications. This reduction might allow for interesting numerical approaches.

Assumption 6.5 *The functions \mathcal{C} and V_B are piecewise constant with jumps (in increasing order) at the points $x_{j,c}$ ($1 \leq j \leq p$) and $x_{j,B}$ ($1 \leq j \leq q$), and the jumps have heights $[\mathcal{C}]_j$ and $[V_B]_j$:*

$$\begin{aligned} \mathcal{C}(x) &= \mathcal{C}_l + \sum_{j=1}^p [\mathcal{C}]_j \mathbf{H}_{j,c}(x), & \mathbf{H}_{j,c}(x) &:= \mathbf{H}(x - x_{j,c}), \\ V_B(x) &= \sum_{j=1}^q [V_B]_j \mathbf{H}_{j,B}(x), & \mathbf{H}_{j,B}(x) &:= \mathbf{H}(x - x_{j,B}), \end{aligned}$$

where \mathbf{H} is the Heaviside function, and $\mathcal{C}_l = \mathcal{C}(0)$, $V_B(0) = 0$ are the values of \mathcal{C} and V_B on the first step.

Lemma 6.6 *Under Assumption 6.5, we have the following identity in distributional sense:*

$$\begin{aligned} \frac{d}{dx} \left(A(\varrho_*^2(x), x) + 2\varepsilon^2 \varrho_{*,x}(x)^2 - \frac{\bar{J}_* x}{\tau_0} - V_*(x) \mathcal{C}(x) - \frac{\lambda_0^2}{2} V_{*,x}(x)^2 \right. \\ \left. - \sum_{j=1}^q \varrho_*^2(x_{j,B}) \cdot [V_B]_j \mathbf{H}_{j,B}(x) + \sum_{j=1}^p V_*(x_{j,c}) \cdot [\mathcal{C}]_j \mathbf{H}_{j,c}(x) \right) = 0. \end{aligned} \quad (6.10)$$

Proof We can write

$$\varrho_*(x)^2 V_{B,x}(x) - V_*(x) C_x(x) = \frac{d}{dx} \left(\sum_{j=1}^q \varrho_*^2(x_{j,B}) \cdot [V_B]_j H_{j,B}(x) - \sum_{j=1}^q V_*(x_{j,C}) \cdot [C]_j H_{j,C}(x) \right),$$

and then the conclusion follows from (6.9). □

A. Appendix

For an illustration of the given functions V_B , C , and for a justification of our chosen boundary conditions (1.5), (1.6), we present here the results of numerical simulations for the equilibrium case by means of finite differences, performed by the authors, using parameter values as in [16] and [17].

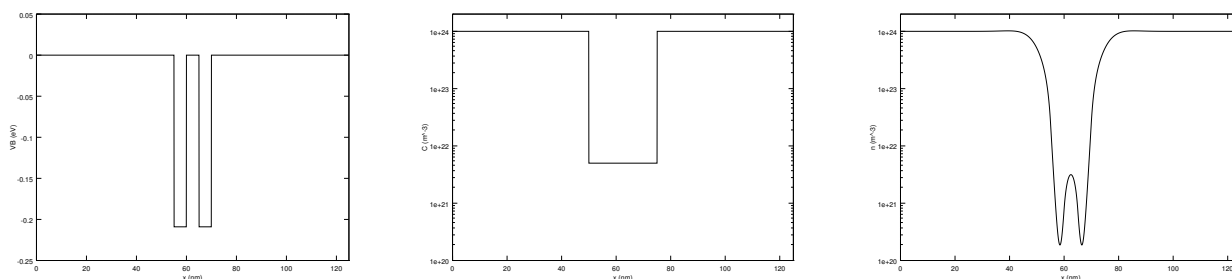


Figure 1. The functions V_B , C , n_* in case of the resonant tunnel diode, cf. [16], [17].

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