NUMERICAL STUDY OF QUANTUM HYDRODYNAMIC MODEL FOR SEMICONDUCTORS

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(Received 26 November 2007)

Abstract

This paper presents a numerical study of the one-dimensional quantum hydrodynamic equations, introducing the quantum hydrodynamic model (QHD) for semiconductors. In the case of QHD, numerical solution of the Schrödinger equation must present higher oscillations as the scaled Planck constant ε becomes smaller ($\varepsilon \sim 10^{-3} \div 10^{-2}$). The numerical studies for general case and for particular isothermal, stationary case are given. Finally, we present different graphical solutions for particle and current densities, in both cases and for different values of ε. Graphical representations allow observing an increasing amplitude of solution oscillations of particle and current densities as ε becomes smaller. For the stationary case one can see that current density remains constant irrespective of ε choice.

1. Introduction

The hydrodynamic model describes propagation of electrons in a semiconductor, the QHD model being a dispersive regularization of hydrodynamic model. This regularization depends on choice of scaled Planck constant ε that gives us some hints about selection of reliable numerical schemes. We derive the QHD equation model starting from the Schrödinger equation via Madelung's transformation. Numerical approach uses the Crank–Nicholson scheme for spatial discretization with a very small time step δt to advance in time, for different values of ε. The nonlinear discrete problem is solved using the Newton–Raphson algorithm, the initial solution for (n+1)-th time step being considered the final solution at n-th time step [1].

2. Derivation of QHD equations

We obtain the one-dimensional QHD equations starting from the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi - qV\psi \tag{1}$$

with the initial condition

$$\psi(x, t=0) = \psi_I(x). \tag{2}$$

Using Madelung's transformation

$$\psi(x,t) = \sqrt{n(x,t)} \cdot e^{-\frac{i}{\hbar} m S(x,t)} \tag{3}$$

and separating the real and imaginary parts in the Schrödinger equation, we obtain two equations in variables (*n,S*)

$$\begin{cases} \dfrac{\partial n}{\partial t} = -div(n \cdot \nabla S) \\ \dfrac{\partial S}{\partial t} = \dfrac{\hbar^2}{2m^2} \dfrac{\Delta\sqrt{n}}{\sqrt{n}} - \dfrac{1}{2}\left|\nabla S\right|^2 + \dfrac{q}{m}V \end{cases}. \tag{4}$$

In the above equations *n(x,t)* is the particle density and *S(x,t)* is the phase of wave function. We define particles density

$$n(x,t) = \left|\psi(x,t)\right|^2 \tag{5}$$

and current density

$$J(x,t) = -\frac{\hbar q}{m}\operatorname{Im}(\overline{\psi}(x,t)\nabla\psi(x,t)\,. \tag{6}$$

Using eq. (3) we obtain for current density

$$J(x,t) = -qn(x,t)\nabla S(x,t)\,. \tag{7}$$

System (4) can be transformed from variables (*n,S*) to (*n,J*). Using eq. (7) we obtain [2, 3]

$$\begin{cases} \dfrac{\partial n}{\partial t} = \dfrac{1}{q}\dfrac{\partial J}{\partial x} \\ \dfrac{\partial J}{\partial t} - \dfrac{1}{q}\dfrac{\partial}{\partial x}\left(\dfrac{J^2}{n} + n\right) + \dfrac{\hbar^2 q}{2m^2} n\nabla\left(\dfrac{\Delta\sqrt{n}}{\sqrt{n}}\right) + \dfrac{q}{m} n\nabla V = 0 \end{cases}. \tag{8}$$

3. Numerical approach

In order to solve numerically system (8) we use the Crank–Nicholson spatial discretization scheme with central finite differences [4, 5, 6], where

$$\begin{cases} \dfrac{\partial n}{\partial t} = \dfrac{n_i^{j+1} - n_i^j}{\delta t} \\ \dfrac{\partial n}{\partial x} = \dfrac{n_{i+1}^{j+1} - n_{i-1}^{j+1} + n_{i+1}^j - n_{i-1}^j}{4h} \\ \dfrac{\partial^2 n}{\partial x^2} = \dfrac{n_{i+1}^{j+1} - 2n_i^{j+1} + n_{i-1}^{j+1} + n_{i+1}^j - 2n_i^j + n_{i-1}^j}{2h^2} \\ \dfrac{\partial^3 n}{\partial x^3} = \dfrac{n_{i+2}^{j+1} - 2n_{i+1}^{j+1} + 2n_{i-1}^{j+1} - n_{i-2}^{j+1} + n_{i+2}^j - 2n_{i+1}^j + 2n_{i-1}^j - n_{i-2}^j}{4h^3} \end{cases}, \tag{9}$$

where $i = 3...M-2,\ j = 0...N-1,\ h = x_{i+1} - x_i$.

The same discretization scheme is valuable for current density.

We solve system (8) for spatial interval S = [0, 1] and temporal interval T = [0, 1]. Using (9) system (8) can be rewritten

$$\begin{cases} \dfrac{n_i^{j+1}-n_i^j}{\delta t} = \dfrac{J_{i+1}^{j+1}-J_{i-1}^{j+1}+J_{i+1}^{j}-J_{i-1}^{j}}{4h} \\ \dfrac{J_i^{j+1}-J_i^j}{\delta t} - 2\dfrac{J_i^j}{n_i^j}\dfrac{J_{i+1}^{j+1}-J_{i-1}^{j+1}+J_{i+1}^{j}-J_{i-1}^{j}}{4h} + \left(\dfrac{J_i^j}{n_i^j}\right)^2 \dfrac{n_{i+1}^{j+1}-n_{i-1}^{j+1}+n_{i+1}^{j}-n_{i-1}^{j}}{4h} - \\ -\dfrac{n_{i+1}^{j+1}-n_{i-1}^{j+1}+n_{i+1}^{j}-n_{i-1}^{j}}{4h} + \dfrac{1}{4}\varepsilon^2\left(\dfrac{n_{i+1}^{j+1}-n_{i-1}^{j+1}+n_{i+1}^{j}-n_{i-1}^{j}}{4h}\right)^3 - \\ -\dfrac{1}{2}\varepsilon^2\dfrac{1}{n_i^j}\dfrac{n_{i+1}^{j+1}-n_{i-1}^{j+1}+n_{i+1}^{j}-n_{i-1}^{j}}{4h}\dfrac{n_{i+1}^{j+1}-2n_i^{j+1}+n_{i-1}^{j+1}+n_{i+1}^{j}-2n_i^{j}+n_{i-1}^{j}}{2h^2} + \\ \dfrac{1}{4}\varepsilon^2\dfrac{n_{i+2}^{j+1}-2n_{i+1}^{j+1}+2n_{i-1}^{j+1}-n_{i-2}^{j+1}+n_{i+2}^{j}-2n_{i+1}^{j}+2n_{i-1}^{j}-n_{i-2}^{j}}{4h^3} + n_i^j\dfrac{V_{i+1}^{j+1}-V_{i-1}^{j+1}+V_{i+1}^{j}-V_{i-1}^{j}}{4h} = 0 \end{cases}, \quad (10)$$

where $i = 3...M-2,\ j = 0...N-1,\ h = x_{i+1} - x_i$.

In eq. (10) we have $\varepsilon \sim 10^{-3} \div 10^{-2}$ and we choose $V(x) = \frac{1}{2}x^2$.

In numerical tests we considered two situations, the general case and the isothermal stationary one. In the stationary case

$$\frac{\partial n}{\partial t} = 0 \Rightarrow \frac{\partial J}{\partial x} = 0. \quad (11)$$

In this situation J remains constant in space and time.

4. Numerical results

Bellow, we present some graphical results for n and J for different values of ε in non-stationary and stationary cases.

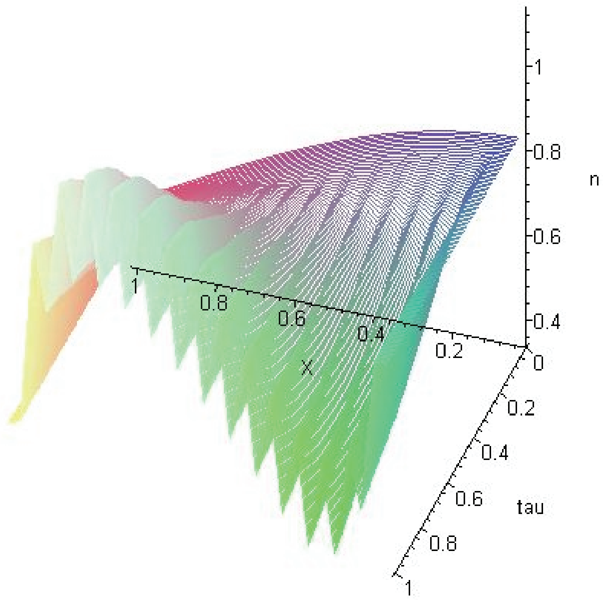

Figure 1. Particle density for ε = 0.00095 at t = 1 s – nonstationary case.

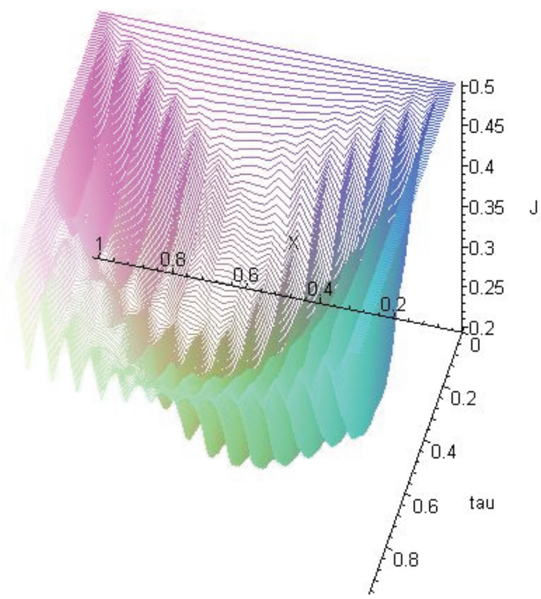

Figure 2. Current density for ε = 0.00095 at t = 1 s – nonstationary case.

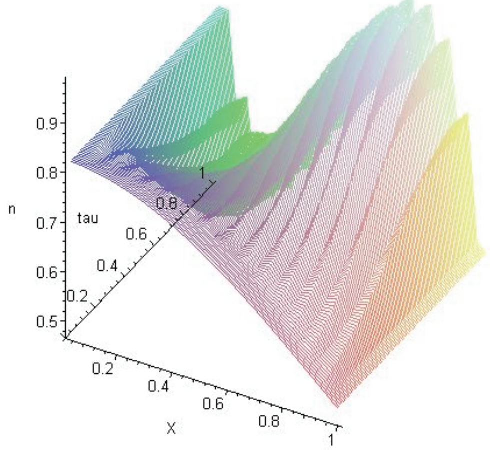

Figure 3. Particle density for ε = 0.0015 at t = 1 s – nonstationary case.

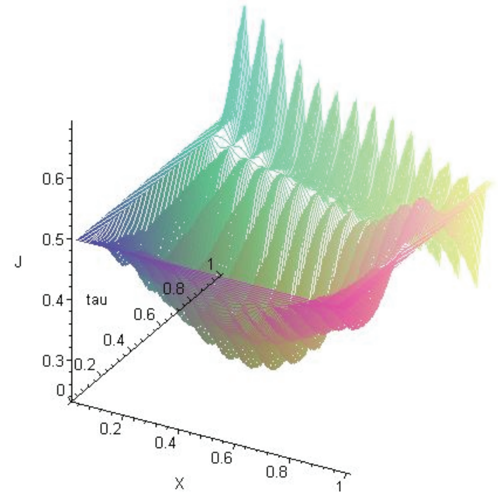

Figure 4. Current density for ε = 0.0015 at t = 1 s – nonstationary case.

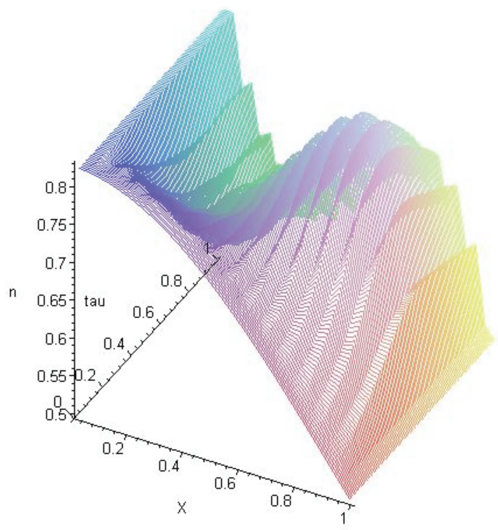

Figure 5. Particle density for ε = 0.0026 at t = 1 s – nonstationary case.

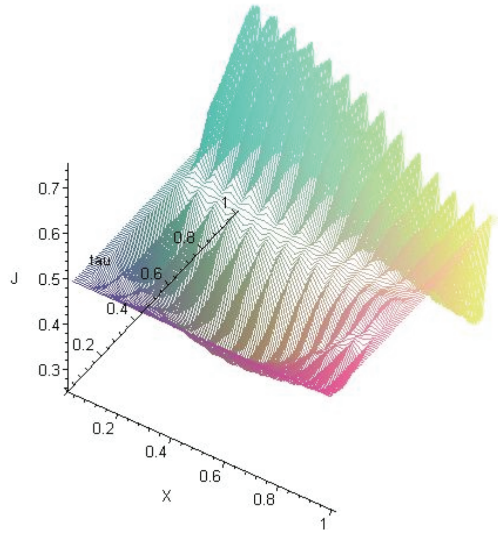

Figure 6. Current density for ε = 0.0026 at t = 1 s – nonstationary case.

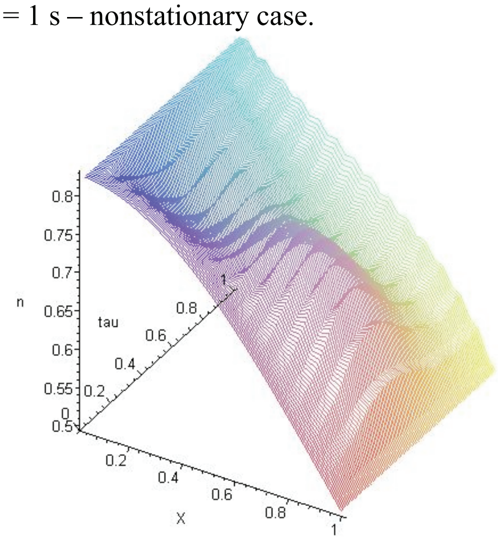

Figure 7. Particle density for ε = 0.0045 at t = 1 s – nonstationary case.

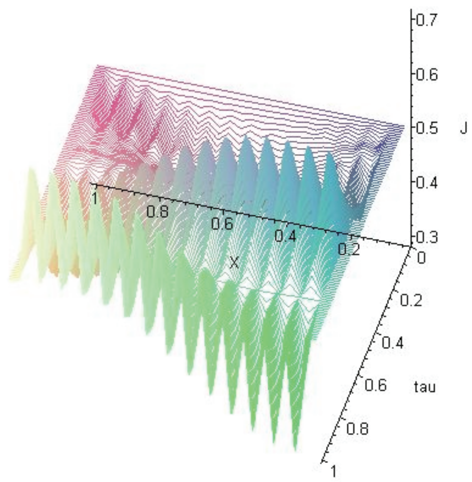

Figure 8. Current density for ε = 0.0045 at t = 1 s – nonstationary case.

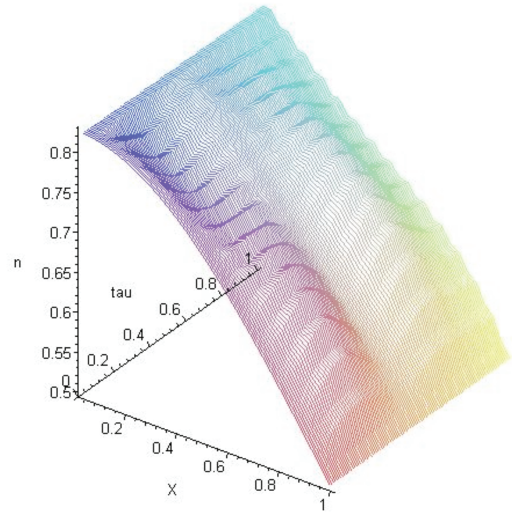

Figure 9. Particle density for ε = 0.008 at t = 1 s – nonstationary case.

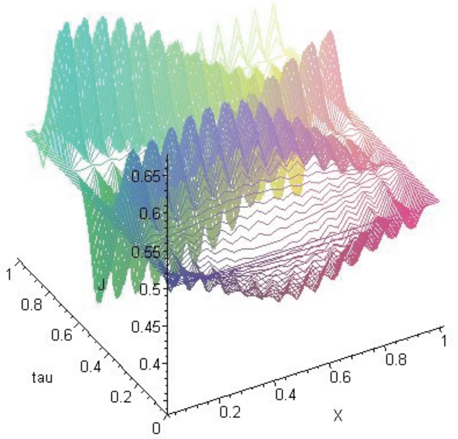

Figure 10. Current density for ε = 0.008 at t = 1 s – nonstationary case.

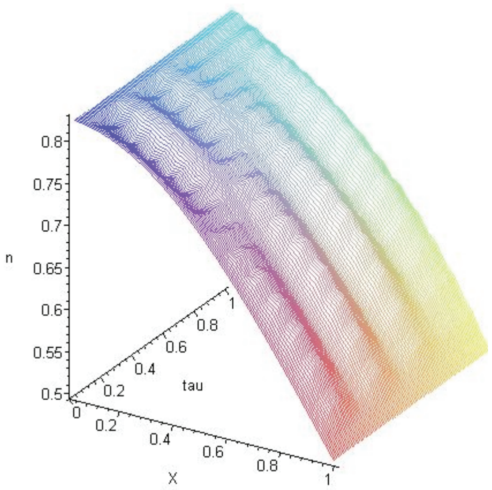

Figure 11. Particle density for ε = 0.015 at t = 1 s – nonstationary case.

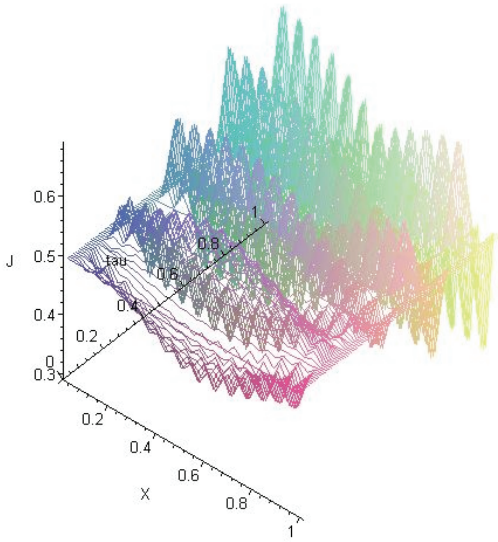

Figure 12. Current density for ε = 0.015 at t = 1 s – nonstationary case.

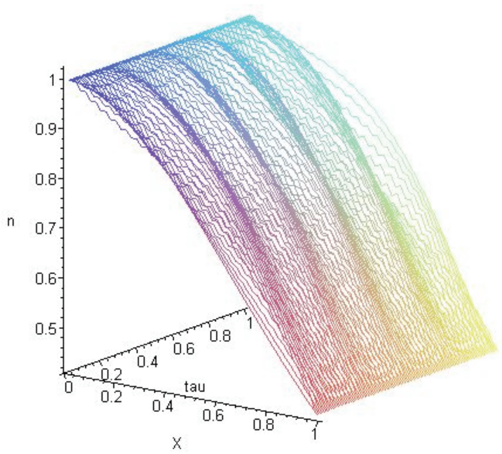

Figure 13. Particle density for ε = 0.0026 at t = 1 s – stationary case.

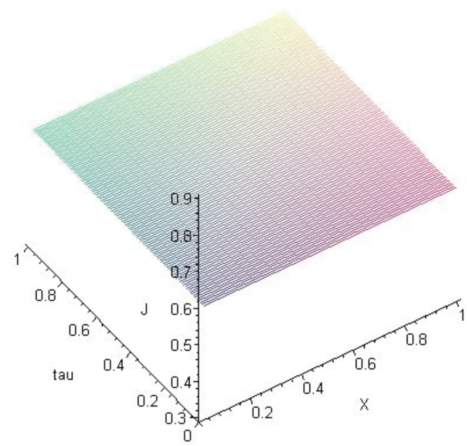

Figure 14. Current density for ε = 0.0026 at t = 1 s. – stationary case.

5. Conclusions

In order to solve numerically system (8) we use the Crank–Nicholson spatial discretization scheme with central finite differences and a very small step δt to advance in time, for different values of ε. The resulted nonlinear discrete problem is solved using the Newton–Raphson algorithm, the initial solution for (n+1)-th time step being considered the final solution at n-th time step. Finally, we present different graphical solutions for particle and current densities, in both cases and for different values of ε. As ε becomes smaller, increasing amplitude of solution oscillations of particles and current densities can be observed. We worked with the potential $V(x) = \frac{1}{2}x^2$. The initial conditions for particle density were obtained solving numerically system (8) at t = 0, or choosing $n(x,0) = \frac{1}{ch^2 x}$. The initial values for J can be chosen between 0.4 and 0.6.

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