Derivation and Numerical Approximation of the Quantum Drift Diffusion Model for Semiconductors

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Abstract

This paper is concerned with the study of the quantum drift diffusion equation for semiconductors. Derivation of the mathematical model, which describes the electron flow through a semiconductor device due to the application of a voltage, is considered and studied in numerical point of view by using some methods.

Introduction

Nowadays, semiconductors are contained in almost all electronic devices. The modern computer and telecommunication industry relies heavily on the use and development of semiconductor devices.

Usually, a semiconductor device can be considered as a device, which needs an input (an electronic signal or light) and produces an output (light or an electronic signal). The device is connected to the outside world by contacts at which a voltage (potential difference) is applied. We are mainly interested in devices, which produce an electronic signal, for instance, the macroscopically measurable electric current (electron flow), generated by the applied bias. In this situation, the input parameter is the applied voltage and the output parameter is the electric current through one contact. Our subject of study is to derive mathematical models, which describe the electron flow through a semiconductor device due to the application of a voltage. Furthermore, the numerical approximations of the model are studied for various types.
Classes of Model For Semiconductors

Generally we can divide semiconductor models into two classes: classical models and quantum models. Moreover we can distinguish microscopic view and macroscopic view. Then we get classical microscopic models, quantum microscopic models, classical macroscopic models and quantum macroscopic models.

Classical microscopic models are modeling for an ensemble of electrons, for instance, for the electrons of mass \( m \) and elementary charge \( q \) without quantum term. They are kinetic models. (Example: Boltzman equation)

Quantum microscopic models are considering for an ensemble of electrons and it is also for electrons of mass \( m \) and elementary charge \( q \) with quantum term. (Example: Schrödinger equation and Wigner equations).

Classical macroscopic models are modeling for system view of electrons, for instance, for the evolution of the particle density \( n \) and the current density \( J \) without quantum term. (Example: Energy Transport equation and Drift Diffusion equation).

Quantum macroscopic models are considering for system view of electrons, for instance, for the evolution of the particle density \( n \) and the current density \( J \) with quantum term. (Example: Quantum Hydrodynamic equation and Quantum Drift Diffusion equation).

We choose to study the Quantum Drift Diffusion equation. The transient quantum drift diffusion model can be derived as a zero-relaxation-time limit in the rescaled Quantum Hydrodynamic model.
Mathematical Modeling

First, we consider the single particle Schrödinger equation in $\mathbb{R}^d$ ($d \geq 1$):

$$i\varepsilon \frac{\partial \Psi}{\partial t} = -\frac{\varepsilon^2}{2} \Delta \Psi - V\Psi, \quad x \in \mathbb{R}^d, \; t > 0$$  \hspace{1cm} (1)

with initial condition:

$$\Psi(x,0) = \Psi_0, \quad x \in \mathbb{R}^d$$

where $\varepsilon > 0$ denotes the scaled Planck constant, $\Psi$ is the wave function, $V$ is the electrostatic potential described by Poisson equation:

$$\lambda^2 \Delta V = n - C$$

where $\lambda > 0$ is scaled Debye length, $C=C(x)$ is the doping profile and $n$ is the particle density which is defined by

$$n(x,t) = |\Psi'(x,t)|^2$$

Then we assume that the scaled phase $S$ of the wave function and the current density $J$ are

$$\Psi(x,t) = \sqrt{n(x,t)} \exp(iS(x,t)/\varepsilon), \quad J(x,t) = \varepsilon \Im(\overline{\Psi(x,t)} \nabla \Psi(x,t)),$$

respectively. By using them in equation (1) and separating real and imaginary parts,
\[
\begin{align*}
   &i\varepsilon \left( \frac{1}{2} \frac{1}{\sqrt{n}} \exp \left( \frac{iS}{\varepsilon} \right) n_t + \frac{i}{\varepsilon} \sqrt{n} \exp \left( \frac{iS}{\varepsilon} \right) S_t \right) = -\frac{\varepsilon^2}{2} \left[ -\frac{1}{4} \frac{1}{\sqrt{n^3}} \exp \left( \frac{iS}{\varepsilon} \right) (\nabla n)^2 \\
   &+ \frac{1}{2} \frac{1}{\sqrt{n}} \exp \left( \frac{iS}{\varepsilon} \right) \Delta n \\
   &+ \frac{i}{\varepsilon} \frac{1}{\sqrt{n}} \exp \left( \frac{iS}{\varepsilon} \right) \nabla n \nabla S \\
   &- \frac{1}{\varepsilon} \sqrt{n} \exp \left( \frac{iS}{\varepsilon} \right) (\nabla S)^2 \\
   &+ \frac{1}{\varepsilon} \sqrt{n} \exp \left( \frac{iS}{\varepsilon} \right) \Delta \\
   &- \sqrt{n} \exp \left( \frac{iS}{\varepsilon} \right)
\end{align*}
\]

for real part,

\[
S_t = \frac{\varepsilon^2}{2} \left[ -\frac{1}{4} \frac{1}{n^2} (\nabla n)^2 + \frac{1}{2} \frac{1}{n} \Delta n - \frac{1}{\varepsilon^2} (\nabla S)^2 \right] + V
\]

\[
= \frac{\varepsilon^2}{2} \left[ -\frac{1}{4} \frac{1}{n^2} (\nabla n)^2 + \frac{1}{2} \frac{1}{n} \Delta n \right]^{-\frac{1}{2}} (\nabla S)^2 + V
\]

\[
= \frac{\varepsilon^2}{2} \left[ \frac{1}{\sqrt{n}} \nabla \sqrt{n} \right]^{-\frac{1}{2}} |\nabla S|^2 + V
\]

then,

\[
n \nabla S_t + \frac{1}{2} n \nabla |\nabla S|^2 - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0
\]

Because of \( n(\nabla S_t) = (n \nabla S)_t - \nabla S n_t \), we get
\[
\frac{\partial J}{\partial t} + \Delta S. \text{div} J + \frac{1}{2} n \Delta \left| \nabla S \right|^2 - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0
\]

\[
\frac{\partial J}{\partial t} + \text{div} \left( \frac{J \otimes J}{n} \right) - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0
\]

where

\[
\left[ \text{div} \left( \frac{J \otimes J}{n} \right) \right] = \sum_{j=1}^{d} \frac{\partial}{\partial x_j} \left( \frac{J_j J_j}{n} \right)
\]

For imaginary part,

\[
n_i = -\varepsilon \left[ \nabla n \cdot \nabla S + n \Delta S \right]
\]

\[
= -\text{div} J
\]

Finally we get,

\[
n_i + \text{div} J = 0 \quad (2a)
\]

\[
\frac{\partial J}{\partial t} + \text{div} \left( \frac{J \otimes J}{n} \right) - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0 \quad (2b)
\]

\[
\lambda^2 \nabla V = n - C \quad (2c)
\]

with the irrotational initial conditions

\[
n(x, 0) = n_0(x), \quad J(x, 0) = n_0(x) S_0(x), \quad x \in \Box^d
\]

where \(n_0\) and \(S_0\) are such that

\[
\Psi_0 = \sqrt{n_0} \exp \left( \frac{i S_0}{\varepsilon} \right).
\]

If \(\varepsilon = 0\), equations (2a) and (2b) are the classical zero temperature Euler equations. For \(\varepsilon > 0\), the quantum correction term:
is the so-called Bohn Potential and

\[ P = -\frac{\varepsilon^2}{4} n(\nabla \otimes \nabla) \ln n \]

is a non diagonal pressure tensor.

Let a mixed quantum state given with occupation probabilities \( \lambda_k, k \in \mathbb{N} \), satisfying

\[ \sum_{k=0}^{\infty} \lambda_k = 1 \]

The total carrier density \( n \) and the total current density \( J \) are defined as:

\[ n = \sum_{k=0}^{\infty} \lambda_k n_k \quad \text{and} \quad J = \sum_{k=0}^{\infty} \lambda_k J_k \]

And the \( k \)th single state is

\[ \frac{\partial n_k}{\partial t} + \text{div} J_k = 0 \]  
\[ \frac{\partial J_k}{\partial t} + \text{div} \left( \frac{J_k \otimes J_k}{n_k} \right) - n_k \nabla V - \frac{\varepsilon^2}{2} n_k \nabla \left( \frac{\Delta \sqrt{n_k}}{\sqrt{n_k}} \right) = 0 \]

with initial condition:

\[ n_k(x,0) = n_{0,k}(x), \quad J_k(x,0) = n_{0,k}(x) \nabla S_{0,k}(x) \]

If we define

\[ -\frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = -\frac{\varepsilon^2}{4} \text{div} \left( n(\nabla \otimes \nabla) \ln n \right) \]
we can derive the following identities

\[
\sum_{k=0}^{\infty} \lambda_k \text{div} \left( \frac{J_k \otimes J_k}{n_k} \right) = \sum_{k=0}^{\infty} \text{div} \left( \lambda_k n_k (u_{c,k} \otimes u_{c,k}) \right)
\]

\[
= \sum_{k=0}^{\infty} \lambda_k \text{div} \left( n_k (u_{c,k} - u_c) \otimes (u_{c,k} - u_c) + 2n_k u_{c,k} \otimes u_c \right) - \text{div} n (u_c \otimes u_c)
\]

\[
= \sum_{k=0}^{\infty} \lambda_k \text{div} \left( n_k (u_{c,k} - u_c) \otimes (u_{c,k} - u_c) + 2 \left( \frac{J_k \otimes J_k}{n} \right) \right) - \text{div} \left( \frac{J \otimes J}{n} \right)
\]

\[
= \text{div} \left( \frac{J \otimes J}{n} \right) + n \theta_c
\]

where \( \theta_c = \sum_{k=0}^{\infty} \frac{\lambda_k}{n} \text{div} \left( (u_{c,k} - u_c) \otimes (u_{c,k} - u_c) \right) \) is called the current temperature. And
\[-\frac{\varepsilon^2}{2} \sum_{k=0}^{\infty} \lambda_k n_k \nabla \left( \frac{\Delta \sqrt{n_k}}{\sqrt{n_k}} \right) = -\frac{\varepsilon^2}{2} \sum_{k=0}^{\infty} \lambda_k \text{div} \left( n_k (\nabla \otimes \nabla) \log n_k \right) \]

\[= -\frac{\varepsilon^2}{2} \sum_{k=0}^{\infty} \lambda_k \text{div} \left[ (\nabla \otimes \nabla) n_k - \left( \frac{\nabla n_k \otimes \nabla n_k}{n_k} \right) \right] \]

\[= -\frac{\varepsilon^2}{2} \sum_{k=0}^{\infty} \lambda_k \text{div} \left[ (\nabla \otimes \nabla) n_k + \left( \frac{\nabla n \otimes \nabla n}{n^3} \right) \right] \]

\[-n_k \left( \frac{\nabla n_k}{n_k} - \frac{\nabla n}{n} \right) \otimes \left( \frac{\nabla n_k}{n_k} - \frac{\nabla n}{n} \right) \]

\[-2 \left( \frac{\nabla n \otimes \nabla n_k}{n} \right) \]

\[= -\frac{\varepsilon^2}{2} \text{div} \left[ (\nabla \otimes \nabla) n - \left( \frac{\nabla n \otimes \nabla n}{n} \right) \right] - \text{div} (n \theta_{os}) \]

where \( \theta_{os} = \sum_{k=0}^{\infty} \lambda_k \frac{n_k}{n} (u_{os,k} - u_{os}) \otimes (u_{os,k} - u_{os}) \) is termed osmotic temperature.

Multiplication of equation (3a) and (3b) by \( \lambda_k \) and summation over \( k \) yields the quantum hydrodynamic equation

\[\frac{\partial n}{\partial t} + \text{div} J = 0\]

\[\frac{\partial J}{\partial t} + \text{div} \left( \frac{J \otimes J}{n} - n \theta_{os} \right) - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0\]

But the temperature tensor cannot be expressed in terms of \( n \) and \( J \) without further assumptions. We assume that the temperature tensor is a scalar (times identity tensor):

\[\theta = T[Id]\]
We assume that $T$ is constant and by adding the relaxation term, we get

$$n_t + \text{div} J = 0$$

$$J_t + \text{div} \left( \frac{J \otimes J}{n} \right) + T \nabla n - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = - \frac{J}{\tau_{\text{relax}}}$$

$$\lambda^2 \Delta V = n - C$$

For physical times of the order of $\frac{1}{\tau_{\text{relax}}}$ we can rescale the equations by introducing

$$t \rightarrow \frac{t_s}{\tau_{\text{relax}}}, \quad \frac{\partial}{\partial t} \rightarrow \tau_{\text{relax}} \frac{\partial}{\partial \hat{t}}, \quad J \rightarrow \frac{J_s}{\tau_{\text{relax}}}$$

Then we get

$$n_t + \text{div} J = 0$$

$$\tau_{\text{relax}}^2 J_t + \tau_{\text{relax}}^2 \text{div} \left( \frac{J \otimes J}{n} \right) + T \nabla n - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = -J$$

$$\lambda^2 \Delta V = n - C$$

In the limit $\tau_{\text{relax}} \rightarrow 0$, we get the quantum drift diffusion equations:

$$n_t + \text{div} J = 0 \quad \text{(4a)}$$

$$T \nabla n - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = -J \quad \text{(4b)}$$

$$\lambda^2 \Delta V = n - C \quad \text{(4c)}$$
We obtain a conservation form from equation (4a) and (4b), i.e.

\[ n_t = \text{div} \left( n \nabla \left( -\frac{\varepsilon^2}{2} \frac{\Delta \sqrt{n}}{\sqrt{n}} + \theta \log(n) - V \right) \right) \]

Introducing the quantum quasi Fermi level

\[ F = -\frac{\varepsilon^2}{2} \frac{\Delta \sqrt{n}}{\sqrt{n}} + \theta \log(n) - V, \]

we obtain the system

\[ n_t = \text{div}(n\nabla F) \] \hspace{1cm} (5a)
\[ F = -\frac{\varepsilon^2}{2} \frac{\Delta \sqrt{n}}{\sqrt{n}} + \theta \log(n) - V \] \hspace{1cm} (5b)
\[ \lambda^2 \Delta V = n - C \] \hspace{1cm} (5c)

**Numerical Approach**

For the first step, we tried to solve numerically a simplified problem. We choose \( v = 0, T = 0, \varepsilon^2 = 1 \), and (space dim.) \( d = 1 \). Then our equation is

\[ n_t = -\n \left( n \left( \frac{\sqrt{n}_x}{\sqrt{n}} \right) \right)_x \right) \right), \quad x \in (0, 1), t > 0 \] \hspace{1cm} (6)

with different boundary conditions:

(i) \( n(0, t) = n(1, t) = 1, \quad n_x(0, t) = n_x(1, t) = 0 \)

or

(ii) \( n(0, t) = n(1, t) = 1, \quad (\sqrt{n})_x(0, t) = (\sqrt{n})_x(1, t) = 0 \)
and initial condition
\[ n(x,0) = n_0(x), \quad x \in (0,1) \]

First, we derive various formally equivalent formulations of equation (6). And then we will try to solve with different numerical methods.

**Type 1**

\[
n_t = -n \left( \frac{\left( \frac{1}{n} \right)_{xx}}{\frac{1}{n}} \right) \\
= -n \left( \frac{1}{2} - \left( \frac{1}{n} \right)_{xx} + \frac{1}{2} \left( \frac{1}{n} \right)_{xxx} \right) \\
= -\left( \frac{1}{2} \left( \frac{1}{n} \right)_{xx} - \frac{1}{n} \left( \frac{1}{n} \right)_{xxxx} + \frac{1}{2} \left( \frac{1}{n} \right)_{xxx} \right) \\
= -\left( \frac{1}{2} \left( \frac{1}{n} \right)_{xx} - \frac{1}{n} \left( \frac{1}{n} \right)_{xxxx} \right) - \frac{1}{2} \left( \frac{1}{n} \right)_{xxx} \\
= -\frac{1}{2} n_{xxx} + \frac{1}{2} \left( \frac{n_{xx}}{n} \right) \\
= \frac{1}{2} \left( n_{xxx} + \left( \frac{n_x}{n} \right)_{xx} \right) 
\]
Type 2

\[
n_t = -\frac{1}{2} \left( n^{-2} n_x^2 - 2n^{-1} n_x n_{xx} + n_{xxx} \right)
\]

\[
= -\frac{1}{2} \left( -n^{-1} n_x^2 - n_{xx} \right)
\]

\[
= -\frac{1}{2} \left( n(-n^{-2} n_x^2 - n^{-1} n_{xx}) \right)
\]

\[
= -\frac{1}{2} \left( n(n^{-1} n_x)_x \right)
\]

\[
= \frac{1}{2} \left( n \log n \right)_x
\]

If \( n = e^u \), then we have

\[
\left( e^u \right)_t = -\frac{1}{2} \left( e^u u_{xx} \right)_x
\]

Type 3

\[
n_t = -\left[ n \left( \frac{(\sqrt{n})_{xx}}{\sqrt{n}} \right) \right]
\]

\[
= -(nF_x)_x
\]

where \( F = \frac{(\sqrt{n})_{xx}}{\sqrt{n}} \)

Let \( \rho = \sqrt{n} \),

\[
\left( \rho^2 \right)_t = -\left( \rho^2 F_x \right)_x
\]

where \( F = \frac{\rho_{xx}}{\rho} \)

A steady state solution of equation (6) is given by \( n(x) = 1, x \in (0,1) \).
**Discretization for Type 1**

\[ n_i = \frac{1}{2} \left( -n_{i-1} + \left( \frac{n_{i}^2}{n_i} \right) \right) \quad x \in (0,1), t > 0 \]

with boundary conditions:

\[ n(0,t) = n(1,t) = 1, \quad n_x(0,t) = n_x(1,t) = 0 \]

and initial condition:

\[ n(x,0) = \cos^2(\pi x) \]

Let \( n_i^j \) be an approximation of \( n(x_i, t_j) \), where \( x_i = (i - 1) \times h, t = (j - i) \times \tau \), \( h > 0, \tau > 0 \) and \( i = 1, 2, ..., N+1, j = 1, 2, ..., M+1, \frac{1}{h} = N, \frac{1}{\tau} = M \).

If we use semi-implicit discretization, we have

\[ \frac{n_i^j - n_i^{j-1}}{\tau} = -\frac{1}{2h^4} \left( n_{i+1}^{j-1} - 4n_i^{j-1} + 6n_i^j - 4n_{i-1}^j + n_{i-1}^{j-1} \right) + \frac{1}{2h^2} (w_i^{j-1} - 2w_i^{j-1} + w_{i+1}^{j-1}) \]

where

\[ w_i^{j-1} = \left( \frac{n_{i+1}^{j-1} - n_{i-1}^{j-1}}{2h} \right)^2 \left( \frac{2}{n_{i+1}^{j-1} + n_{i-1}^{j-1}} \right) = \frac{(n_{i+1}^{j-1} - n_{i-1}^{j-1})^2}{2h^2(n_{i+1}^{j-1} + n_{i-1}^{j-1})} \]

and

\[ n_1^j = n_2^j = n_N^j = n_{N+1}^j = 1 \]

Then we get Figure 1, the solution is convergent to 1. If we use \( \tau \) large enough the temporal convergence of the solution to the constant steady state 1 is faster than when used small \( \tau \).
Figure 1

**Discretization for Type 2**

Let $n = e^u$, then the problem is

$$\left( e^u \right)_t = -\frac{1}{2} \left( e^u u_{xx} \right)_{xx} \quad x \in (0,1), t > 0$$

with boundary condition,

$$u(0,t) = 0, \quad u(1,t) = 0$$

$$u_x(0,t) = 0, \quad u_x(1,t) = 0$$

and initial condition,

$$u(x,0) = \log(\cos^2(\pi x))$$
By using semi-implicit discretization,

\[ e^{u_i^{n+1}} \cdot \frac{1}{\tau} (u_i^{n} - u_i^{n-1}) = -\frac{1}{2} (w_i^{n+1} - 2w_i^n + w_i^{n-1}) \]

where \( w_i^n = e^{u_i^n} (u_i^{n+1} - 2u_i^n + u_i^{n-1}) \)

and \( u_1^n = u_2^n = u_N^n = u_{N+1}^n = 1 \).

Then we get Figure 2, the solution is convergent to 1. The behavior of solution is the same as Type 1.

![Figure 2](image-url)
Discretization for Type 3

We set $\rho = V_n$, then the problem is

$$\left( \rho^2 \right)_t = 2 \rho \rho_x = -\left( \rho^2 F^r \right)_x, \quad x \in (0,1), t > 0,$$

with boundary conditions:

$$\rho(0,t) = 1, \quad \rho(1,t) = 1,$$

$$\rho_{xx}(0,t) = 0, \quad \rho_{xx}(1,t) = 0$$

and initial condition

$$\rho(x,0) = |\cos(\pi x)|$$

We will try to use two methods to solve this problem. First we use explicit discretization.

**Type 3(A)**

$$2 \rho_i^{j+1} \frac{1}{\tau} (\rho_i^j - \rho_i^{j-1}) = -\frac{1}{h^2} \left( (\rho_{i+1}^j)^2 (F_{i+1}^{j-1} - F_i^{j-1}) - (\rho_{i-1}^j)^2 (F_i^{j-1} - F_{i-1}^{j-1}) \right)$$

where

$$F_{i}^{j-1} = \frac{1}{\rho_{i-1}^{j-1}} \frac{1}{h^2} (\rho_{i+1}^{j-1} - 2 \rho_i^{j-1} + \rho_{i-1}^{j-1})$$

and $\rho_i^j = \rho_{n+1} = 1$. 
Then we get Figure 3, but we need the condition $\frac{1}{h^4} \ll 1$. This means that $\tau$ must be very small. Therefore the solution is slowly convergent to 1. But the formula of type 3 is easier than Type 1 and Type 2 to solve the conservation form of Quantum Drift Diffusion equation. Then we will try by semi-implicit method to be faster to converge.

**Type 3(B)**

$$\frac{1}{h^2} (\rho_{i+1}^j - 2\rho_i^j + \rho_{i-1}^j) = \rho_i^{j-1} F_i^{j-1}$$

and
The boundary condition $p_{xx} = 0$ is equivalent to $F = 0$. Therefore $F_i' = F_{N+1}' = 0$. Then we get Figure 4, the solution is faster than Type 3(A) to be convergent to 1 but sometimes it is larger than 1.

If we use given value for $\frac{p_{xx}}{p}$, we get Figure 5. The solution is better than above condition. It is not larger than 1 because we can reduce the truncation error. The disadvantage of semi-implicit discretization is we cannot use very small $\tau$. 

![Figure 4](image-url)
Figure 5

Numerical Approximation of QDD Equation

In this section we derive the semi-implicit discretization of equations (5a), (5b) and (5c) in one space dimension case (d=1).

Set $\rho = \sqrt{n}$. Then we read:

\[(\rho^2)_t = (\rho^2 F_x)_x \]  \hspace{1cm} (7a)

\[F = - \frac{\varepsilon^2 \rho_{xx}}{2 \rho} + 2\theta \log(\rho) - V \]  \hspace{1cm} (7b)

\[\lambda^2 V_{xx} = \rho^2 - C \]  \hspace{1cm} (7c)

with boundary conditions:
\[ \rho(0,t) = 1, \quad \rho(1,t) = 1, \]
\[ \rho_{xx}(0,t) = 0, \quad \rho_{xx}(1,t) = 0 \]
\[ V(0,t) = 0, \quad V(1,t) = U \quad \text{where} \quad U > 0. \]
\[ F(0,t) = 0, \quad F(1,t) = U \]

and initial conditions:
\[ \rho(x,0) = \sqrt{n(x,0)} \quad \text{where} \quad n(x,0) = \cos^2(\pi x) \quad (8) \]

With the boundary conditions, the steady-state solution is given by
\[ \rho(x,0) = 1, \quad V(x,0) = xU \quad x \in (0,1) \]

Then we get Figure 6.

There are some problems because of truncation error of \( \frac{\rho_{xx}}{\rho} \), by using given value for \( \frac{\rho_{xx}}{\rho} \), we get Figure 7.

Figure 6
Figure 7

If we use $U = 0$, we get Figure 8. And if we use $U > 0$ we get Figure 9.

But we cannot change $\tau$. By numerical experiments, it can be seen that this procedure leads to numerical instability whenever $\tau$ change.
**Acknowledgement**

The author acknowledges the support of short-term research grants of DAAD (German Academic Exchange Service). The receipt of research funding for this research under the project code: "ARCHU/013/2002/MATHEMATICS (1)" from the Asia Research Centre, Yangon University is gratefully acknowledged.

**References**


