NUMERICAL STUDY OF TWO DIMENSIONAL QUANTUM HYDRODINAMIC MODEL FOR SEMICONDUCTORS

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1. Introduction

This paper presents a numerical study of the two dimensional quantum hydrodynamic equations, introducing the quantum hydrodynamic model (QHD) for semiconductors. We derive the QHD equations model starting from Schrödinger equation via Madelung's transformation. Numerical approach uses a Crank – Nicholson spatial discretization scheme with central finite differences and a very small step δt to advance in time, for different values of ε. In the case of QHD, the numerical solution of Schrödinger equation must present higher oscillations, as the scaled Planck constant ε becomes smaller ($\varepsilon \sim 10^{-3} \div 10^{-2}$). The resulted non – linear discrete problem is solved using a Newton – Raphson algorithm, the initial solution for (n+1)-th time step being considered the final solution at n-th time step.

2. Derivation of QHD equations

We obtain the two dimensional QHD equations starting from Schrödinger equation

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

with the initial condition

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

Scaling the equations (1) - (2) by introducing reference values for the time, length and potential

$$t = \tau \cdot t_S, \qquad x = L \cdot x_S, \qquad V = U \cdot V_S \tag{3}$$

and assuming that the kinetic energy is of the same order as the electric energy

$$m\left(\frac{L}{\tau}\right)^2 = qU \tag{4}$$

the Schrödinger equation becomes

$$i\varepsilon \frac{\partial \psi(x,y,t)}{\partial t} = -\frac{\varepsilon^2}{2}\Delta \psi(x,y,t) - V\psi(x,y,t) \tag{5}$$

where the scaled Planck constant is

$$\varepsilon = \frac{\hbar \tau}{mL^2} \tag{6}$$

Using Madelung's transformation

$$\psi(x,y,t) = \sqrt{n(x,y,t)} \cdot e^{-\frac{i}{\varepsilon}S(x,y,t)} \tag{7}$$

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

$$
\begin{cases}
\dfrac{\partial n(x,y,t)}{\partial t} = -div\left(n \cdot \nabla S(x,y,t)\right) \\
\dfrac{\partial S(x,y,t)}{\partial t} = \dfrac{\varepsilon^2}{2} \dfrac{\Delta\sqrt{n(x,y,t)}}{\sqrt{n(x,y,t)}} - \dfrac{1}{2}\left|\nabla S(x,y,t)\right|^2 + V(x,y)
\end{cases}
\tag{8}
$$

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

$$
n(x,y,t) = \left|\psi(x,y,t)\right|^2 \tag{9}
$$

and current density

$$
J(x,y,t) = -\varepsilon\,\mathrm{Im}\left(\overline{\psi}(x,y,t)\nabla\psi(x,y,t)\right) \tag{10}
$$

Using eq. (7) we obtain for current density

$$
J(x,y,t) = -n(x,y,t)\nabla S(x,y,t) \tag{11}
$$

Transforming system (8) from variables (n,S) to (n,J) and using eq. (11) we obtain

$$
\begin{cases}
\dfrac{\partial n}{\partial t} - \nabla \cdot \vec{J} = 0 \\
\dfrac{\partial \vec{J}}{\partial t} - \nabla \cdot \left(\dfrac{\vec{J} \otimes \vec{J}}{n}\right) + \dfrac{\varepsilon^2}{2} n \nabla\left(\dfrac{\Delta\sqrt{n}}{\sqrt{n}}\right) + n\nabla V = 0
\end{cases}
\tag{12}
$$

3. Numerical approach

In order to solve numerically the system (12) we use a Crank – Nicholson spatial discretization scheme with central finite differences where

$$
\begin{cases}
\dfrac{\partial n}{\partial t} = \dfrac{n_{i,j}^{k+1} - n_{i,j}^{k}}{\delta t} \\
\dfrac{\partial n}{\partial x} = \dfrac{n_{i+1,j}^{k+1} - n_{i-1,j}^{k+1} + n_{i+1,j}^{k} - n_{i-1,j}^{k}}{4h_1} \\
\dfrac{\partial^2 n}{\partial x^2} = \dfrac{n_{i+1,j}^{k+1} - 2n_{i,j}^{k+1} + n_{i-1,j}^{k+1} + n_{i+1,j}^{k} - 2n_{i,j}^{k} + n_{i-1,j}^{k}}{2{h_1}^2} \\
\dfrac{\partial^3 n}{\partial x^3} = \dfrac{n_{i+2,j}^{k+1} - 2n_{i+1,j}^{k+1} + 2n_{i-1,j}^{k+1} - n_{i-2,j}^{k+1} + n_{i+2,j}^{k} - 2n_{i+1,j}^{k} + 2n_{i-1,j}^{k} - n_{i-2,j}^{k}}{4{h_1}^3} \\
\dfrac{\partial n}{\partial y} = \dfrac{n_{i,j+1}^{k+1} - n_{i,j-1}^{k+1} + n_{i,j+1}^{k} - n_{i,j-1}^{k}}{4h_2} \\
\dfrac{\partial^2 n}{\partial y^2} = \dfrac{n_{i,j+1}^{k+1} - 2n_{i,j}^{k+1} + n_{i,j-1}^{k+1} + n_{i,j+1}^{k} - 2n_{i,j}^{k} + n_{i,j-1}^{k}}{2{h_2}^2} \\
\dfrac{\partial^3 n}{\partial y^3} = \dfrac{n_{i,j+2}^{k+1} - 2n_{i,j+1}^{k+1} + 2n_{i,j-1}^{k+1} - n_{i,j-2}^{k+1} + n_{i,j+2}^{k} - 2n_{i,j+1}^{k} + 2n_{i,j-1}^{k} - n_{i,j-2}^{k}}{4{h_2}^3}
\end{cases}
\tag{13}
$$

with $i = 3\ldots,M-2,\ j = 3,\ldots,N\text{-}2,\ k = 0,\ldots,T\text{-}1,\ h_1 = x_{i+1} - x_i,\ h_2 = y_{i+1} - y_i,\ \delta t = t_{k+1} - t_k$.
The same scheme is valuable for current density.

References

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