

ON A QUANTUM HYDRODYNAMIC MODEL FOR A PHOTOVOLTAIC CELL

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Abstract

We present a theoretical model for the behavior of the propagation of electrons in a photovoltaic cell with some Bohm quantum potential corrections. The system describes the dynamic of the electron density and the current density functions. A numerical solution for the 1-dimensional case based on the method of the backward finite differences is given. Also, some analytical solutions for 3-dimensional case are proposed.

1. Introduction

The first approach in modelling the behaviour of the electrons in a photovoltaic cell was a hydrodynamic model. The hydrodynamic model treats the propagation of electrons in a semiconductor as a flow of a charge in an electric field.

Semiconductor models based on classical or semi-classical mechanics (like drift-diffusion equation, hydrodynamic models and the semi-classical solid state physics Boltzmann equation) cannot be used to reasonably describe the performance of ultra-integrated devices, which are based on quantum effects. Typical examples of such devices are resonant tunneling diodes [1]. In the last years the so-called quantum hydrodynamic model (QHD) has been introduced [2]. The quantum hydrodynamic model has the advantage of dealing with macroscopic fluid-type unknowns and it is able to describe quantum phenomena, such as negative differential resistance in a resonant tunneling diode [5]. Mathematically, the QHD system is a dispersive regularization of the hydrodynamic equations.

2. A QHD model for a photovoltaic cell

The starting point of our investigation is the Schrödinger equation for a QHD model which describes the electrons evolution in a semiconductor medium adding the Bohm quantum corrections. More exactly we have the following equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi - qV\psi, \quad (1)$$

where $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant, m is the electron mass, q is the elementary charge and V is the electrostatic potential. The function $\psi = \psi(\vec{r}, t)$ is called the wave function and, mathematically, is a complex function.

The solving of the Schrödinger equation in the above form concerned many mathematicians from different domains: ordinary differential equations, partial differential equations, complex analysis, operator theory, differential geometry, numerical analysis, computational geometry, etc. Different approaches to solve this variant of the Schrödinger equation have been proposed. An elegant and interesting method is based on the Madelung's transform:

$$n(\vec{r}, t) = |\Psi(\vec{r}, t)|^2 \text{ and } J(\vec{r}, t) = -\frac{\hbar q}{m} \text{Im}(\Psi^* \nabla \Psi),$$

which yield a system of two equations

$$\begin{cases} \frac{\partial n}{\partial t} = \frac{1}{q} \text{div}(\vec{J}) \\ \frac{\partial \vec{J}}{\partial t} = \frac{1}{q} \text{div} \left(\frac{\vec{J} \otimes \vec{J}}{n} \right) - \frac{q \hbar^2}{2m^2} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) + \frac{q^2}{m} n \nabla V \end{cases} \quad (2)$$

but with two unknown real functions. The function $n(\vec{r}, t)$ denotes the electron density and it is the modulus of the complex function $\Psi(\vec{r}, t)$. The function $J(\vec{r}, t)$ denotes the electron current density and it is proportional with the imaginary part of the function $\Psi^* \nabla \Psi$. The above system describes the behaviour of the electrons in a single thin layer in a photovoltaic cell, see [3, 4, 6]. It is easy to see that the second equation of (2) has some non-linear terms as for example the square root of the function $n(\vec{r}, t)$.

We remark that the Madelung's transform is based on the Wentzel-Kramers-Brillouin-Ansatz (WKB-Ansatz) expression $\psi = \sqrt{n} e^{\frac{im}{\hbar} S}$, which means that it is considered a transform $\psi \rightarrow (n, S)$ and if we denote with $\vec{J} = -qn \nabla S$ then we have the above functions (the function S is called the scaled phase of the wave function Ψ).

In the second equation of the system (2) we denote with “ $\otimes$ ” the tensor product (outer or exterior product) of two vectors which is a matrix and then, divergence of this tensor product is a vector. More exactly, if $\vec{J} = \begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix}$, then $\vec{J} \otimes \vec{J} = \begin{pmatrix} J_1 J_1 & J_1 J_2 & J_1 J_3 \\ J_2 J_1 & J_2 J_2 & J_2 J_3 \\ J_3 J_1 & J_3 J_2 & J_3 J_3 \end{pmatrix}$ and

$$\text{div}(\vec{J}) = \begin{pmatrix} \frac{\partial J_1 J_1}{\partial x} + \frac{\partial J_2 J_1}{\partial y} + \frac{\partial J_3 J_1}{\partial z} \\ \frac{\partial J_1 J_2}{\partial x} + \frac{\partial J_2 J_2}{\partial y} + \frac{\partial J_3 J_2}{\partial z} \\ \frac{\partial J_1 J_3}{\partial x} + \frac{\partial J_2 J_3}{\partial y} + \frac{\partial J_3 J_3}{\partial z} \end{pmatrix}. \quad (3)$$

3. A numerical approach

The solving of the differential system (2) was studied by many authors. Because, it is almost impossible to obtain an analytic solution for the differential system (2) (in general case), some numerical methods were proposed. Almost all methods are based on the approximation of the first, second and third derivative with some finite differences in forward, central or backward form between some up wind scheme for the derivative of the product of two functions.

In general, the numerical approaches for the QHD models are concerned with just the 1-dimensional case. In the following we will also study this case.

From (2), we have the following system in the 1-dimensional case

$$\begin{cases} \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J}{\partial x} \\ \frac{\partial J}{\partial t} = \frac{1}{q} \frac{\partial}{\partial x} \left(\frac{J^2}{n} \right) - \frac{q\hbar^2}{2m^2} n \frac{\partial}{\partial x} \left(\frac{\frac{\partial^2 \sqrt{n}}{\partial x^2}}{\sqrt{n}} \right) + \frac{q^2}{m} n \frac{\partial V}{\partial x} \end{cases} \quad (4)$$

or, after simplifying

$$\begin{cases} \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J}{\partial x} \\ \frac{\partial J}{\partial t} = \frac{2}{q} \frac{J}{n} \frac{\partial J}{\partial x} - \frac{q\hbar^2}{2m^2} \left(\frac{1}{2n^3} \left(\frac{\partial n}{\partial x} \right)^3 - \frac{1}{n^2} \frac{\partial n}{\partial x} \frac{\partial^2 n}{\partial x^2} + \frac{1}{2n} \frac{\partial^3 n}{\partial x^3} \right) - \frac{1}{q} \frac{J^2}{n^2} \frac{\partial n}{\partial x} - \frac{q^2}{m} n \frac{\partial V}{\partial x} \end{cases} \quad (5)$$

For the numerical solving of the system (5) we use the backward finite differences:

$$\begin{aligned} \frac{df_i}{dx} &= \frac{f(x_i, t_j) - f(x_{i-1}, t_j)}{x_i - x_{i-1}} \\ \frac{d^2 f_i}{dx^2} &= \frac{f(x_i, t_j) - 2f(x_{i-1}, t_j) + f(x_{i-2}, t_j)}{(x_i - x_{i-1})^2} \\ \frac{d^3 f_i}{dx^3} &= \frac{f(x_i, t_j) - 3f(x_{i-1}, t_j) + 3f(x_{i-2}, t_j) - f(x_{i-3}, t_j)}{(x_i - x_{i-1})^3} \\ \frac{df_j}{dt} &= \frac{f(x_i, t_j) - f(x_i, t_{j-1})}{t_j - t_{j-1}} \end{aligned}$$

where f is any function $n(x, t)$ or $J(x, t)$, and a point (i, j) is a node of some discrete mesh. We will consider i for spatial variable x and j for time variable t .

Replacing in the system (5) the partial derivatives with the finite differences we obtain a non-linear algebraic system

$$\begin{cases} \frac{n(i, j) - n(i, j-1)}{k} = \frac{1}{q} \frac{J(i, j) - J(i-1, j)}{h} \\ \frac{J(i, j) - J(i, j-1)}{k} = \frac{2}{q} \frac{J(i, j)}{n(i, j)} \frac{J(i, j) - J(i-1, j)}{h} - \frac{q\hbar^2}{2m^2} \left[\frac{1}{2n(i, j)^3} \left(\frac{n(i, j) - n(i-1, j)}{h} \right)^3 - \right. \\ \left. - \frac{1}{n(i, j)^2} \cdot \frac{n(i, j) - n(i-1, j)}{h} \cdot \frac{n(i, j) - 2n(i-1, j) + n(i-2, j)}{h^2} + \right. \\ \left. + \frac{1}{2n(i, j)} \cdot \frac{n(i, j) - 3n(i-1, j) + 3n(i-2, j) - n(i-3, j)}{h^3} \right] - \\ \left. - \frac{1}{q} \frac{J(i, j)^2}{n(i, j)^2} \frac{n(i, j) - n(i-1, j)}{h} - \frac{q^2}{m} n(i, j) \frac{V(i) - V(i-1)}{h} \right] \end{cases} \quad (6)$$

for $i = 4, \dots, m$ and $j = 2, \dots, n$ in a $m \times n$ discrete mesh and $h = \delta x = x_i - x_{i-1}$ and $k = \delta t = t_i - t_{i-1}$.

Starting with some initial values (borders conditions) we observe that the next values - $n(i, j)$ or $J(i, j)$ result as a solution of a non-linear system and this can be made using a Newton-Raphson iterative procedure.

If, we use an iterative scheme for the above system, it is not possible to directly obtain the next numerical value. We propose the following scheme:

$$\begin{array}{ccc} f(i-1, j-1) & \rightarrow & f(i, j-1) \\ \downarrow & & \downarrow \\ f(i, j-1) & \rightarrow & f(i, j) \end{array} \quad (7)$$

This scheme corresponds from the physical point of view to the time-stationary (the vertical case) and respectively to homogeneous states (the horizontal case).

Using this observations, we will take first the time-stationary case and we have that $\frac{\partial n}{\partial t} = \frac{\partial J}{\partial t} \equiv 0$ and then from the system (5) we have that

$$\begin{cases} 0 = \frac{1}{q} \frac{\partial J}{\partial x} \\ 0 = \frac{2}{q} \frac{J}{n} \frac{\partial J}{\partial x} - \frac{q\hbar^2}{2m^2} \left(\frac{1}{2n^3} \left(\frac{\partial n}{\partial x} \right)^3 - \frac{1}{n^2} \frac{\partial n}{\partial x} \frac{\partial^2 n}{\partial x^2} + \frac{1}{2n} \frac{\partial^3 n}{\partial x^3} \right) - \frac{1}{q} \frac{J^2}{n^2} \frac{\partial n}{\partial x} - \frac{q^2}{m} n \frac{\partial V}{\partial x} \end{cases} \quad (8)$$

and then we have that $\frac{\partial J}{\partial x} = 0$ and thus $J = \text{constant}$ in this case and the second equation can be written as follows

$$\frac{q\hbar^2}{2m^2} \left(\frac{1}{2n^2} \left(\frac{\partial n}{\partial x} \right)^3 - \frac{1}{n} \frac{\partial n}{\partial x} \frac{\partial^2 n}{\partial x^2} + \frac{1}{2} \frac{\partial^3 n}{\partial x^3} \right) + \frac{1}{q} \frac{J^2}{n} \frac{\partial n}{\partial x} + \frac{q^2}{m} n^2 \frac{\partial V}{\partial x} = 0, \quad (9)$$

which is a kind type of the Korteweg de Vries equation (non-linear and non-homogenous case). If we replace in the system (6) we obtain

$$\begin{cases} J(i-1, j) = J(i-1, j-1) \\ \frac{q\hbar^2}{2m^2} \left[\frac{1}{2n(i, j-1)^3} \left(\frac{n(i, j-1) - n(i-1, j)}{h} \right)^3 - \right. \\ \left. - \frac{1}{n(i, j-1)^2} \cdot \frac{n(i, j-1) - n(i-1, j)}{h} \cdot \frac{n(i, j-1) - 2n(i-1, j-1) + n(i-2, j-1)}{h^2} + \right. \\ \left. + \frac{1}{2n(i, j-1)} \cdot \frac{n(i, j-1) - 3n(i-1, j-1)}{h^3} + \frac{3n(i-2, j-1) - n(i-3, j-1)}{h^3} \right] + \\ \left. + \frac{1}{q} \frac{J(i-1, j-1)^2}{n(i, j-1)^2} \frac{n(i, j-1) - n(i-1, j-1)}{h} + \frac{q^2}{m} n(i, j-1)^2 \frac{V(i) - V(i-1)}{h} = 0 \right. \end{cases} \quad (10)$$

and we can compute the next value of the function $n(i, j-1)$.

Using the values computed from the system (10) we consider the homogeneous case, and we have that $\frac{\partial n}{\partial x} = \frac{\partial^2 n}{\partial x^2} = \frac{\partial^3 n}{\partial x^3} = \frac{\partial J}{\partial x} \equiv 0$ and then $n = \text{constant}$ and we obtain

$$\begin{cases} n(i-1, j) = n(i-1, j-1) \\ J(i-1, j) = J(i-1, j-1) \end{cases} \quad (11)$$

and then J is a constant function.

Now, we can compute the values $n(i, j)$ and $J(i, j)$ using the system (6).

A computational result was obtained using a mathematical software (Mathematica) with the values $q = 1.6 \cdot 10^{-19} [C]$, $\hbar = 6.6025/2 \pi [J \cdot s]$, $m = 9.1 \cdot 10^{-31} [kg]$ and $i = 1, \dots, 200$, $j = 1, \dots, 200$ with the electronic potential $V(x) = x^3/3$. The below graphs correspond to the unknowns function $n(x, t)$ (Fig. 1).

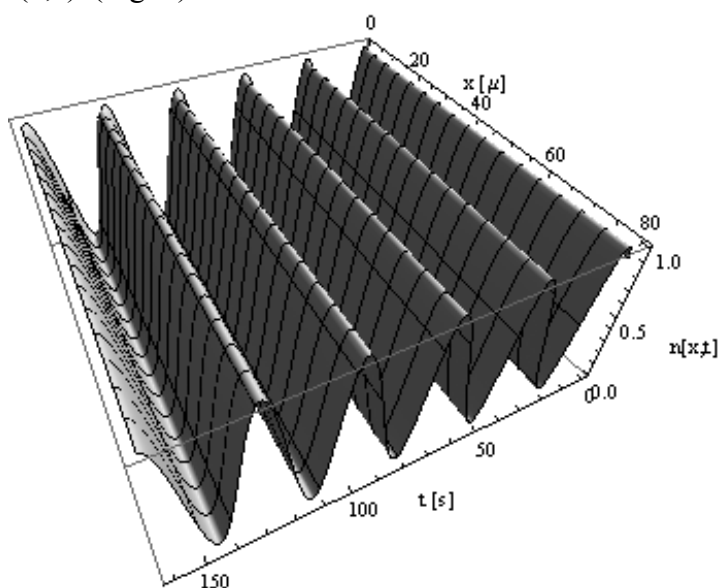


Fig. 1. Electron density.

The obtained results are comparable with the other reported results.

4. Some analytical results

The above results suggest us to study the generalized Kortweg de Vries equations in the 3-dimensional case for our investigation on some models for QHD in 3-dimensional way. In this equation x is direction of propagation while y and z are the transverse variables.

We remark, that in our case, if we use similar scheme as (7) we can obtain some similar equation if we consider a stationary case.

In 1997, Bouard and Saut [7] obtained the three-dimensional generalization of the KdV equation which can be written as the form

$$[u_t + f(u)u_x + u_{xxx}]_x + u_{yy} + u_{zz} = 0 \quad (12)$$

Some numerical results in 2 or 3 dimension can be obtained using a similar scheme as in (7), but there are not interesting for a graphical representations.

An analytical solution for the equation (12) was obtained by the authors using a results of Chen and Wen [8], where the authors look for the real-valued traveling wave solution of the form $U(s) = u(x, y, z, t)$ with $s = ax + by + cz - vt$ where a, b, c are some real constants (v is the velocity).

Without loss the generality we can suppose that all constants equal one and we consider for our case two real functions $U(s)=n(x, y, z, t)$ and $W(s)=J(x, y, z, t)$ with $s=x+y+z-vt$. We replace with this new functions in the system (2) and we have the following system

$$\begin{cases} -vU' = \frac{3}{q}W' \\ -vW' = \frac{3}{q}\left(\frac{2WW'U - W^2U'}{U^2}\right) - \frac{q\hbar^2}{2m^2}\left(-\frac{9}{2}\frac{(U')^2}{U^2} + \frac{27}{4}\frac{U''}{U} - \frac{9}{2}U'''\right) + \frac{q^2}{m}v s U \end{cases} \quad (13)$$

From the first equation we have that $W=-qvU+K$ and we suppose that $K=0$. With this relation we have, in the second equation, the following

$$\frac{q}{3}vU' = 2qU' - 3q\frac{U'}{U^2} - \frac{q\hbar^2}{2m^2}\left(-\frac{9}{2}\frac{(U')^2}{U^2} + \frac{27}{4}\frac{U''}{U} - \frac{9}{2}U'''\right) + \frac{q^2}{m}sU \quad (14)$$

or equivalent (multiplying with U^2/q and suppose that $v=1$)

$$-\frac{5}{3}U'U^2 + 3U' + \frac{\hbar^2}{2m^2}\left(-\frac{9}{2}(U')^2 + \frac{27}{4}UU'' - \frac{9}{2}U^2U'''\right) - \frac{q}{m}sU^3 = 0 \quad (15)$$

Using some similar results [6] we take the initial values

$$U(0) = \frac{q}{\cosh^2(0)} = q, U'(0) = \left(\frac{q}{\cosh^2(0)}\right)' = 0, U''(0) = \left(\frac{q}{\cosh^2(0)}\right)'' = -2q \quad (16)$$

Now, we search a solution by the form

$$-c_1 + \frac{c_2}{\cosh^2\left(\frac{s}{c_3}\right)} \quad (17)$$

and from the initial values we obtain

$$c_1 = q(-1 + c_3^2), \quad c_2 = qc_3^2 \quad (18)$$

and from the equation (15) we find the best value form the constant $c_3=100$. With this values we have

$$U(s) = -(10^4 - 1)q + \frac{10^4 q}{\cosh^2\left(\frac{s}{100}\right)}, \quad (19)$$

which equals the numerical solutions of the equation (15), see the bellow graph

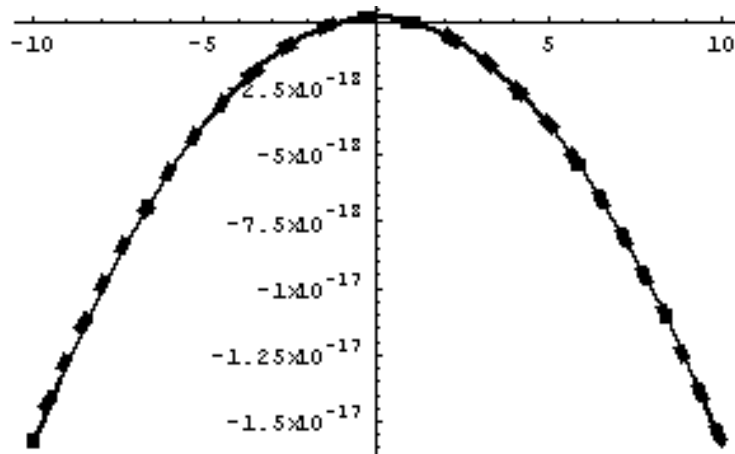


Fig. 2. The graphs of the both solutions.

where the dashed line is the function (19) and the continuous line is the numerical solution of the equation (15).

Therefore, some analytical solutions for our system can be

$$n(x, y, z, t) = U(s) = -(10^4 - 1)q + \frac{10^4 q}{\cosh^2\left(\frac{x + y + z - vt}{100}\right)} \quad (20)$$

and respectively

$$J(x, y, z, t) = -\frac{q}{3}U(s) = \frac{(10^4 - 1)q^2}{3} - \frac{10^4 q^2}{3 \cosh^2\left(\frac{x + y + z - vt}{100}\right)}. \quad (21)$$

Of course, these solutions are in some restrictive hypothesis about the considered constants, but the more generalizations are open.

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