A Fully Discrete Finite Element Scheme for the Derrida-Lebowitz-Speer-Spohn Equation

Jorge Mauricio Ruiz Vera [1]   and Ignacio Mantilla Prada [2]

Abstract

The Derrida-Lebowitz-Speer-Spohn (DLSS) equation is a fourth order in space non-linear evolution equation. This equation arises in the study of interface fluctuations in spin systems and quantum semiconductor modelling. In this paper, we present a finite element discretization for a exponential formulation of a coupled-equation approach to the DLSS equation. Using the available information about the physical phenomena, we are able to set the corresponding boundary conditions for the coupled system. We prove existence of the discrete solution by fixed point argument. Numerical results illustrate the quantum character of the equation. Finally a test of order of convergence of the proposed discretization scheme is presented.

Key words: Finite elements, Nonlinear evolution equations, Semiconductors.

[1]   Doctor en Ciencias Matemáticas, jmruizv@unal.edu.co, Departamento de matemáticas, Universidad Nacional de Colombia, Bogotá, Colombia.
[2]   Dr. rer. nat. in Mathematik, imantillap@unal.edu.co, Departamento de matemáticas, Universidad Nacional de Colombia, Bogotá, Colombia.

Highlights

• Exponential formulation of a coupled-equation approach to the DLSS equation. • Existence proof of the discrete solution by means of a fixed point argument. • Numerical results suggest optimal convergence of the method in the $H^1(\Omega)$-norm.

Un esquema de elementos finitos completamente discreto para la ecuación de Derrida-Lebowitz-Speer-Spohn

Resumen

La ecuación de Derrida-Lebowitz-Speer-Spohn (DLSS) es una ecuación de evolución no lineal de cuarto orden. Esta aparece en el estudio de las fluctuaciones de interface de sistemas de espín y en la modelación de semiconductores cuánticos. En este artículo, se presenta una discretización por elementos finitos para una formulación exponencial de la ecuación DLSS abordada como un sistema acoplado de ecuaciones. Usando la información disponible acerca del fenómeno físico, se establecen las condiciones de contorno para el sistema acoplado. Se demuestra la existencia de la solución discreta global en el tiempo via un argumento de punto fijo. Los resultados numéricos ilustran el carácter cuántico de la ecuación. Finalmente se presenta un test del orden de convergencia de la discretización porpuesta.

Palabras clave: Elementos finitos, Ecuaciones no lineales de evolución, Semiconductores.

1   Introduction

The Derrida-Lebowitz-Speer-Spohn (DLSS) equation is a nonlinear fourth order parabolic equation which was proposed to study the interface fluctuations in a spin system [1], [2]. Coincidentally, in the mathematical modelling of the charge transport in quantum semiconductor devices the DLSS equation appears as the zero temperature and zero electric field quantum drift diffusion equation [3].

In this paper, we discuss a new numerical technique to solve the DLSS equation

$$n_t + \frac{\varepsilon^2}{2}(n(\log n)_{xx})_{xx} = 0, \qquad \text{in} \ \ \Omega \times (0, T), \tag{1a}$$

subject to the initial and boundary conditions

$$n(x, 0) = n_0 \geq 0 \qquad \text{in } \Omega, \tag{1b}$$
$$n(0, t) = n(1, t) = 1 \qquad t \in [0, T], \tag{1c}$$
$$n_x(0, t) = n_x(1, t) = 0 \qquad t \in [0, T], \tag{1d}$$

where n_0 is a given function, Ω is the bounded interval $(0, 1)$, and $T > 0$ is a fixed positive time. Regarding semiconductor modelling, $n(x, t)$ denotes the electron concentration, and ε is the scaled Planck constant; it is of order $O(10^{-2, \ldots, -4})$. The Dirichlet boundary conditions (1c) model charge neutrality at the boundary contacts, while Neumann boundary conditions (1d) describe no current flow passing through the boundary.

Due to the several difficulties and challenges that fourth order differential equations have (see e.g. [4]), several researchers have analyzed the problem (1). For instance, existence results of a positive classical solution locally in time and nonnegative solutions globally in time of (1) are found in [1] and [5] respectively. More recently, in [6] the existence of the solution for the multidimensional equation is proven. Furthermore, in [7], [8] and [9] the long-time behavior of solutions is studied. However, concerning its numerical solution not much work is known. In [1] and [5] a fully implicit finite difference discretization scheme was employed to the equivalent formulation

$$n_t = -\frac{\varepsilon^2}{2} \left(n_{xxxx} - \left(\frac{n_x^2}{n} \right)_{xx} \right) \tag{2}$$

in order to verify the preservation of the non negativity by the solution n. An alternative numerical treatment is presented in [10], where a fully discrete variant of the minimizing movement scheme is developed based on the particular structure of (1a). The numerical experiments in [10] suggest that this scheme is unconditionally stable and second-order convergence.

With this paper, we pursue a different numerical approach based on the following two main steps: First, in order to guarantee the positivity of the solution n, we perform an exponential transformation of variable $n = e^{2u}$. Such transformation has been already used in [5] and [8]

for theoretical purposes but not for numerical tasks. After that, we introduce a new variable $w = -\varepsilon^2 e^{2u} u_{xx}$ in order to write Equation (1) as two coupled partial differential equations, which require less stringent smoothness constrains over the solution as well as for the finite elements approximation than consider the single fourth order equation. Finally, the resulting problem is discretized by a fully discrete finite element scheme.

The paper is organized as follows. In section 2 we present a coupled equation decomposition after an exponential transformation of variables for DLSS equation and discuss the corresponding boundary conditions in the context of the quantum charge transport in semiconductors. We formulate the fully discrete finite element scheme and numerical treatment of the nonlinearities in section 3. Existence of the discrete solution is proved in 3.1. Finally, section 4 is devoted to the numerical results. Concluding remarks are given in section 5.

2   Exponential and coupled equation formulation

It is well known, that for a fourth order differential equation the nonnegativity of the initial data does not imply the same property of solutions at any time. This motivated us to perform the change of variable $n = e^{2u}$, which yields the following exponential form of problem (1)

$$(e^{2u})_t = -\varepsilon^2 (e^{2u} u_{xx})_{xx} \qquad \text{in } \Omega \times (0, T), \qquad (3a)$$

$$u(x, 0) = u_0 := \frac{1}{2} \log(n_0) \qquad \text{in } \Omega, \qquad (3b)$$

$$u(0, t) = u(1, t) = 0 \qquad t \in [0, T], \qquad (3c)$$

$$u_x(0, t) = u_x(1, t) = 0 \qquad t \in [0, T]. \qquad (3d)$$

Such formulation of (1) has been proposed in [5] as a crucial step to prove the existence of nonnegative weak solutions, but it has not been used for finding an approximate solution of (1). In fact, in [5] it was proved that, if the initial condition u_0 is a measurable function such that $\int_\Omega (\exp(2u_0) - 2u_0) dx < \infty$, then problem (3) has a solution $u \in H_0^2(\Omega)$.

Furthermore, note that the existence of positive solution n of the problem (1) is a consequence of the existence solution u of (3).

In order to relax the smoothness constrains on the solution as well as the finite element approximation, we introduce an auxiliary variable $w = -\varepsilon^2 e^{2u} u_{xx}$. Then we may write problem (3) as a coupled second order system of a nonlinear parabolic and nonlinear elliptic equations

$$(e^{2u})_t = w_{xx} \qquad \text{on } \Omega \times (0, T), \tag{4a}$$

$$-\varepsilon^2 u_{xx} = e^{-2u} w \qquad \text{on } \Omega \times (0, T). \tag{4b}$$

Now, we state the corresponding boundary conditions. For the unknown u it is easy to see that conditions (3c) and (3d) hold. However the values of w or w_x at the boundary can not be derived straightforwardly, hence we need to consider additional information about the electron transport at the boundary. For this purpose, let us assume smooth non vacuum solutions ($n \neq 0$) of (1a), then

$$n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x = \frac{1}{2}(n(\log n)_{xx})_x . \tag{5}$$

In addition, from [11] it is known that the quantum current has to vanish at the semiconductors contacts, that is

$$\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x = 0 \text{ on } \partial\Omega \ \ t > 0. \tag{6}$$

Combining (5) with (6) and taking $n = e^{2u}$ we obtain

$$0 = n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x = (e^{2u} u_{xx})_x = -\frac{1}{\varepsilon^2} w_x \qquad \text{for all } x \in \partial\Omega \ \ t > 0.$$

This lead us to impose homogeneous Neumann conditions for $w(x, t)$ i.e,

$$w_x(0, t) = w_x(1, t) = 0 \qquad t \in [0, T]. \tag{7}$$

Remark 2.1. The differential operator $(\sqrt{n})_{xx}/\sqrt{n}$ is the so called Bohm potential and appears as the quantum correction term of the classical drift-diffusion model for semiconductors [3], [12].

3   Numerical discretization

In this section we describe the construction of finite element method for the coupled system of nonlinear partial differential Equation (4) with boundary conditions (3c) and (7). To give a variational formulation of this boundary value problem, we introduce the spaces

$$H^1(\Omega) = \{\psi \in L^2(\Omega) : \psi_x \in L^2(\Omega)\}$$

and

$$H_0^1(\Omega) = \{\phi \in H^1(\Omega) : \phi(0) = \phi(1) = 0\}.$$

Now we multiply (4a) and (4b) by $\phi \in H_0^1(\Omega)$ and $\psi \in H^1(\Omega)$ respectively and integrating by parts over Ω, we find that

$$\int_\Omega (e^{2u})_t \phi dx + \int_\Omega \partial_x w \partial_x \phi dx = 0, \qquad \forall \phi \in H_0^1(\Omega), \qquad \text{(8a)}$$

$$\varepsilon^2 \int_\Omega \partial_x u \partial_x \psi dx - \int_\Omega e^{-2u} w \psi dx = 0, \qquad \forall \psi \in H^1(\Omega), \qquad \text{(8b)}$$

$$u(x,0) = u_0, \qquad \text{(8c)}$$

since $w_x(0,t) = w_x(1,t) = 0$ and $u_x(0,t) = u_x(1,t) = 0$ for all $t \geq 0$.

If $(\cdot, \cdot)$ denotes the $L^2(\Omega)$ inner product and the mapping $a(\cdot, \cdot) : H^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ is defined by

$$a(\psi, \phi) := \int_\Omega (\partial_x \psi, \partial_x \phi) \text{ for all } \psi \in H^1(\Omega) \text{ and } \phi \in H_0^1(\Omega),$$

then the variational formulation of (4) with boundary condition (3c) and (7) is: Find the pair $(w, u)(t) \in H^1(\Omega) \times H_0^1(\Omega)$ for all $t \in (0, T)$ such that

$$((e^{2u})_t, \phi) + a(w, \phi) = 0 \qquad \forall \phi \in H_0^1(\Omega) \qquad \text{(9a)}$$

$$\varepsilon^2 a(\psi, u) - (e^{-2u} w, \psi) = 0 \qquad \forall \psi \in H^1(\Omega) \qquad \text{(9b)}$$

$$u(x,0) = u_0. \qquad \text{(9c)}$$

In order to discretize (9) in time, first we apply the chain rule to the time derivative term in (9a), then

$$(e^{2u})_t = 2e^{2u} u_t.$$

Next, we divide the interval $(0, T]$ into M equal parts, i.e. time step $\tau = T/M$, and each time level $t_k = k\tau$, with $k = 0, 1, .., M$. Then we approximate the quantity u_t by finite difference. After that, if the index k signifies the most recent known time level, then evaluating the non linear term e^{2u} at the time level k and the spatial terms at the next unknown time level $k + 1$ produces the semi-discrete problem: Find the pair $(w^{k+1}, u^{k+1}) \in H^1(\Omega) \times H_0^1(\Omega)$ for $k = 0, ..., M - 1$ such that

$$\frac{2}{\tau}(e^{2u^k}(u^{k+1} - u^k), \phi) + a(w^{k+1}, \phi) = 0 \qquad \forall \phi \in H_0^1(\Omega), \qquad (10a)$$

$$\varepsilon^2 \, a(\psi, u^{k+1}) - (e^{-2u^{k+1}} w^{k+1}, \psi) = 0 \qquad \forall \psi \in H^1(\Omega) \qquad (10b)$$

with $u^0 = u_0$.

We now discretize also in space, let $0 = x_0 < x_1 < ... < x_N = 1$ be mesh on the interval $\Omega = (0, 1)$ with $h_i := x_i - x_{i-1}, i = 1, ..., N$. In addition, let $W_h \subset H^1(\Omega)$ be the corresponding subspace of continuous piecewise linear functions on Ω and $V_h \subset H_0^1(\Omega)$ be the subspace of continuous piecewise linear functions on Ω vanishing at $x = 0$ and $x = 1$. Furthermore, let us equip V_h and W_h with a basis $\{b_i\}_{i=1}^{N-1}$ and $\{b_i\}_{i=0}^{N}$ respectively, where

$$b_i(x) = \begin{cases} \frac{x - x_{i-1}}{h_i} & x \in [x_{i-1}, x_i] \\ \frac{x_{i+1} - x}{h_{i+1}} & x \in [x_i, x_{i+1}] \\ 0 & \text{otherwise.} \end{cases}$$

Then for any $w_h^k \in W_h$ and $u_h^k \in V_h$, these can be written as $u_h^k(x) = \sum_{i=1}^{N-1} u_i^k b_i(x)$ and $w_h^k(x) = \sum_{i=0}^{N} w_i^k b_i(x)$ in the k-th time level. We now approximate the nonlinear terms in (10a) and (10b) by their linear interpolants on the mesh, that is

$$e^{2u^k}(u^{k+1} - u^k) \approx (e^{2u^k}(u^{k+1} - u^k))^I := \sum_{i=1}^{N-1} e^{2u_i^k}(u_i^{k+1} - u_i^k)b_i(x)$$

and

$$e^{-2u^{k+1}} w^{k+1} \approx (e^{-2u^{k+1}} w^{k+1})^I := \sum_{i=0}^{N} e^{-2u_i^{k+1}} w_i^{k+1} b_i(x).$$

Therefore, the fully finite element method for (9) reads as follows: Find for $k = 0, ..., M - 1$, the pair $(w_h^{k+1}, u_h^{k+1}) \in W_h \times V_h$ such that

$$\frac{2}{\tau}(e^{2u_h^k}(u_h^{k+1} - u_h^k), b_i)_h + a(w_h^{k+1}, b_i) = 0, \qquad i = 1, \ldots, N - 1, \quad (11a)$$

$$\varepsilon^2\, a(b_j, u_h^{k+1}) - (e^{-2u_h^{k+1}} w_h^{k+1}, b_j)_h = 0, \qquad j = 0, \ldots, N, \qquad (11b)$$

$$u_h^0 = u_{0h}, \qquad (11c)$$

where $(f, g)_h := (f^I, g)$.

Finally, computing the integrals exactly in system of Equations (11a)-(11b), we obtain the nonlinear system of equations

$$2\mathbf{AD}(\mathbf{u}^k)\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\tau_k} + \mathbf{Bw}^{k+1} = 0,$$

$$\varepsilon^2\mathbf{B}^T\mathbf{u}^{k+1} - \mathbf{C}\widetilde{\mathbf{D}}(\mathbf{u}^{k+1})^{-1}\mathbf{w}^{k+1} = 0, \qquad (12)$$

where the vectors $\mathbf{u}^{k+1} \in \mathbb{R}^{N-1}$ and $\mathbf{w}^{k+1} \in \mathbb{R}^{N+1}$ contain the nodal unknowns $u_i^{k+1}(t)$ and $w_i^{k+1}(t)$ respectively. The matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}$ are given by

$$\mathbf{A} = (a_{i,j}), \quad a_{i,j} = (b_j, b_i) \quad \text{for} \quad i = 1, ..., N - 1, \quad j = 1, ..., N - 1$$
$$\mathbf{B} = (b_{i,j}), \quad b_{i,j} = a(b_j, b_i) \quad \text{for} \quad i = 1, ..., N - 1, \quad j = 0, ..., N$$
$$\mathbf{C} = (c_{i,j}), \quad c_{i,j} = (b_j, b_i) \quad \text{for} \quad i = 0, ..., N, \qquad j = 0, ..., N$$

while the diagonal matrices $\mathbf{D}(\mathbf{u}^k)$ and $\widetilde{\mathbf{D}}(\mathbf{u}^{k+1})$ are

$$\mathbf{D}(\mathbf{u}^k) = \text{diag}(e^{2u_1^{k-1}}, e^{2u_2^{k-1}}, \ldots, e^{2u_{N-2}^{k-1}}, e^{2u_{N-1}^{k-1}})$$
$$\widetilde{\mathbf{D}}(\mathbf{u}^{k+1}) = \text{diag}(e^{2u_0^k}, e^{2u_1^k}, \ldots, e^{2u_{N-1}^k}, e^{2u_N^k}). \qquad (13)$$

In order to solve the nonlinear system (12), let us denote by $\mathbf{y} \in \mathbb{R}^{2N}$ the unknown vector $\begin{bmatrix} \mathbf{u}^{k+1} \\ \mathbf{w}^{k+1} \end{bmatrix}$ and employ the Newton method

$$\mathbf{y}^{(m+1)} = \mathbf{y}^{(m)} + \Delta\mathbf{y}$$

where $\Delta\mathbf{y}$ is the solution of the linear system

$$\mathbf{J}(\mathbf{y}^{(m)})\Delta\mathbf{y} = -\mathbf{F}(\mathbf{y}^{(m)})$$

with $\mathbf{F}(\mathbf{y}) : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ given by (12) and Jacobi matrix

$$\mathbf{J}(\mathbf{y}) = \begin{bmatrix} \frac{2}{\tau}\mathbf{AD}(\mathbf{u}^k) & \mathbf{B} \\ \varepsilon^2\mathbf{B}^T & 2\mathbf{C}\widetilde{\mathbf{D}}(\mathbf{u})^{-1}\mathrm{diag}(\mathbf{w}) \end{bmatrix}.$$

We choose $\mathbf{y}^{(0)} = \begin{bmatrix} \mathbf{u}^k \\ \mathbf{w}^k \end{bmatrix}$ as a initial guess for the Newton iteration, provided that the time step τ is small enough.

3.1 Existence of the discrete solutions

In this section, we prove the existence of the discrete solution by means of a fixed point argument.

First, let us observe that from the symmetric positive definiteness of matrices $\mathbf{A}$ and $\mathbf{D}(\mathbf{z})$ with given $\mathbf{z} \in \mathbb{R}^{N-1}$, the bilinear form on $\mathbb{R}^{N-1}$ defined by

$$\langle \mathbf{u}, \mathbf{v} \rangle := \mathbf{u}^T\mathbf{AD}(\mathbf{z})\mathbf{v} \qquad \forall \mathbf{u}, \mathbf{v} \in \mathbb{R}^{N-1} \tag{14}$$

is an inner product on $\mathbb{R}^{N-1}$.

Theorem 3.1. *The nonlinear system of Equations* (12)*, has a solution.*

Proof: Since the mass matrices $\mathbf{A}$ and $\mathbf{C}$ are symmetric positive definite and the terms $e^{\pm u_i(t)} \neq 0$ for $i = 0, 1, ..., N$ in (13), we are able to eliminate the unknown $\mathbf{w}$ from the second Equation of (12). Then we may write (12) as the Equation $\mathbf{G}(\mathbf{u}^{k+1}) = 0$ for each time level k, where $\mathbf{G}$ is a continuous function from $\mathbb{R}^{N-1}$ to $\mathbb{R}^{N-1}$ given by

$$G(\mathbf{u}) := \mathbf{u} - \mathbf{u}^k + \frac{\varepsilon^2\tau}{2} \mathbf{D}(\mathbf{u}^k)^{-1}\mathbf{A}^{-1}\mathbf{B}\widetilde{\mathbf{D}}(\mathbf{u})\mathbf{C}^{-1}\mathbf{B}^{\mathbf{T}}\mathbf{u}. \tag{15}$$

Let us now introduce the inner product on $\mathbb{R}^{N-1}$ defined by

$$\langle \mathbf{u}, \mathbf{v} \rangle := \mathbf{u}^T\mathbf{AD}(\mathbf{u}^k)\mathbf{v}$$

for a given $\mathbf{u}^k$. Hence, it defines a norm $\| \cdot \|_{\mathbf{D}}$ equivalent to the usual euclidian norm in $\mathbb{R}^{N-1}$. Further, we define the ball $B_R(0) := \{u \in \mathbb{R}^{N-1} : \|\mathbf{u}\|_{\mathbf{D}} \leq R\}$ with $R = \|\mathbf{u}^k\|_{\mathbf{D}}$. Then

$$\langle \mathbf{u}, \mathbf{G}(\mathbf{u}) \rangle = \langle \mathbf{u}, \mathbf{u} - \mathbf{u}^k \rangle + \frac{\varepsilon^2\tau}{2} \langle \mathbf{u}, \mathbf{D}(\mathbf{u}^k)^{-1}\mathbf{A}^{-1}\mathbf{B}\widetilde{\mathbf{D}}(\mathbf{u})\mathbf{C}^{-1}\mathbf{B}^{\mathbf{T}}\mathbf{u} \rangle$$

$$\begin{aligned}
&= \langle \mathbf{u}, \mathbf{u} - \mathbf{u}^k \rangle + \frac{\varepsilon^2 \tau}{2} \, \mathbf{u}^T \mathbf{A} \, \mathbf{D}(\mathbf{u}^k) \mathbf{D}(\mathbf{u}^k)^{-1} \mathbf{A}^{-1} \mathbf{B} \widetilde{\mathbf{D}}(\mathbf{u}) \mathbf{C}^{-1} \mathbf{B}^{\mathbf{T}} \mathbf{u} \\
&= \langle \mathbf{u}, \mathbf{u} \rangle - \langle \mathbf{u}, \mathbf{u}^k \rangle + \frac{\varepsilon^2 \tau}{2} \, (\mathbf{B}^{\mathbf{T}} \mathbf{u})^T \widetilde{\mathbf{D}}(\mathbf{u}) \mathbf{C}^{-1} \mathbf{B}^{\mathbf{T}} \mathbf{u} \\
&\geq \|\mathbf{u}\|_D^2 \; - \; \langle \mathbf{u}, \mathbf{u}^k \rangle \\
&\geq 0
\end{aligned}$$

for all $\mathbf{u}$ such that $\|\mathbf{u}\|_{\mathbf{D}} \geq R$. Therefore, by the Minty-Brower's fixed point theorem [13], $G(\mathbf{u})$ has a solution in $B_R(0)$.

Remark 3.1. We observe that it is possible to solve the nonlinear system of Equations $\mathbf{G}(\mathbf{u}^{k+1}) = 0$ by Newton's method instead of (12). However, the presence of the inverse matrices of $\mathbf{A}$ and $\mathbf{C}$ yields a loss of sparseness of the Jacobi matrix of $\mathbf{G}(\mathbf{u})$. Hence, it is not computationally efficient to solve such equation even though it has $N - 1$ unknowns.

4 Numerical results

To demonstrate the efficacy of the finite element described before, we consider the fourth-order nonlinear parabolic problem (1) with non-negative initial condition

$$n(x, 0) = \epsilon + \cos^{2m}(\pi x) \ \text{ in } \ [0, 1],$$

for $m = 1, 8$ and $\epsilon = 10^{-6}$. Further we give a physical interpretation of the results as well as an experimental error convergence analysis for the proposed spatial discretization.

We apply the fully finite element method (11) for solving the problem (1) up to $T = 10^{-2}$. Since the method is semi-implicit, we choose $\tau \leq \frac{1}{2} h^2$ to keep it stable. We present in Figure 1 numerical results for $m = 1$ with space discretization step $h = 1/30$, and time step $\tau = 10^{-5}$ and in Figure 2 for $m = 8$ with space discretization step $h = 1/30$, and time step $\tau = 10^{-6}$. In each time step we have solved the nonlinear system of Equations (12) by means of the Newton's method (See section 3).

4.1   Physical interpretation of the solution

Physical processes modelled by fourth order parabolic equations are very similar to the diffusion phenomena but the oscillatory data is damped more rapidly. Indeed, from Figure 1 we observe that at the instant $t = 0$ there is high concentration of electron on the boundaries $x = 0$, $x = 1$ and it decrease in the interior of the semiconductor until reach the zero at $x = 0.5$. Then, the electrons move from the higher concentration parts to the lower concentration part. This movement finishes when the distribution of electrons in the semiconductor is almost uniform, i.e the steady state is reached $t = t_\infty$. In contrast, when $m = 8$ the electron density evolution does not behave like classical diffusion (Figure 2).
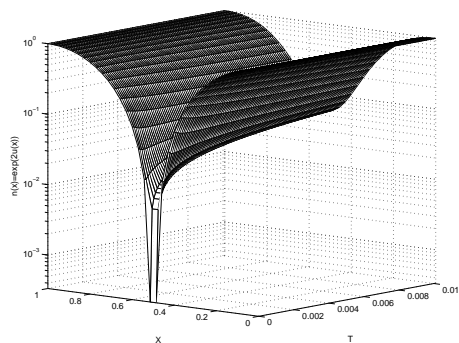

Figure 1: Density evolution $N = 30$, $\tau = 10^{-5}$, $t \in (0, 10^{-2}]$, $m = 1$.
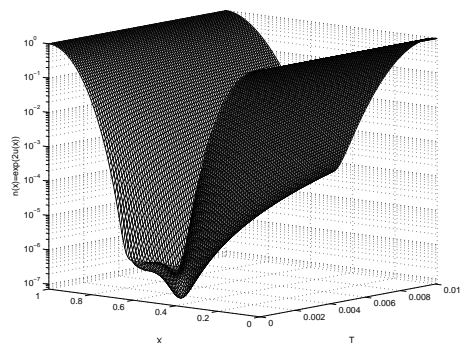
Figure 2: Density evolution $N = 30$, $\tau = 10^{-6}$, $t \in (0, 10^{-2}]$, $m = 8$.

In this case the initial electrons density is very low in a neighborhood of $x = 0.5$, hence the electrons diffuse to this low density region and move almost freely, without many collisions, during some period of time. As a consequence, they start to accumulate in the center of the semiconductor (see the small peak at $t = 2 \times 10^{-4}$) leaving two areas with lower density. Afterwards, the electrons are redistributed rapidly, vanishing the peak. Then, the situation behaves like in the case $m = 1$. Such behavior on the electron density gives an evidence of the quantum effect due to the Bohm potential.

Similar behaviors for the electron density n have been obtained in

[1], [5] and [10]. However, in [5] Equation (2) is solved for the variable n using a finite difference scheme, while we solve (1a) for the variable $u = \frac{1}{2}\log(n)$.

4.2 Convergence rates

In order to examine the convergence properties with respect to the spatial step size h, we use a solution $\hat{u}$ on a very fine grid ($h = 1/1600$) as a reference solution in computing the approximation errors in the $L_2(\Omega)$-norm and $H^1(\Omega)$-norm. Furthermore, we solved the system (4) on five grids with sizes $h = 1/(2^k \cdot 50), k = 0, \ldots, 4$. Let u_h^T denote the numerical solution corresponding to the space grid with size h at final time $t = T$ and let $\hat{u}^h$ be the restriction of the fine grid solution to the h-grid, so that we can define the approximate error $e(h) = \|u_h^T - \hat{u}_h^T\|$. Since we expect that the method is r'th order accurate, that is $e(h) \approx Ch^r$ as $h \to 0$, then the convergence order r can be estimated as

$$r \approx \log_2\big(e(h)/e(h/2)\big).$$

Table 1 presents for various space step sizes, numerical errors for u_h^T and convergence rates when $m = 1$. One can see from the table optimal orders of convergence in the $L_2(\Omega)$-norm and $H^1(\Omega)$-norm. On the other hand, Table 2 shows numerical results for $m = 8$ where the $L_2(\Omega)$-norm of the error decreases to order one; while the $H^1(\Omega)$-norm error remains to be first order.

h	$\|\hat{u}^T - u_h^T\|_{L_2}$	Rate	$\|\hat{u}^T - u_h^T\|_{H^1}$	Rate
$\frac{1}{50}$	0.007253	—	1.627803	—
$\frac{1}{100}$	0.001606	2.17	0.771415	1.07
$\frac{1}{200}$	0.000394	2.02	0.358607	1.10
$\frac{1}{400}$	0.000096	2.03	0.153536	1.22
$\frac{1}{800}$	0.000019	2.33	0.051164	1.58

Table 1: Convergence rates for $m = 1$

h	$\|\hat{u}^T - u_h^T\|_{L_2}$	Rate	$\|\hat{u}^T - u_h^T\|_{H^1}$	Rate
$\frac{1}{50}$	0.0403960	—	0.290222	—
$\frac{1}{100}$	0.0201442	1.00	0.139242	1.05
$\frac{1}{200}$	0.0095811	1.07	0.064717	1.10
$\frac{1}{400}$	0.0041818	1.19	0.027723	1.22
$\frac{1}{800}$	0.0014613	1.51	0.009321	1.57

Table 2: Convergence rates for $m = 8$

5 Conclusions

In this paper we have presented a new numerical approach for a fourth order nonlinear problem based on piecewise linear finite element method. We applied a semi implicit discretization in time to construct the fully discrete solution and prove the existence of the fully finite element discrete solution. Due to the used exponential transformation of variables, the proposed method guarantee the positivity of the solution. Numerical calculations show that the proposed scheme is convergent but it has only an optimal convergence rate in the $H^1(\Omega)$-norm. Future work will focus on a consistency analysis of the proposed method.

Acknowledgments

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