ON A NONLINEAR PARABOLIC PROBLEM ARISING IN THE QUANTUM DIFFUSIVE DESCRIPTION OF A DEGENERATE FERMION GAS[*]

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Abstract. This article studies, both theoretically and numerically, a nonlinear drift-diffusion equation describing a gas of fermions in the zero-temperature limit. The equation is considered on a bounded domain whose boundary is divided into an "insulating" part, where homogeneous Neumann conditions are imposed, and a "contact" part, where nonhomogeneous Dirichlet data are assigned. The existence of stationary solutions for a suitable class of Dirichlet data is proven by assuming a simple domain configuration. The long-time behavior of the time-dependent solution, for more complex domain configurations, is investigated by means of numerical experiments.

Key words. quantum drift diffusion, fermions, nonlinear parabolic equations, mixed boundary conditions

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1. Introduction. The derivation of quantum fluid equations from quantum kinetic equations [5, 17, 23] is a natural problem in quantum statistical mechanics, in exactly the same way as the derivation of classical fluid equations from Boltzmann equation is a standard topic in classical statistical mechanics [2, 3, 4, 8, 9, 11, 12, 14, 15]. It allows us, indeed, to clarify the relationships between two levels of descriptions and to obtain "quantum corrections" to the classical fluid equations that are difficult (if not impossible) to identify only on the grounds of physical intuition. This is particularly true in the case of a quantum system of identical particles, i.e. obeying either Bose–Einstein or Fermi–Dirac statistics [6, 23].

Quantum fluid equations, whose prototype are the Madelung equations [20], are not only important from a theoretical point of view, but they are also very interesting for applications, in particular, in semiconductor devices modeling [5, 17, 16, 18]. Indeed, the fluid description of a quantum system has many practical advantages: first of all, it provides a description in terms of macroscopic variables with a direct physical interpretation (such as density, current, temperature); moreover, it allows one to model open systems in a very natural way, by imposing suitable semiclassical boundary conditions.

In this article, we study a very specific model, namely, the diffusive equation for a degenerate (i.e., at zero absolute temperature) gas of fermions in two space dimensions. The two-dimensional case is rather peculiar since, remarkably, the third-order "quantum pressure" term vanishes [6, 23]. The resulting diffusive equation

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hence has the form of a purely semiclassical equation [19], although being (formally) exact up to order $\hbar^4$. Such an equation (after a suitable rescaling of variables) reads as follows [6, 23]:

$$u_t = \nabla \cdot (u\nabla(u + V)), \tag{1}$$

where V is a given potential and $\nabla = (\partial/\partial x_1, \partial/\partial x_2)$, and has therefore the form of a two-dimensional "porous media" equation [24] endowed with a drift term. In this paper we choose to work on (1), not only because of its particularly neat form, but also because the use of two-dimensional models is natural in many instances of semiconductor devices [17, 21].

The mathematical study of (1) has been partially developed in the literature. In particular, existence and uniqueness of a weak solution in the evolutionary case has been proven in [1] and in [13], whereas an analysis of the long-time behavior has been provided in [10] and [7]. In [1], the time-dependent equation is endowed with mixed homogeneous Neumann and nonhomogeneous Dirichlet boundary data; in [10], the stationary equation is also considered, but only in the case of homogeneous Neumann boundary data.

However, a semiconductor device cannot be fully described by imposing only homogeneous Dirichlet boundary conditions. Indeed, for describing real situations, a portion of the boundary (corresponding to metallic contacts) should be described by using nonhomogeneous Dirichlet data, whereas other regions of the boundary (corresponding to insulating boundaries) should be supplemented with homogeneous Neumann conditions [17, 21].

The main aim of this article is hence to investigate, both theoretically and numerically, some aspects of (1) by allowing both nonhomogeneous Dirichlet boundary data and homogeneous Neumann conditions.

The structure of the article is the following. In the next section we will formulate the mathematical problem and review some basic results on the evolutionary case. Then, in section 3, we will study the stationary case. Particular attention will be given to the situation in which the domain is rectangular and both the data and the potential depend only on one space variable, in which case solutions that depend only on that variable can be considered. A theorem of existence and uniqueness for such solutions, requiring some restrictions on the Dirichlet data, will be proven. Finally, in section 4, we will describe a numerical procedure for studying the initial/boundary value problem and provide some numerical experiments.

2. The mathematical problem. Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a piecewise smooth boundary $\partial\Omega$, and let Γ_D and Γ_N be two nonempty subsets of $\partial\Omega$ such that

$$\Gamma_D \cap \Gamma_N = \emptyset \quad \text{and} \quad \partial\Omega = \Gamma_D \cup \Gamma_N.$$

The gas of fermions in the zero-temperature limit is described by a density function $u : \mathbb{R}^+ \times \Omega \to \mathbb{R}^+$, whose time evolution is governed by the following nonlinear drift-diffusion equation [6]

$$\begin{cases} u_t + \nabla \cdot J = 0, \\ J = -u\nabla(u + V), \end{cases} \quad (t, x) \in \mathbb{R}^+ \times \Omega. \tag{2}$$

Here $V : \overline{\Omega} \to \mathbb{R}$ is a given potential which, for the sake of simplicity, will be assumed to be continuously differentiable. The problem is supplemented with the initial datum

$$u(0, x) = u_{\text{in}}(x), \quad x \in \Omega, \tag{3}$$

and mixed boundary conditions

$$u(t,x) = u_D(x), \quad (t,x) \in \mathbb{R}^+ \times \Gamma_D,$$

(4)

$$J(t,x) \cdot n_x = 0, \quad (t,x) \in \mathbb{R}^+ \times \Gamma_N,$$

where $u_{\text{in}}(x) > 0$ for a.e. $x \in \Omega$, $u_D(x) > 0$ for a.e. $x \in \Gamma_D$, and n_x is the outward normal to Γ_N at $x \in \Gamma_N$.

Equation (2), with nonnegative mixed Neumann/Dirichlet boundary conditions (3) and (4) has been studied in several works, and its main properties have been analyzed. In particular, existence, uniqueness, and preservation of the cone of non-negative functions for problem (2)–(4) are the specialization to the uncoupled case (without reaction terms) of the results obtained in [13]. More precisely, by adapting to our case the theorems proven in sections 2 and 3 of [13], we can state the following.

THEOREM 1. *Let* $u_{\text{in}} \in L^p(\Omega)$, $u_D \in L^p(0,T;W^{1,p}(\Omega)) \cap L^\infty((0,T) \times \Omega)$, $p \geq 1$, *and* $\partial_t u_D \in L^1(0,T;L^\infty(\Omega))$, *with nonnegative* u_{in} *and* u_D. *Then, there exists a unique nonnegative weak solution* $u \in L^p(0,T;W^{1,p}(\Omega)) + L^p(0,T;\Xi)$ *of the initial/boundary value problem* (2)–(4), *where*

$$\Xi = \{\xi \in W^{1,p}(\Omega) \ : \ \xi = 0 \ on \ \Gamma_D\}.$$

Another approach for proving this result consists in transforming (2) into the equation

(5)
$$\partial_t b(u) = \frac{1}{2}\Delta u + \nabla \cdot (b(u)\nabla V)$$

by means of the transformation

(6)
$$b(z) := \text{sign}(z)\sqrt{|z|},$$

i.e.,

$$z = u^2\text{sign}(u),$$

and then by using the existence and uniqueness theory of Alt and Luckhaus, which studied the class of nonlinear parabolic equations written above, with boundary conditions of type (4), in [1].

In the next section we shall investigate the stationary case and prove (at least for a particular class of initial/boundary conditions) a theorem of existence and uniqueness of the stationary solution. Despite the general result on the evolutionary equation, we are able to prove a sufficient condition which guarantees the well-posedness of the stationary problem only for a restricted class of "supercritical" Dirichlet data (see Theorem 11).

It is worth remarking that the well-posedness of the initial value problem for (2) with only Neumann conditions ($\Gamma_D = \emptyset$) has been proven by Carrillo et al. [10]. Then, the origin of troubles is clearly in the nonhomogeneous Dirichlet conditions.

3. The stationary problem. The study of nonnegative stationary solutions of (2), satisfying the prescribed mixed boundary conditions (4), leads us to consider the problem

(7)
$$\nabla \cdot [u\nabla (u + V)] = 0, \quad x \in \Omega,$$

with boundary conditions

$$u(x) = u_D(x), \quad x \in \Gamma_D,$$

(8)

$$u\nabla (u + V) \cdot n_x = 0, \quad x \in \Gamma_N.$$

3.1. A general result in the two-dimensional case. A peculiar feature of the stationary problem is the lack of uniqueness of the stationary solution, as shown in the following proposition.

PROPOSITION 2. *Let us suppose that $u_D \equiv 0$. If $u \in H^1(\Omega)$ is a nonnegative weak solution of the boundary value problem (7)–(8), then, for every $x \in \Omega$, either $u = 0$ or $\nabla(u + V) = 0$ in x.*

Proof. We multiply (7) by $u + V$ and then integrate with respect to x in Ω. After integrating by parts, we obtain that

$$\int_\Omega u \left| \nabla (u + V) \right|^2 \mathrm{d}x = 0$$

because of the boundary conditions (8) with $u_D = 0$. Since $u \geq 0$, by assumption, the statement follows. □

This simple result shows that, depending on V, the homogeneous stationary problem may have a nonunique solution. For example, if $V \leq 0$ with compact support $K \subset \Omega$, then both $u \equiv 0$ and the function

$$u(x) = \begin{cases} 0, & x \in \overline{\Omega} \setminus K, \\ -V(x), & x \in K, \end{cases}$$

are nonnegative solutions of (7). Moreover, if $\Gamma_D = \emptyset$, then $u = \gamma - V$ is a strictly positive solution for all constants γ such that $\gamma > V(x)$ for all $x \in \overline{\Omega}$ (in particular, if V is allowed to go to $+\infty$, no positive solution may exist at all).

3.2. Reduction to a one-dimensional problem. We now examine the stationary problem in a particular case, which is basically one dimensional. Let $\Omega = (0, 1) \times (a, b) \subset \mathbb{R}^2$, let

$$\Gamma_D = \{0, 1\} \times [a, b], \qquad \Gamma_N = [0, 1] \times \{a, b\},$$

and let $u = u(x_1, x_2)$, so that the Dirichlet boundary conditions read as follows:

$$u(0, x_2) = u_0(x_2), \qquad u(1, x_2) = u_1(x_2), \qquad x_2 \in [a, b],$$

and the Neumann conditions are imposed on the two other sides of the rectangle.

Moreover, let us assume that

$$\frac{\partial V}{\partial x_2} = \frac{\partial u_0}{\partial x_2} = \frac{\partial u_1}{\partial x_2} = 0,$$

i.e., both the potential V and the Dirichlet data u_D only depend on the variable x_1. Then, clearly, $u(x_1, x_2) = u(x_1)$ is a solution of the stationary problem provided that $u(x_1)$ solves the one-dimensional problem

$$(9) \qquad \frac{d}{dx_1} \left[u(x_1) \frac{d}{dx_1} \left(u(x_1) + V(x_1) \right) \right] = 0, \quad x_1 \in [0, 1],$$

$$u(0) = u_0, \quad u(1) = u_1,$$

where we recall that $V : [0, 1] \to \mathbb{R}$ is assumed to be continuously differentiable. We are going to prove that problem (9) has a unique positive solution for positive Dirichlet data, $u_0 > 0$ and $u_1 > 0$, subject to suitable restrictions (see Theorem 11).

For the sake of simplicity, from here to the end of this section, we shall denote with x the one-dimensional variable x_1; then, recall that

$$x \equiv x_1.$$

From (9) we immediately obtain that a constant $c \in \mathbb{R}$ exists such that

$$(10) \qquad u(x)\left[u'(x) + V'(x)\right] = c, \qquad x \in [0,1]$$

(where the derivatives are now denoted by apices). The case $c = 0$ corresponds to all situations in which either $u(x) = 0$ or $u'(x) = -V'(x)$ for some $x \in [0,1]$; in such a case, as discussed above, we cannot expect to have uniqueness. Then, we assume $c \neq 0$ and, consequently, we are forced to consider strictly positive Dirichlet data. If $c \neq 0$, then any regular solution of (10) cannot vanish in $[0,1]$ and then we can assume u to be strictly positive in $[0,1]$ and write the differential equation in the normal form

$$(11) \qquad u'(x) = \frac{c}{u(x)} - V'(x).$$

Let us first consider the case of constant V', for which we have an explicit representation of the solution of the Cauchy problem for the ODE (11). We denote by

$$W : [-1/e, +\infty) \to [-1, +\infty) \qquad \text{and} \qquad \tilde{W} : [e, +\infty) \to [1, +\infty),$$

respectively, the inverse functions of $f(x) = xe^x$ and $g(x) = e^x/x$ (W is known as the *Lambert W-function* [22]). It is readily proven that the functions W and $\tilde{W}$ satisfy the differential equations

$$(12) \qquad W'(y) = \frac{W(y)}{y\left(W(y) + 1\right)} \qquad \text{and} \qquad \tilde{W}'(y) = \frac{\tilde{W}(y)}{y\left(\tilde{W}(y) - 1\right)}.$$

LEMMA 3. *Let $u_0 > 0$, $c > 0$, and $\alpha \in \mathbb{R}$. Then, the solution of the Cauchy problem*

$$(13) \qquad u'(x) = \frac{c}{u(x)} - \alpha, \qquad u(x_0) = u_0,$$

is given by $u(x) = \phi(x - x_0, u_0, c, \alpha)$, where

$$(14) \qquad \phi(\Delta x, u_0, c, \alpha) = \begin{cases} \dfrac{c}{\alpha}\left\{1 + W\left[\left(\dfrac{\alpha u_0}{c} - 1\right)e^{-\frac{\alpha^2}{c}\Delta x + \frac{\alpha u_0}{c} - 1}\right]\right\} & \text{if } \alpha > 0, \\[12pt] \sqrt{u_0^2 + 2c\,\Delta x} & \text{if } \alpha = 0, \\[12pt] \dfrac{c}{\alpha}\left\{1 - \tilde{W}\left[\left(1 - \dfrac{\alpha u_0}{c}\right)^{-1}e^{\frac{\alpha^2}{c}\Delta x + 1 - \frac{\alpha u_0}{c}}\right]\right\} & \text{if } \alpha < 0. \end{cases}$$

Moreover, for fixed $x > x_0$, we have that $\phi(x, u_0, c, \alpha)$ is strictly increasing with respect to u_0 and c, and strictly decreasing with respect to α.

Proof. The fact that ϕ satisfies (13) comes straightforwardly from (12). Then we just prove the growth properties with respect to α and c. Although they could be

checked directly on expression (14), it is easier to use the differential equation satisfied by ϕ, i.e.,

$$(15) \qquad \frac{\partial \phi}{\partial x} = \frac{c}{\phi} - \alpha.$$

Defining $\psi = \partial \phi / \partial c$ we obtain

$$(16) \qquad \frac{\partial \psi}{\partial x} = -\frac{c\,\psi}{\phi^2} + \frac{1}{\phi}$$

and, since $\phi_{|x=0} = u_0$ for all $\alpha \in \mathbb{R}$, we also have

$$(17) \qquad \psi_{|x=0} = 0.$$

If $x_0 \in (0,1]$ existed such that $\psi \leq 0$ in $(0, x_0)$, then from (16) one would obtain

$$\frac{\partial \psi}{\partial x} \geq \frac{1}{\phi} > 0$$

in $(0, x_0)$ (where the fact that $\phi > 0$ can be easily checked from (14)) which, together with (17), would give $\psi > 0$ in $(0, x_0)$. Then $\psi > 0$ in $(0, 1]$, which of course implies that ϕ is strictly increasing with respect to $c > 0$.

The proof that ϕ is strictly decreasing with respect to $\alpha \in \mathbb{R}$ can be carried out analogously. $\square$

In addition to the properties listed in Lemma 3 let us also note that $\phi(\Delta x, u_0, c, \alpha)$, as Δx increases from 0 to $+\infty$,

(i) increases monotonically from u_0 to $+\infty$ if $\alpha \leq 0$;

(ii) increases monotonically from u_0 to the asymptotic value c/α if $\alpha > 0$ and $u_0 < c/\alpha$;

(iii) is identically equal to c/α if $\alpha > 0$ and $u_0 = c/\alpha$;

(iv) decreases monotonically from u_0 to the asymptotic value c/α if $\alpha > 0$ and $u_0 > c/\alpha$.

Lemma 3 will allow us to prove properties of the more general differential equation (11) by approximating $V'(x)$ with piecewise constant functions.

LEMMA 4. *Let $x_0 = 0 < x_1 < \cdots < x_n = 1$ be a partition of $[0,1]$ and let $V_n'(x)$ be a piecewise constant function, taking the value α_i in the interval (x_i, x_{i+1}) such that $V_n \to V$ uniformly in $[0,1]$ as $n \to +\infty$. Let $u(x)$ be the solution of the Cauchy problem*

$$(18) \qquad u'(x) = \frac{c}{u(x)} - V'(x), \quad x \in [0,1], \qquad u(0) = u_0 > 0,$$

with $c > 0$, and let $v_n(x)$ be defined by

$$v_n(x) = \phi(x, u_0, c, \alpha_0), \qquad\qquad x \in [0, x_1],$$

$$v_n(x) = \phi(x - x_i, v_n(x_i), c, \alpha_i), \quad x \in (x_i, x_{i+1}], \quad i = 1, 2, \ldots, n-1$$

(in other words, v_n solves $v_n'(x) = \frac{c}{v_n(x)} - \alpha_i$ in $[x_i, x_{i+1}]$, taking as initial value in each interval the final value of the preceding interval, starting with u_0 in the first interval). Then $v_n \to u$ uniformly in $[0,1]$ as $n \to +\infty$.

Proof. Note that u and v_n are continuous solutions of the integral equations

$$u(x) = u_0 + \int_0^x \frac{c}{u(y)}\, dy - V(x) + V(0)$$

and

$$v_n(x) = u_0 + \int_0^x \frac{c}{v_n(y)}\, dy - V_n(x) + V(0),$$

respectively (where, of course, $V_n(x) := V(0) + \int_0^x V_n'(y)\, dy$ is a piecewise linear approximation of $V(x)$). Then,

$$|u(x) - v_n(x)| \le c \int_0^x \frac{|u(y) - v_n(y)|}{|u(y)\, v_n(y)|}\, dy + |V(x) - V_n(x)|.$$

We note that $u(x)$ can be decreasing only in the set

$$\{x \in [0,1] \mid V'(x) > 0 \text{ and } u(x) > c/V'(x)\}.$$

Since $u(0) = u_0 > 0$, we have that

$$u(x) > \min\{u_0, c/V_+'\},$$

where V_+' denotes the maximum positive value of $V'(x)$ in $[0,1]$. Similar considerations hold for v_n (with a lower bound that can be supposed to be independent on n). Then, $\epsilon > 0$ exists such that $u(x)v_n(x) \ge \epsilon$ for all $x \in [0,1]$ and, therefore,

$$|u(x) - v_n(x)| \le \frac{c}{\epsilon} \int_0^x |u(y) - v_n(y)|\, dy + |V(x) - V_n(x)|.$$

Since $V_n(x) \to V(x)$ uniformly in $[0,1]$, the thesis follows from Gronwall's lemma. □

LEMMA 5. *Let u as in the previous lemma and let*

$$\alpha_M = \max_{0 \le x \le 1} V'(x), \qquad \alpha_m = \min_{0 \le x \le 1} V'(x).$$

Then,

(19) $$\underline{v}(x) \le u(x) \le \overline{v}(x), \qquad x \in [0,1],$$

where

$$\underline{v}(x) = \phi(x, u_0, c, \alpha_M), \qquad \overline{v}(x) = \phi(x, u_0, c, \alpha_m).$$

Proof. Let V_n' and v_n be as in the previous lemma, and assume, without loss of generality, that $\alpha_m \le V_n'(x) \le \alpha_M$ for all $x \in [0,1]$. In the first interval, $[0, x_1]$, we have $\underline{v}(x) \le v_n(x) \le \overline{v}(x)$, because

$$\phi(x, u_0, c, \alpha_M) \le \phi(x, u_0, c, \alpha_0) \le \phi(x, u_0, c, \alpha_m),$$

as ϕ is increasing for decreasing α (Lemma 3). Then, in each of the successive intervals we still have $\underline{v}(x) \le v_n(x) \le \overline{v}(x)$, because, a fortiori,

$$\phi(x, \underline{v}(x_i), c, \alpha_M) \le \phi(x, v_n(x_i), c, \alpha_0) \le \phi(x, \overline{v}(x_i), c, \alpha_m),$$

being ϕ increasing also with respect to the initial value. Thus $\underline{v}(x) \le v_n(x) \le \overline{v}(x)$ in the whole interval $[0,1]$. Since, from Lemma 4, $v_n \to u$ uniformly in $[0,1]$ the inequalities are also true for u, which proves our claim. □

Note that the result of Lemma 5 implies, in particular, that $u(x) > 0$ for all $x \in [0, 1]$.

LEMMA 6. *Let us denote by $u(x, c)$, with $x \in [0, 1]$ and $c > 0$, the solution of the Cauchy problem* (18). *Then, $u(x, c)$ is strictly increasing with respect to c for every fixed $x \in (0, 1]$.*

Proof. We resort again to the uniformly approximating sequence defined in Lemma 4, that we now denote by $v_n(x, c)$ in order to stress the dependence on c. We can assume, as in Lemma 5, that $\alpha_m \leq V_n'(x) \leq \alpha_M$ (independently on n).

From definition (14) it is apparent that $\phi(\Delta x, u_0, c, \alpha)$ is a C^1-function of $c > 0$, piecewise continuous with respect to $\alpha \in \mathbb{R}$. However, if we prove that $\frac{\partial \phi}{\partial c}$ is actually continuous with respect to α also at $\alpha = 0$, then $\frac{\partial \phi}{\partial c}$ has a (positive) lower bound when α varies in $[\alpha_m, \alpha_M]$ and, therefore, for any given $\Delta x \in (0, 1]$, $u_0 > 0$ and $c > 0$, a constant $\mu > 0$ exists such that

$$(20) \qquad \frac{\partial}{\partial c} \phi(\Delta x, u_0, c, \alpha_i) \geq \mu \quad \text{for all } i = 0, 1, \ldots, n-1.$$

We now prove the continuity of $\frac{\partial \phi}{\partial c}$ (and of ϕ as well) as $\alpha \to 0^+$. For $\alpha > 0$ the expression of ϕ (which is now seen as a function of c and α) is the first one in (14), i.e.,

$$\phi(c, \alpha) = \frac{c}{\alpha} \left\{ 1 + W[g(c, \alpha)] \right\},$$

where

$$g(c, \alpha) = \left(\frac{\alpha u_0}{c} - 1 \right) e^{-\frac{\alpha^2}{c} \Delta x + \frac{\alpha u_0}{c} - 1}.$$

By using (12) we easily get

$$\frac{\partial}{\partial \alpha} \{ 1 + W[g(c, \alpha)] \}^2 = \frac{2\alpha W[g(c, \alpha)](u_0^2 + 2c\Delta x - 2\alpha u_0 \Delta x)}{\alpha c u_0 - c^2}.$$

Since $W[g(c, \alpha)] \to -1$ as $\alpha \to 0^+$, by applying l'Hôpital's theorem we obtain

$$\lim_{\alpha \to 0^+} \frac{c^2}{\alpha^2} \{ 1 + W[g(c, \alpha)] \}^2 = u_0^2 + 2c\Delta x$$

so that

$$(21) \qquad \lim_{\alpha \to 0^+} \phi(c, \alpha) = \lim_{\alpha \to 0^+} \frac{c}{\alpha} \{ 1 + W[g(c, \alpha)] \} = \sqrt{u_0^2 + 2c\Delta x},$$

which, according to (14), proves the continuity of ϕ for $\alpha \to 0^+$.

Coming to the c-derivative, after straightforward calculations, we have (for $\alpha > 0$)

$$\frac{\partial \phi}{\partial c}(c, \alpha) = \frac{1}{\alpha} \{ 1 + W[g(c, \alpha)] \} + \frac{\alpha W[g(c, \alpha)](\alpha u_0 \Delta x - c\Delta x - u_0^2)}{c \{ 1 + W[g(c, \alpha)] \}(\alpha u_0 - c)}.$$

By using (21) we obtain therefore

$$\lim_{\alpha \to 0^+} \frac{\partial \phi}{\partial \alpha}(c, \alpha) = \frac{\Delta x}{\sqrt{u_0^2 + 2c\Delta x}} = \frac{\partial}{\partial c} \sqrt{u_0^2 + 2c\Delta x},$$

which proves the continuity of $\frac{\partial \phi}{\partial c}$ as $\alpha \to 0^+$.

The continuity of $\frac{\partial \phi}{\partial c}$ (and ϕ) for $\alpha \to 0^-$ is proven in the same way by using the expression of ϕ for $\alpha < 0$ in (14). This, according to the discussion above, proves (20). We stress the fact that μ only depends on α_m and α_M, and does not depend on the

sequence of the α_i's. Then, from the definition of v_n (see Lemma 4) we have that

$$v_n(x, c + \Delta c) - v_n(x, c) \geq \mu \Delta c$$

for all $x \in (0, 1]$ and $\Delta c \geq 0$ (small enough), with μ independent on n. Then, passing to the limit for $n \to \infty$ we obtain that $u(x, c)$ is strictly increasing with respect to c for every $0 < x \leq 1$. $\qquad \square$

LEMMA 7. *Referring to Lemma 6 for the notations, we have that $u(x, c)$ converges uniformly to a continuous limit $u(x, 0)$ as $c \to 0^+$.*

Proof. It is not difficult to show that

$$(22) \qquad \lim_{c \to 0^+} \phi(\Delta x, u_0, c, \alpha) = \max\{u_0 - \alpha x, 0\},$$

uniformly with respect to Δx, u_0, and α. Then, still assuming $\alpha_m \leq V_n'(x) \leq \alpha_M$, we obtain that $\lim_{c \to 0^+} v_n(x, c) = v_n(x, 0)$, uniformly with respect to x and n, where $v_n(x, 0)$ is a continuous, piecewise linear, limit function. Since $c \mapsto v_n(x, c)$ (seen as a sequence in c) is uniformly Cauchy with respect to x and n, it is straightforward to prove that $c \mapsto u(x, c)$ is in turn uniformly Cauchy (with respect to x) and, therefore, converges uniformly to a continuous limit $u(x, 0)$. $\qquad \square$

DEFINITION 8. *To any given data (u_0, V) of the Cauchy problem (18) we associate the set of points*

$$0 < x_1 \leq y_1 < x_2 \leq y_2 < \cdots < x_n = y_n = 1$$

by means of the following recursive rule (where $V_0 = V(0)$):

1. *We start by putting*

$$x_1 = \sup\{x \in [0, 1] \mid u_0 + V_0 - V(\xi) > 0 \ \forall \ \xi \in [0, x)\};$$

   if $x_1 = 1$, then we put $y_1 = 1$ and the procedure ends with $n = 1$, otherwise we proceed to Step 2.

2. *If $x_1 < 1$ we put*

$$y_1 = \sup\{x \in [x_1, 1] \mid -V'(\xi) \leq 0 \ \forall \ \xi \in [x_1, x)\};$$

   if $y_1 = 1$, then the procedure ends with $n = 1$, otherwise we proceed to Step 3.

3. *If $y_{i-1} < 1$ we put*

$$x_i = \sup\{x \in (y_{i-1}, 1] \mid V(y_{i-1}) - V(\xi) > 0 \ \forall \ \xi \in (y_{i-1}, x)\};$$

   if $x_i = 1$, then we put $y_i = 1$ and the procedure ends with $n = i$, otherwise we proceed to Step 4.

4. *If $x_i < 1$ we put*

$$y_i = \sup\{x \in [x_i, 1] \mid -V'(\xi) \leq 0 \ \forall \ \xi \in [x_i, x)\};$$

   if $y_i = 1$, then the procedure ends with $n = i$, otherwise we increment the index i and repeat Steps 3 and 4 until we find $x_i = 1$ or $y_i = 1$ for some i. (For the sake of simplicity we can assume that V changes sign a finite number of times, so that the procedure stops at a finite n.)

Finally, we define the continuous function

$$(23) \qquad U(x) = \begin{cases} u_0 + V_0 - V(x), & x \in [0, x_1], \\ 0, & x \in [x_i, y_i], \\ V(y_i) - V(x), & x \in [y_i, x_{i+1}]. \end{cases}$$

LEMMA 9 (asymptotic behavior for $c \to 0^+$). *Let u be the solution of the Cauchy problem* (18). *Then,*

$$\lim_{c \to 0^+} u(x) = U(x),$$

where U is the function defined in Definition 8.

Proof. We divide the proof into three recursive steps.

Step 1. Let $\epsilon > 0$ be arbitrarily small and let $x \in [0, x_1 - \epsilon]$. From Definition 8 we have that $\eta > 0$ exists such that $u_0 + V_0 - V(\xi) \geq \eta$ for all $\xi \in [0, x]$. Then, from the obvious inequality

$$u(x) = u_0 + V_0 - V(x) + \int_0^x \frac{c}{u(\xi)} \, d\xi > u_0 + V_0 - V(x),$$

we obtain

$$u(x) - u_0 - V_0 + V(x) \leq \frac{cx}{\eta}, \qquad x \in [0, x_1 - \epsilon],$$

which proves that $\lim_{c \to 0^+} u(x) = U(x)$, for all $x \in [0, x_1)$. Since the limit has to be a continuous function (Lemma 7), from the arbitrariness of ϵ we also have

$$\lim_{c \to 0^+} u(x_1) = U(x_1) = 0.$$

Step 2. In the interval $[x_1, y_1]$ we have that $\lim_{c \to 0^+} u(x_1) = 0$ (from the previous step) and, by definition, $\alpha_m = \min_{x \in [x_1, y_1]} V'(x) \geq 0$. Then, from Lemma 5

$$\lim_{c \to 0^+} u(x) \leq \lim_{c \to 0^+} \sqrt{u^2(x_1) + 2c(x - x_1)} = 0$$

for all $x \in [x_1, y_1]$.

Step 3. In the subsequent intervals of the form $[y_i, x_{i+1}]$ or $[x_i, y_i]$, we repeat the same proofs of the steps 1 and 2 (respectively), with the only difference being that $U(y_i) = 0$ instead of $U(0) = u_0 > 0$ (which implies that Step 1 has to be slightly modified by using an $\eta > 0$ such that $V(y_i) - V(\xi) \geq \eta$ for all $\xi \in [y_i + \epsilon, x_{i+1} - \epsilon]$). $\square$

Note that the limiting process $c \to 0^+$ selects one particular solution among the infinitely many solutions of the case $c = 0$, for which we have seen that there is not uniqueness (see section 3.1).

DEFINITION 10. *We define the critical values for the Dirichlet data $u_0 > 0$ and $u_1 > 0$ as follows:*

$$(24) \qquad u_0^{\mathrm{crit}} = V_M - V_0, \qquad u_1^{\mathrm{crit}} = V_M - V_1,$$

where we put $V_0 = V(0)$, $V_1 = V(1)$, and

$$V_M = \max_{x \in [0,1]} V(x).$$

If a boundary term is greater than the corresponding critical value, then it is said to be supercritical, otherwise it is said to be subcritical.

We can finally prove that the solution of the the Dirichlet problem (9) exists and is unique, provided that the Dirichlet data $u_0 > 0$ and $u_1 > 0$ are not both subcritical.

THEOREM 11. *If $u_0 > u_0^{\mathrm{crit}}$, then the Dirichlet problem* (9) *has a unique, strictly positive, solution u for all $u_1 > 0$. If $u_1 > u_1^{\mathrm{crit}}$, then the Dirichlet problem* (9) *has a unique, strictly positive, solution u for all $u_0 > 0$.*

Proof. Consider first the case $u_0 > u_0^{\mathrm{crit}}$ and assume, temporarily, that $c > 0$.

We know that the mapping $c \mapsto u(1)$, obtained by solving the Cauchy problem (18) is strictly monotone. Moreover, from Lemma 5, we have that

$$\lim_{c \to +\infty} u(1) \geq \lim_{c \to +\infty} \underline{v}(1) = +\infty,$$

since it is easy to see that $\phi(x, u_0, c, \alpha) \to +\infty$ as $c \to +\infty$ for all $x > 0$ and $\alpha \in \mathbb{R}$. Moreover, since $u_0 > u_0^{\mathrm{crit}}$, from Definition 8 and Lemma 9 we have that

$$\lim_{c \to 0^+} u(x) = U(x) = u_0 + V_0 - V(x) > 0,$$

i.e., in particular,

$$\lim_{c \to 0^+} u(1) = u_0 - \Delta V > 0, \quad \text{where} \quad \Delta V = V_1 - V_0.$$

What we have proven so far is that the left-Dirichlet datum $u_0 > u_0^{\mathrm{crit}}$ can be uniquely linked to any right-Dirichlet datum $u_1 = u(1) \in [u_0 - \Delta V, +\infty)$ by solving the Cauchy problem (18) with a suitable $c \geq 0$. To go below the threshold $u_0 - \Delta V$ we have to consider negative values of c. However, the case $c < 0$ can always be recast into the case $c > 0$ by noticing that, if u satisfies $u'(x) = c/u(x) - V'(x)$, then $\tilde{u}(x) = u(1 - x)$ satisfies

$$\tilde{u}'(x) = -\frac{c}{\tilde{u}(x)} - \tilde{V}'(x), \quad \text{where} \quad \tilde{V}(x) = V(1 - x).$$

In other words, the forward Cauchy problem with $c < 0$ is equivalent to the backward Cauchy problem with $c > 0$. Hence, if we fix the right-Dirichlet datum $0 < u_1 < u_0 - \Delta V$ and take $c < 0$, we can consider the Cauchy problem

$$(25) \qquad \tilde{u}'(x) = \frac{|c|}{\tilde{u}(x)} - \tilde{V}'(x), \quad x \in [0, 1], \qquad \tilde{u}(0) = u_1,$$

that is, the backward Cauchy problem for u with right-Cauchy datum u_1. What we want to prove is that u_1 can be linked to u_0 with a suitable choice of $c < 0$, i.e., that $c < 0$ exists such that $\tilde{u}(1) = u(0) = u_0$. Since the datum u_1 is not necessarily supercritical for problem (25), then in the limit $c \to 0^-$ we have in general that $\tilde{u}$ tends to the asymptotic solution $\tilde{U}(x)$ (with the obvious definition) and, according to the theory we already know, for $\tilde{u}(1)$ there are three possibilities:

$$\lim_{c \to 0^-} \tilde{u}(1) = \begin{cases} u_1 - \Delta \tilde{V} & \text{(that is } u_1 + \Delta V), \\ 0, \\ V(y) - V(0) & \text{for some point } y \in (0, 1). \end{cases}$$

In the first case (corresponding to u_1 supercritical for problem (25) we have $\lim_{c \to 0^-} \tilde{u}(1) = u_1 + \Delta V < u_0$ (since we have assumed $u_1 < u_0 - \Delta V$). In the second case, obviously, $\lim_{c \to 0^-} \tilde{u}(1) = 0 < u_0$ and in the third case

$$u_0 > -V_0 + V(y) = \lim_{c \to 0^-} \tilde{u}(1),$$

(because u_0 is supercritical). In each of the three cases, therefore,

$$\lim_{c \to 0^-} u(0) = \lim_{c \to 0^-} \tilde{u}(1) < u_0$$

and then (owing to the monotonic growth with respect to $|c|$), $u_0 = u(0)$ for a suitable $c < 0$. In conclusion, we have shown that the left-Dirichlet datum $u_0 > u_0^{\text{crit}}$ can be uniquely linked to any right-Dirichlet datum $u_1 = u(1) > 0$, by solving the Cauchy problem (18) with a suitable $c \in \mathbb{R}$.

The proof of the second part of the claim, i.e., the case $u_1 > u_1^{\text{crit}}$, is completely equivalent to the proof of the first part since, as we have just shown, it suffices to change c into $-c$. $\square$

4. Numerical simulations. Let $x = (x_1, x_2)$ and let Ω the square in $\mathbb{R}^2$ defined as

$$\Omega = \{x \in \mathbb{R}^2 \, : \, 0 \le x_1 \le 1 \text{ and } 0 \le x_2 \le 1\}.$$

We denote moreover

$$\partial\Omega := \Gamma = \sum_{i=1}^5 \Gamma_i,$$

where

$$\Gamma_1 := \{x \in \mathbb{R}^2 \, : \, 0 < x_1 \le 1 \text{ and } x_2 = 0\},$$
$$\Gamma_2 := \{x \in \mathbb{R}^2 \, : \, x_1 = 1 \text{ and } 0 < x_2 \le 1\},$$
$$\Gamma_3 := \{x \in \mathbb{R}^2 \, : \, 0 \le x_1 < 1 \text{ and } x_2 = 1\},$$
$$\Gamma_4 := \{x \in \mathbb{R}^2 \, : \, x_1 = 0 \text{ and } 1/2 \le x_2 < 1\},$$
$$\Gamma_5 := \{x \in \mathbb{R}^2 \, : \, x_1 = 0 \text{ and } 0 \le x_2 < 1/2\},$$

and consider the unknowns $u : \mathbb{R}^+ \times \Omega \to \mathbb{R}$ and $J : \mathbb{R}^+ \times \Omega \to \mathbb{R}^2$.

We now introduce, for $n = 0, \ldots, N$, a semidiscrete weak formulation of (2) for the semidiscrete density unknowns $u^n(x) = u(n\Delta t, x)$ and the semidiscrete flux $J^n(x) = J(n\Delta t, x)$, where $\Delta t > 0$ is the time step.

Let $\phi \in H^1(\Omega)$ and $\psi \in H^1(\Omega) \times H^1(\Omega)$. We approximate the weak formulation of (2) by means of the following coupled system

$$(26) \quad \begin{cases} \displaystyle\int_\Omega \frac{1}{\Delta t}(u^n - \max\{u^{n-1}, 0\})\phi \, dx + \int_{\partial\Omega} \phi J^n \cdot n_x \, dS - \int_\Omega J^n \cdot \nabla\phi \, dx = 0, \\[4mm] \displaystyle\int_\Omega J^n \cdot \psi \, dx + \frac{1}{2\pi}\int_\Omega \max\{u^{n-1}, 0\}[\nabla u^n \cdot \psi] \, dx + \int_\Omega u^n[\nabla V \cdot \psi] \, dx = 0, \end{cases}$$

where n_x is the outward normal with respect to Ω starting from a point $x \in \partial\Omega$.

The boundary term (i.e., the integral on $\partial\Omega$ in the formulation written above) will be treated in agreement with the different boundary conditions specified for each numerical simulation.

The "positive part" term in the weak formulation (26) is pleonastic at the continuous level, since the solution of the problem is known to be nonnegative by Theorem 1. At the discrete level, this strategy helps in controlling the nonnegativity of the numerical solution.

The numerical experiments aim at showing some peculiar properties of (2) under different choices of the potential V and of the boundary conditions, and have been obtained by using the finite element method.

From the semidiscrete formulation, by using quadratic P_2 Lagrangian elements on a triangular mesh, we obtain a linear system whose size is given by twice the number of vertices and the number of mididedges in the triangulation. The system is solved by a multifrontal Gauss LU factorization.

The simulations are written in `FreeFem++`. The mesh discretization used in our simulations is composed by 19514 triangles, with 9940 vertices.

4.1. Long-time behavior of the solution in the one-dimensional case. We consider here the boundary conditions

$$(27) \qquad J|_{\Gamma_1} = J|_{\Gamma_3} = 0, \quad u|_{\Gamma_2} = u_1, \qquad u|_{\Gamma_4 \cup \Gamma_5} = u_0,$$

and assume that both the initial datum and the potential only depend on x_1. Then, as already discussed in section 3.2 in the stationary case, the two-dimensional problem reduces to the one-dimensional problem

$$(28) \qquad \frac{\partial u}{\partial t} = \frac{\partial}{\partial x_1}\left[u \frac{\partial}{\partial x_1}(u + V)\right] = 0, \quad x_1 \in [0,1], \ t > 0,$$

$$u(0,t) = u_0, \quad u(1,t) = u_1, \quad u(x_1, 0) = u_{\text{in}}(x_1),$$

where the initial datum, $u_{\text{in}}(x_1)$, and the (constant) Dirichlet data, u_0 and u_1, are positive. In this subsection we report a set of numerical simulations showing that the solution to (28) tends asymptotically to the stationary solution discussed in section 3.2 (see, in particular, Theorem 11). In Figure 1 the spatial profile of the solution along the direction x_1 (recall that the solution is homogeneous in the direction x_2) is shown at different instants of time. This first set of simulations has been performed with the potential

$$(29) \qquad V(x_1) = \sin(2\pi x_1).$$

Note that, according to Definition 10, for such a potential we have

$$u_0^{\text{crit}} = u_1^{\text{crit}} = 1.$$

The initial datum $u_{\text{in}}(x_1)$ is chosen as a linear function interpolating the values u_0 and u_1 and the evolution of such a datum towards the asymptotic, stationary solution (dotted black curve) is illustrated for different choices of u_0 and u_1.

In panels (a), (b), (c), and (d) we have chosen, respectively,

$$(u_0, u_1) = (1.2, 2.2), \qquad (u_0, u_1) = (1.2, 1.2),$$
$$(u_0, u_1) = (1.2, 0.2), \qquad (u_0, u_1) = (0.6, 1.2).$$

Then, in cases (a) and (b) both data are supercritical while, in case (c), u_1 is subcritical and, in case (d), u_0 is subcritical. We recall that Theorem 11 guarantees the well-posedness of the stationary problem if at least one of the Dirichlet data is supercritical.

In case (b) since the potential (29) is compatible with equal Dirichlet data, the asymptotic solution is exactly $u(x_1, \infty) = U(x_1) = u_0 - V(x_1)$ (corresponding to $c = 0$; see definition (23) and Lemma 9). In cases (a) and (d), since $u_1 > u_0$, we
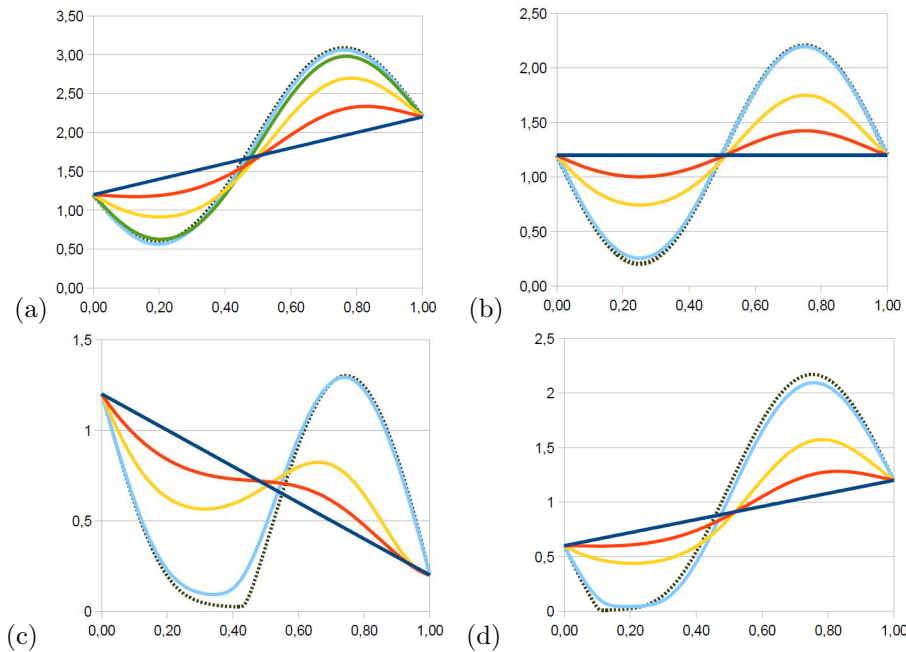
FIG. 1. *Evolution towards the stationary state in the one-dimensional case with sinusoidal potential* (29). *In each panel the initial datum is the straight line and the asymptotic solution is the dotted black curve. The other lines correspond to* $t = 0.012$, $t = 0.024$, $t = 0.048$, $t = 0.1$. *In panels* (a) *and* (b) *the two Dirichlet data are both supercritical (in particular, in panel* (b) *the asymptotic solution is* $u_0 - V(x_1)$). *In panels* (c) *and* (d), *one of the data is subcritical (respectively,* u_1 *and* u_0).

have that $c > 0$ and in case (c), where $u_1 < u_0$, we have that $c < 0$ (see the proof of Theorem 11 with $\Delta V = 0$). In the three cases (a), (c), and (d), therefore, the asymptotic solution is *not* $U(x_1)$ (which corresponds to $u_1 = u_0$ in the present case, where $\Delta V = 0$). Nevertheless, it is interesting to see that the asymptotic curves in Figure 1 tend to have the same character as $U(x_1)$, i.e., regular in the supercritical cases and piecewise regular in the subcritical casesn (however, as long as t is finite, the solution is everywhere regular).

4.2. Analysis of the current in the one-dimensional case: monotone potentials. We consider again (2) with the conditions (27) and the following data and boundary conditions:

$$u_{\text{in}} = 2 - x_1, \qquad u_0 = 2, \qquad u_1 = 1.$$

For this experiment, we have chosen the potential

$$V(x_1) = -x_1.$$

Since

$$u_0^{\text{crit}} = 0, \qquad u_1^{\text{crit}} = 1,$$

the boundary condition u_0 in this simulation is supercritical. In Figure 2, we plot the current versus time that passes through the boundaries Γ_2 (blue dotted line) and $\Gamma_4 \cup \Gamma_5$ (red continuous line), i.e., we visualize the time evolution of

$$J_R := \int_{\Gamma_2} J \cdot n_x \, dx_2 \quad \text{and} \quad J_L := \int_{\Gamma_4 \cup \Gamma_5} J \cdot n_x \, dx_2,$$
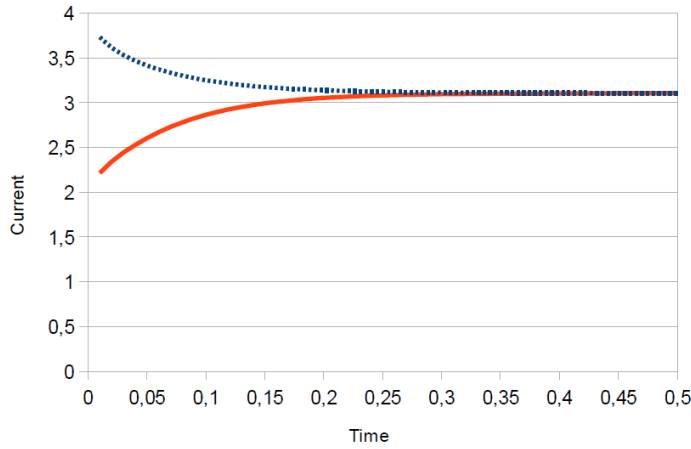
respectively.

FIG. 2. *Currents J_L (blue dotted line) and J_R (red continuous line) versus time under the action of the potential $V(x_1) = -x_1$.*

We note that, after a transient period, both currents at the extremities of the device tend monotonically to the common value 3.11.

In the second numerical simulation, we have left unchanged the initial and boundary conditions, but we have chosen a different potential, namely,

$$V(x_1) = -x_1 + e^{-x_1^2}.$$

This potential is nonlinear, but is still monotone. Here

$$u_0^{\text{crit}} = 0, \qquad u_1^{\text{crit}} = 2 - 1/e \approx 1.63,$$

hence the boundary condition u_1 is supercritical.

In Figure 3, we plot the current versus time that passes through the boundaries Γ_2 (blue dotted line) and $\Gamma_4 \cup \Gamma_5$ (red continuous line), respectively.

We note a different behavior of J_L and J_R with respect to the previous simulation in the transient period before reaching the equilibrium: J_L is still a monotone increasing function, but J_R is no longer monotone. At time $t = 1.4$ (not plotted in Figure 3) the two currents at the extremities of the domain have reached the common asymptotic value 4.01.

4.3. Analysis of the current in the one-dimensional case: a potential barrier. We now consider (2) under the action of the potential

$$V(x_1) = e^{-(x_1 - .5)^2}.$$

Here the critical values of the problem are

$$u_0^{\text{crit}} = u_1^{\text{crit}} = 1 - e^{1/4} \approx 0.22.$$

We compare the time evolution of the current at the extremities of the device in two situations. The first one, whose results are plotted in Figure 4, has been obtained with the initial data and the boundary conditions

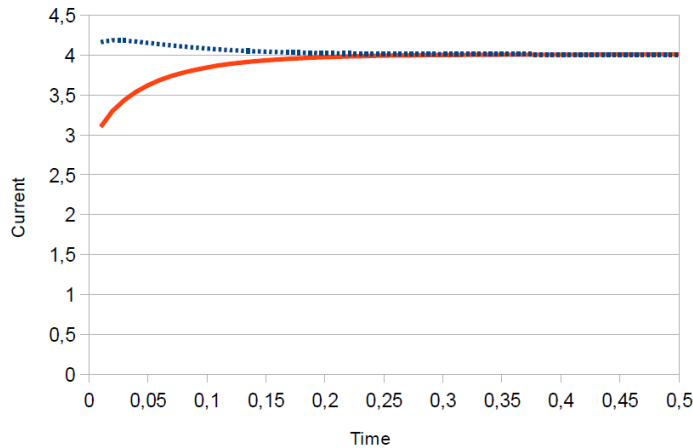$$u_{\text{in}} = 2 - x_1, \qquad u_0 = 2, \qquad u_1 = 1.$$

FIG. 3. *Currents J_L (blue dotted line) and J_R (red continuous line) versus time under the action of the potential $V(x_1) = -x_1 + e^{-x_1^2}$.*
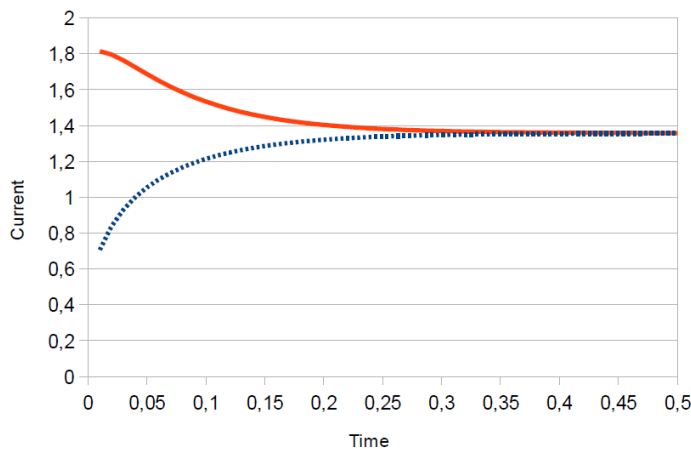

FIG. 4. *Currents J_L (blue dotted line) and J_R (red continuous line) versus time under the action of the potential $V(x_1) = e^{-(x_1-.5)^2}$ and a small gap between the boundary data in Γ_2 and Γ_4.*

The second situation, whose results are plotted in Figure 5, has been obtained by imposing the following initial data and boundary conditions:

$$u_{\text{in}} = 6 - 5x_1, \qquad u_0 = 6, \qquad u_1 = 1.$$

The numerical results of Figures 4 and 5 show that the stationary current flowing through the device in the case of a small density gap differ considerably from the one that is obtained in the case of a wide density gap (numerically we get a value which is close to 1.36 in the first case and the value 16.84 in the second). Moreover, in the first case, the convergence speed to the asymptotic state is slower than in the second case.

We have finally computed, for $a \in [0,3]$, the asymptotic common value at the ends of the device versus a, which is a parameter that controls the gap of the boundary data
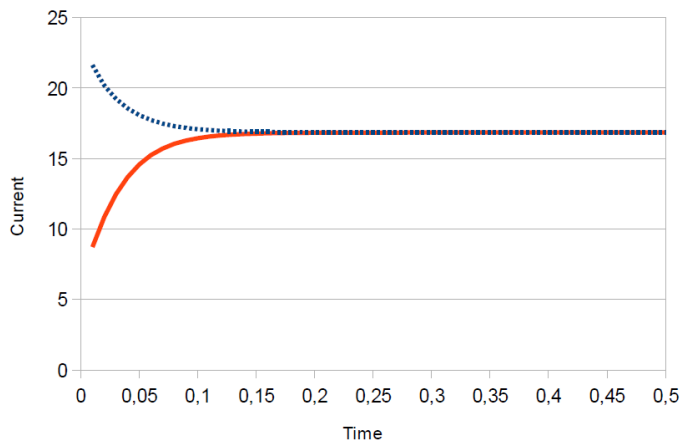
FIG. 5. *Currents J_L (blue dotted line) and J_R (red continuous line) versus time under the action of the potential $V(x_1) = e^{-(x_1 - .5)^2}$ and a wide gap between the boundary data in Γ_2 and Γ_4.*
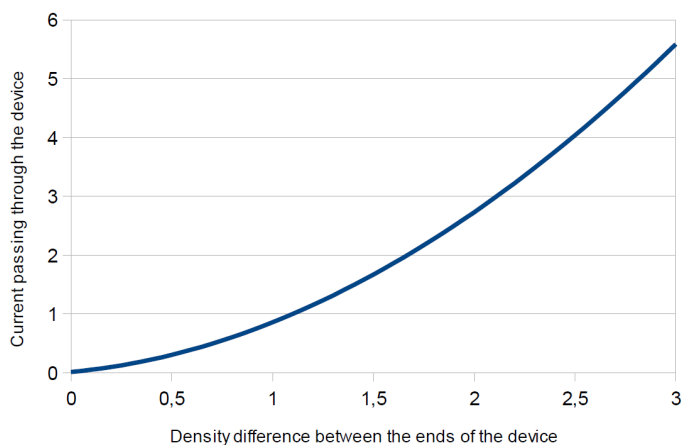

FIG. 6. *Asymptotic current at the ends of the device under the action of the potential $V(x_1) = e^{-(x_1 - .5)^2}$ versus the gap between the boundary data in Γ_2 and Γ_4.*

between the ends Γ_2 and Γ_4, through the choice of the following initial and boundary conditions:

$$u_{\mathrm{in}} = .5 + a(1 - x), \qquad u_0 = .5 + a, \qquad u_1 = .5.$$

Both boundary data are supercritical.

The results, plotted in Figure 6, show that the current is zero when $a = 0$ and that it is strictly monotone. The profile is parabolic with a good approximation. This simulation has been very time consuming, since we had to repeat, for each element of the discretization of $a \in [0, 3]$, a computation in long time that gives the asymptotic common value of the currents at the ends of the device. The discretization between the values of a is $\Delta a = 0.05$, and the final time of each simulation has been $t = 2.5$. The discrepancies observed between the numerical values of $J_R(t = 2.5)$ and $J_L(t = 2.5)$ are, for each value of a, beyond the resolution of Figure 6.
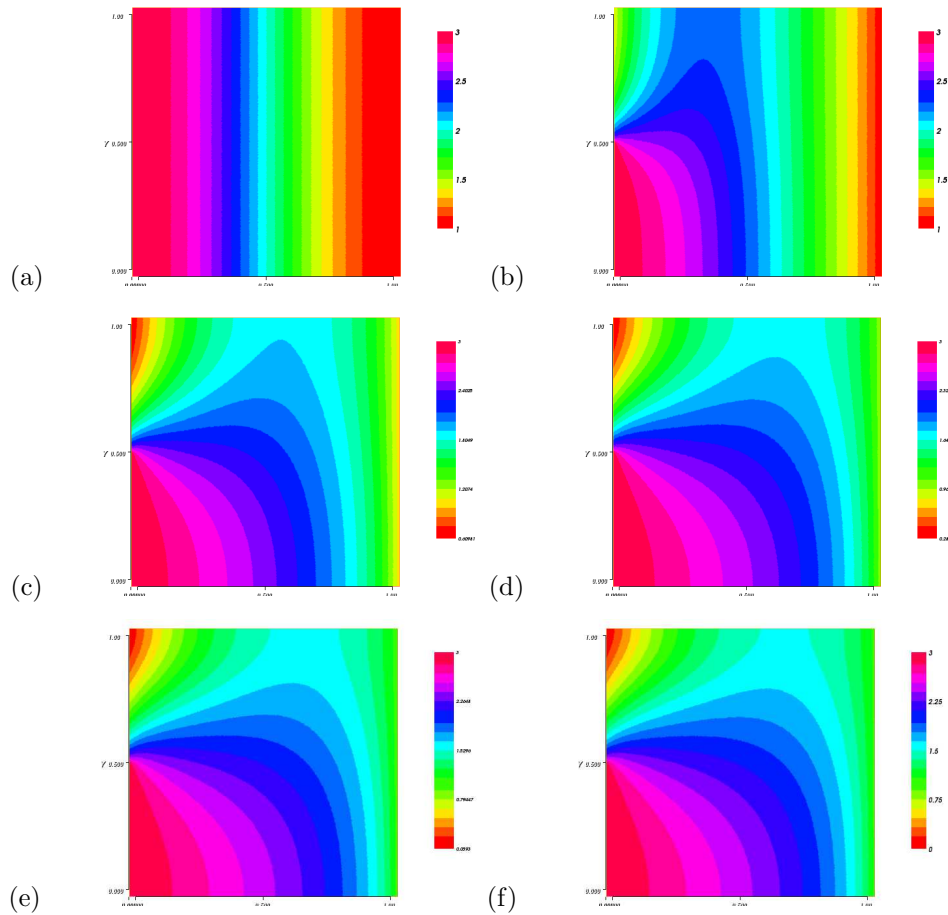
FIG. 7. *Contours of the density* u *at six different instants:* (*a*) $t = 0$ *(initial condition),* (*b*) $t = 0.10$, (*c*) $t = 0.30$, (*d*) $t = 0.50$, (*e*) $t = 0.80$ *and* (*f*) $t = 1.00$.

4.4. Analysis of the current in a two-dimensional device in a non-symmetric situation. We conclude the description of our simulations with a test case that is widely used in the literature [21]. Consider the system defined by (2) under the action of the linear potential

$$V(x) = 1 - x_1.$$

In this case, the initial data and boundary conditions are

$$u_{\text{in}}(x) = \cos(\pi x_1) + 2$$

and

$$J|_{\Gamma_1} = J|_{\Gamma_3} = J|_{\Gamma_4} = 0, \qquad u|_{\Gamma_2} = 1, \qquad u|_{\Gamma_5} = 3.$$

Note that, even though u_{in} and V depend only on the first variable x_1, the problem is genuinely two dimensional because of the boundary conditions.

In Figure 7, we show the time evolution of the unknown density u. At time $t = 1$ the system has already reached an almost stationary configuration.
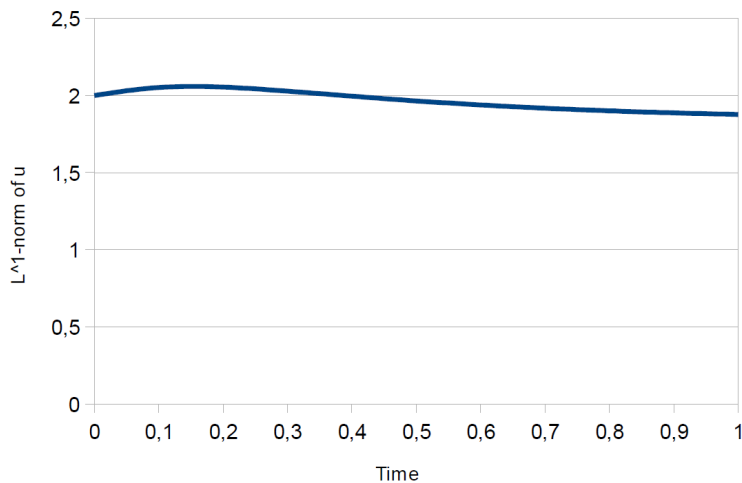
Fig. 8. *Time evolution of* $\|u\|_1$.

We also show in Figure 8 the time evolution of the L^1-norm of the density u. Note that the total mass of the problem is not conserved in time, but has a nonmonotone behavior around the value $\|u_{\mathrm{in}}\|_{L^1(\Omega)} = 2$.

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