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AN ANALYSIS OF QUANTUM CORRECTION OF THE ONE-DIMENSIONAL AND STATIONARY HYDRODYNAMIC MODELS FOR SEMICONDUCTORS

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Abstract
The one-dimensional and stationary case of the HD-model and the QHD-model for semiconductors with constant temperature are mathematically and numerically studied. The Quantum Hydrodynamic Model (QHD) shows a remarkable potential to describe the nanostructured devices, as well as quantum solar cells. By simulating a semiconductor device it is shown that the quantum Bohm potential (the quantum correction) changes significantly the behavior of the solutions.
Keywords: *quantum hydrodynamics; ballistic transport, differential equations*

1. Introduction

In this paper we study the ballistic transport of the carriers in symmetrical n^+-n-n^+ devices. At work temperature it is assumed that the impurity atoms are completely ionized, which means that in the Poisson equation the doping concentration C is added to the electron distribution. This kind of doping creates an internal electrical field, which eliminates the electrons from the central place (middle) of the device. The ***QHD***-model consists of the conservation laws of mass moment for the particle density n, the particle current density $\vec{J}$ and the Poisson's equation for the electric potential V (see [5]). Neglecting the quantum term on obtain the ***HD***-model. *We study the 1-dimensional and stationary case.* In the both models the current density J is a constant. In our situation the ***QHD***-model and the ***HD***-model have the form:

$$(1)\qquad (a)\begin{cases} -\dfrac{J^2}{n}\dfrac{d}{dx}(\dfrac{1}{n})+\dfrac{dV}{dx}+\dfrac{\varepsilon^2}{2}\dfrac{d}{dx}\left(\dfrac{\frac{d^2\sqrt{n}}{dx^2}}{\sqrt{n}}\right)=0 \\ \lambda^2\dfrac{d^2V}{dx^2}=n-C \end{cases}\qquad (b)\begin{cases} -\dfrac{J^2}{n}\dfrac{d}{dx}(\dfrac{1}{n})+\dfrac{dV}{dx}=0 \\ \lambda^2\dfrac{d^2V}{dx^2}=n-C, \end{cases}$$

Here C denote the doping profile of the semiconductor, ε and λ denote the scaled Planck constant and the scaled Debye length and x is in *[0,L]* with L the device diameter . The quantum term, the so-called Bohm potential, is $\dfrac{\varepsilon^2}{2}\dfrac{\Delta_x\sqrt{n}}{\sqrt{n}}$.

The total charge C-n vanishes at the boundary:

(2) $$n(0) = C(0),\ \ n(L) = C(L).$$

The main objectives of this paper are: to present the mathematical method used, to design for some particular cases the particle density *n* and the electric potential *V*, to underline that the quantum aspects are suggestive.

2. The study of HD-Model

The form of the electric potential *V* is the consequence of the first equation of problem (1.b). Using the second equation we obtain the equation of particle density *n.*

(3) $$V = \frac{J^2}{2n^2} + q,\quad \frac{d^2 n}{dx^2} - \frac{3}{n}\left(\frac{dn}{dx}\right)^2 + \frac{1}{\lambda^2 J^2} n^3 (n - C) = 0$$

where *q* is a real constant. To find the particle density must solve the boundary-value problem of second-order differential equation $(3)_2$ and boundary conditions (2).

For the numerical study we consider the scaled parameters $L = 1,\ \lambda = 0.1$ and the doping profile $C(x) = 1 - x(1 - x),\quad x \in [0,1]$. To solve the boundary value problem $(3)_2$+(2) we use the software package MAPLE 9.5. We consider the Cauchy problem with the differential equation $(3)_2$ and initial conditions $n(0) = C(0),\ \frac{dn}{dx}(0) = n_0$. The parameter n_0 is obtained using the boundary conditions *n(1)=C(1).* We find a numerical solution of the Cauchy problem using a Fehlberg fourth-fifth order Runge-Kutta method with degree four interpolant.

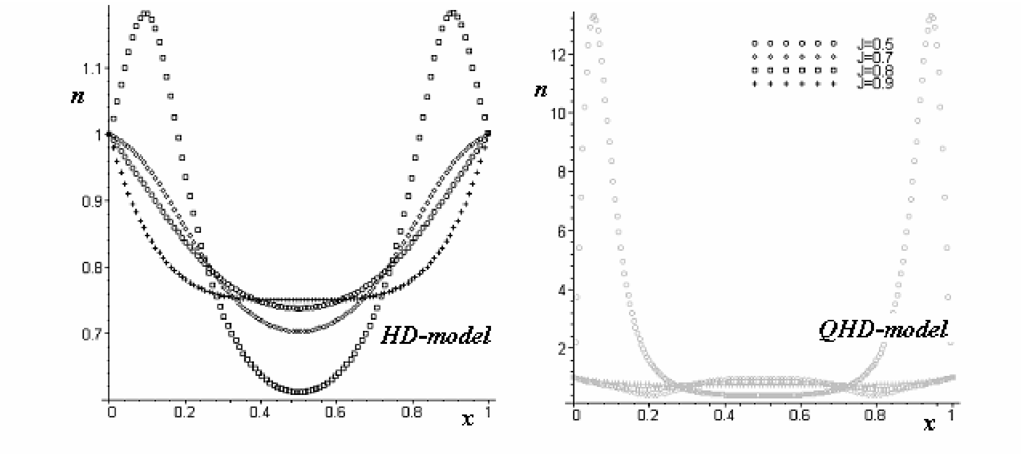

Figure 1: the particle density *n*

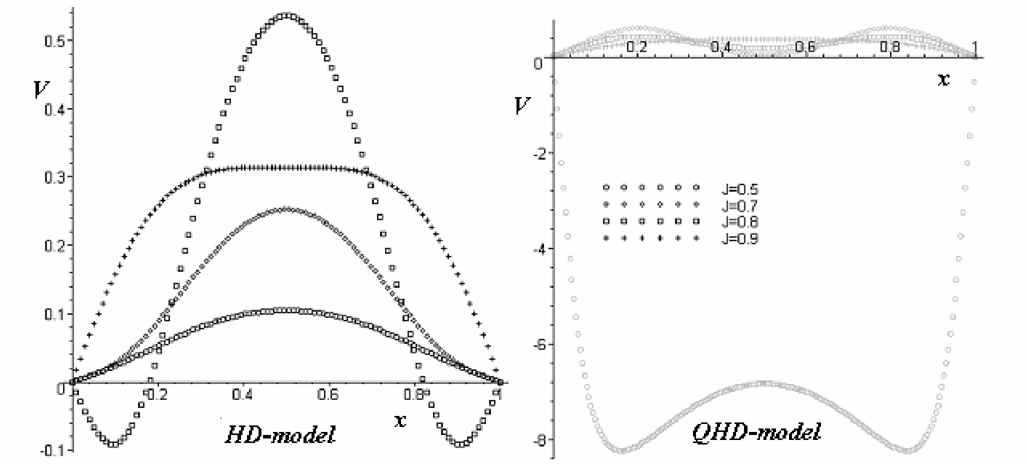

Figure 2: the electric potential V

3. The study of QHD-Model

The first equation of problem (1.a) implies:

(4) $$V = \frac{J^2}{2n^2} - \frac{\varepsilon^2}{2\sqrt{n}} \frac{d^2\sqrt{n}}{dx^2} + q$$

where q is a real constant. Using the change of variables $w = \sqrt{n}$ and the expression of V we obtain the forth-order differential equation:

(5) $$\varepsilon^2 w^5 \frac{d^4 w}{dx^4} - 2\varepsilon^2 w^4 \frac{dw}{dx}\frac{d^3 w}{dx^3} - \varepsilon^2 w^4 (\frac{d^2 w}{dx^2})^2 + 2\varepsilon^2 w^3 (\frac{dw}{dx})^2 \frac{d^2 w}{dx^2} + 4J^2 w \frac{d^2 w}{dx^2} - 20J^2 (\frac{dw}{dx})^2 + \frac{2}{\lambda^2} w^6 (w^2 - C) = 0$$

In this paper we study the symmetric solutions of this equation; the solutions which verifies the relation $w(x) = w(L-x)$ for all $x \in [0, L]$. In this situation it is sufficient to study the function w on the interval $[L/2, L]$. We use the symmetry of the function w and supplementary we consider that the second-derivative of particle density n has the same value on $L/2$ in the classical ***HD***-model and in the ***QHD***-model. We obtain:

(6) $$w(\frac{L}{2}) = w_0,\ \frac{dw}{dx}(\frac{L}{2}) = 0,\ \frac{d^2 w}{dx^2}(\frac{L}{2}) = \frac{1}{2w_0}\frac{d^2 C}{dx^2}(\frac{L}{2}),\ \frac{d^3 w}{dx^3}(\frac{L}{2}) = 0.$$

The main mathematical problem is to find the solutions w of the Cauchy problem (5)-(6) having the properties: w is defined on the interval $[L/2, L]$ and $w(L) = \sqrt{C(L)}$ (the total charge C-n vanishes at the boundary).

Our method of investigation is: to determine (numerically) a solution w of the **main mathematical problem,** to find (numerically) the particle density n and to find (numerically) the electric potential V using (4).

We consider the scaled parameters $L = 1$, $\varepsilon = 0.114$, $\lambda = 0.1$ and the doping profile $C(x) = 1 - x(1 - x), \quad x \in [0,1]$.

To solve **the main mathematical problem** we use the software package MAPLE 9.5. For the electric potential *V* we consider the boundary conditions *V(0)=V(1)=0.*

4. Conclusions

The employed theory is applicable to un-polarized devices, when internal transport of carriers is present due to structure inhomogeneity.

The numerical study implemented in MAPLE interpreter (see figures) points out a significant difference between classical and quantum aspects at low currents. For high particle currents the system goes beyond physical limit. This limit of the applicability of the ***QHD*** model is about 10 mA/μm^2.

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References

1. Dong J., Electronic Journal of Diff. Eq., Vol 2005, No. 123, pp. 1-8, (2005)
2. Dreher M., Konstanzer Schriften in Mathematik ind Informatik, Nr. 215, Mai (2006).
3. Gamba I.M., Jüngel A., Arch. Ration. Mech. Anal., 156 , pp. 183-203, (2001)
4. Jüngel A., Milišić J-P., Bull. Inst. Math., Acad. Sinica (New Series), Vol. 2, No. 2, pp. 251-279, (2007)
5. Jüngel A., Tang S., Appl. Num. Math., vol. 56, Issue 7 (July), pp. 899-915, (2006)
6. Jüngel A., Mariani M. C., Rial D., Konst. Math. und Inf., Nr. 145, Mai (2001).
7. Tulcan-Paulescu E., Comănescu D., On the quantum correction in the hydrodynamic models for electronic transport in nanoscale semiconductor devices, to appear.