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Review of Numerical Solutions of Differential Equations Applied to Semiconductor Materials

Asmaa A. Salama[1], Mohamed S. Abdel-wahed[1,2], D. A. Hammad[1], Mourad S. Semary[1]
[1]Department of Basic Engineering Sciences, Faculty of Engineering at Benha, Benha University, Egypt.
[2]Department of Basic Engineering Sciences, Faculty of Engineering, BADR University in Cairo BUC, Egypt
Email address: asmaa.salama@bhit.bu.edu.eg, Mohamed.sayed@bhit.bu.edu.eg, doaa.hammad@bhit.bu.edu.eg, mourad.semary@yahoo.com

***Abstract*—** *Many differential equations can't be solved analytically, and for many applications, such as in electronic engineering – numerical solution is often more sufficient. Schrodinger equation, Poisson equation and Continuity equations are the most popular differential equations used in semiconductor materials. In this paper, the numerical solution of these equations is reviewed while focusing on some specific methods which are compared and evaluated. Schrodinger equation is solved using both Numerov method and Finite Difference method. Poisson equation is solved using Finite Difference method at various types of boundary conditions. Continuity equation is solved using Scharfetter-Gummel method. Numerical solutions are compared with the exact results and the dependence of error on the mesh size is shown.*

Keywords*—Numerov method; Finite Difference Method; Scharfetter-Gummel Method*.

I. INTRODUCTION

Semiconductor is a class of solids which have intermediate electrical conductivity between insulators and conductors. Semiconductors are used in the manufacture of different kinds of electronic devices, including transistors, diodes, and integrated circuits. Such devices have been used in a lot of application because of their reliability, compactness, power efficiency, and low cost.

Hereinafter, we will discuss the most popular differential equations used in modelling semiconductor materials. We will focus on three main equations: Schrodinger equation Eq. (1.1), Poisson equation Eq. (1.2) and Continuity equation for electrons Eq. (1.3) and for holes Eq. (1.4).

First, The Schrödinger equation is a differential equation that governs the wave function of a quantum-mechanical system. It is the basis of in quantum mechanics, and its discovery was a significant landmark in the development of the subject. The form of Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+V(x)\psi(x)=E\psi(x) \qquad (1.1)$$

(Where m is the particle mass, $\hbar$ is the reduced Planked constant, $\psi(x)$ is the wave function, $V(x)$ is the potential, E is the particle energy).In these paper, The 1-D time-independent Schrodinger equation [1, 2] is solved using two methods: Numerov method [3, 4] and Finite Difference method. Numerov method is used to solve ordinary differential equations [5] of second order in which the first-order term does not exist. To be able to derive Numerov Method we start with the expansion of the solution in a Taylor series. Numerical outcomes from Numerov method and Finite Difference method are compared with exact solution. From comparison we know that Numerov method is more accurate than Finite Difference method.

Second, the solution to Poisson's equation is the potential field caused by a given electric charge or mass density distribution; with the potential field known, one can then calculate electrostatic or gravitational (force) field. Also, Poisson equation is a powerful tool for modelling electrostatic systems behaviour. Poisson equation form is

$$u''(x)=g(x) \qquad (1.2)$$

(Where $u''(x)$ is second derivative of a given function and, $g(x)$ is a given function). In this paper, Poisson equation is solved using Finite Difference method [6, 7] with different boundary conditions (Dirichlet-Dirichlet boundary condition, Neumann-Dirichlet and Dirichlet-Neumann boundary condition). Numerical outcomes are compared with exact solution in all cases and absolute error between numerical and exact outcomes is shown.

Third, the continuity equation can describe the transfer of various quantities, such as gas or fluid. The continuity equation can be written in integral form, which is applied at finite region, or in differential form, which is applied at a point. Continuity equation takes two forms as in Eq. (1.3) which is for electrons and Eq. (1.4) which is for holes.

$$\frac{\partial(\delta p)}{\partial t}=-\frac{1}{q}\frac{\partial J_p}{\partial x}+G_{\text{ext}}-\frac{\delta p}{\tau_p} \qquad (1.3)$$

$$\frac{\partial(\delta n)}{\partial t}=+\frac{1}{q}\frac{\partial J_n}{\partial x}+G_{\text{ext}}-\frac{\delta n}{\tau_n} \qquad (1.4)$$

Where

$$J_p=q\mu_p p\mathrm{E}-qD_p\frac{dp}{dx} \qquad (1.5)$$

$$J_n=q\mu_n p\mathrm{E}+qD_n\frac{dn}{dx} \qquad (1.6)$$

(where J_n is current density for electrons, J_p is current density for holes, n is the electrons concentration, p is the

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holes concentrations, G_{ext} is the external generation).In these paper, Continuity equation is solved numerically using Scharfetter-Gummel method [8-15]. The numerical outcomes also are compared with the exact solution. The Scharfetter-Gummel scheme provides a good way to discretise the continuity equation for particle transport.

II. NUMERICAL METHODS FOR SOLVING SCHRODINGER EQUATION

This section presents some of numerical methods which used to solve Schrodinger equation. Firstly, paper presents Numerov method and its principle. Secondly, Numerov method will be applied to solve Schrodinger equation. Thirdly, Schrodinger equation is also solved using finite difference method. Finally, numerical comparisons are showed.

A. The Numerov Method

Presenting of mathematical conclusion of Numerov method and how to apply it to solve Schrodinger equation:

For linear ordinary differential equations [3, 5, 16, 17] without a y' term, like the Schrödinger equation, the Numerov method can be used.

$$y'' + m(x)\,y = l(x), a \le x \le b \tag{2.1}$$

Using Taylor expansion we have

$$y_{n+1} = y_n + hy_n' + \frac{1}{2}h^2 y'' + \frac{1}{3!}h^3 y''' + \frac{1}{4!}h^4 y^{(4)} + \frac{1}{5!}h^5 y^{(5)} + O\left(h^6\right) \tag{2.2}$$

$$y_{n-1} = y_n - hy_n' + \frac{1}{2}h^2 y'' - \frac{1}{3!}h^3 y''' + \frac{1}{4!}h^4 y^{(4)} - \frac{1}{5!}h^5 y^{(5)} + O\left(h^6\right). \tag{2.3}$$

Eq.(2.2) and Eq.(2.3)are added and simplifying to produce y''

$$y_n'' = \frac{y_{n+1} - 2y_n + y_{n-1}}{h^2} + O\left(h^2\right) \tag{2.4}$$

Our previous second-order formula for the difference approximation to y''_n is used to apply on Eq. (2.1).

$$y^{(4)} = \frac{d^2}{dx^2}(-m(x)y + l(x)) \tag{2.5}$$

Using the same procedure as before Eq. (2.4), we can calculate the fourth derivative.

$$y_n^{(4)} = \frac{-m_{n+1}y_{n+1} + 2m_n y_n}{h^2} + \frac{-m_{n-1}y_{n-1} + l_{n+1} - 2l_n + l_{n-1}}{h^2} + O\left(h^2\right) \tag{2.6}$$

The next term in Taylor series for y is

$$\frac{1}{12}h^4 y_n^{(4)} = \frac{1}{12}h^2(-m_{n+1}y_{n+1} + 2m_n y_n - m_{n-1}y_{n-1} + l_{n+1} - 2l_n + l_{n-1}) + O\left(h^6\right) \tag{2.7}$$

Using Eq. (2.7) to substituting into equation Eq. (2.1) and simplifying we get a new expression for y''

$$h^2 y_n'' = \left(1 + \frac{1}{12}h^2 m_{n+1}\right)y_{n+1} - 2\left(1 + \frac{1}{12}h^2 m_n\right)y_n + \left(1 + \frac{1}{12}h^2 m_{n-1}\right)y_{n-1} - \frac{1}{12}h^2\left(l_{n+1} - 2l_n + l_{n-1}\right) \tag{2.8}$$

After simplifying Eq. (2.8) we get this form

$$\left(1 + \frac{1}{12}h^2 m_{n+1}\right)y_{n+1} - 2\left(1 - \frac{5}{12}h^2 m_n\right)y_n + \left(1 + \frac{1}{12}h^2 m_{n-1}\right)y_{n-1} = \frac{1}{12}h^2\left(l_{n+1} + 10l_n + l_{n-1}\right) \tag{2.9}$$

The nonhomogeneous boundary value problem is now solvable as a matrix equation and then gets the Eigen values and Eigen vectors which is the results.

The Numerov method [3, 18, 19] will be applied to solve Schrodinger equation due to Numerov method is a numerical method for solving ordinary differential equations of the form

$$\frac{d^2\psi(x)}{dx^2} = g(x)\psi(x) \tag{2.10}$$

The 1-D Schrodinger equation without regard to time (Eq. (1.1)) Can be expressed as Eq. (2.10)

$$\psi^{(2)}(x) = -\frac{2m}{\hbar^2}(E - F(x))\psi(x) = g(x)\psi(x) \tag{2.11}$$

Using Wave function expansions in the Taylor series $\psi(x)$ we will go through the same procedures of the Numerov method then we get

$$\psi^{(2)}(x) = \frac{\psi(x+d) + \psi(x-d) - 2\psi(x)}{d^2} - \frac{1}{12}d^2\psi^{(4)}(x) + O\left(d^4\right) \tag{2.12}$$

Using Eq. (2.11) and Eq. (2.12) we obtained

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$$g_i\psi_i = \frac{\psi_{i+1}+\psi_{i-1}-2\psi_i}{d^2} - \frac{1}{12}\left(g_{i+1}\psi_{i+1}+g_{i-1}\psi_{i-1}-2g_i\psi_i\right) \tag{2.13}$$

Where

$$g_{i-1}\equiv g\left(x-d\right), g_i \equiv g\left(x\right), g_{i+1}\equiv g\left(x+d\right) \tag{2.14}$$

$$\psi_{i-1}\equiv \psi\left(x-d\right), \psi_i \equiv \psi\left(x\right), \psi_{i-1}\equiv \psi\left(x-d\right) \tag{2.15}$$

Rearranging Eq. (2.13) will get

$$\frac{\psi_{i+1}+\psi_{i-1}-2\psi_i}{d^2} = \frac{1}{12}\left(g_{i+1}\psi_{i+1}+g_{i-1}\psi_{i-1}+10g_i\psi_i\right) \tag{2.16}$$

$$f_{i-1} = -\frac{2m}{\hbar^2}\left(E-F_{i-1}\right),\ f_i = -\frac{2m}{\hbar^2}\left(E-F_i\right),\ f_{i+1} = -\frac{2m}{\hbar^2}\left(E-F_{i+1}\right) \tag{2.17}$$

$$-\frac{\hbar^2}{2m}\frac{\psi_{i-1}-2\psi_i+\psi_{i+1}}{d^2} + \frac{F_{i-1}\psi_{i-1}+10F_i\psi_i+F_{i+1}\psi_{i+1}}{12} = E\frac{\psi_{i-1}+10\psi_i+\psi_{i+1}}{12} \tag{2.18}$$

$$-\frac{\hbar^2}{2m}A\psi + BF\psi = EB\psi \tag{2.19}$$

$$A = \frac{1}{d^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & 0 & \dots \\ 0 & 1 & -2 & 1 & 0 & \dots \\ 0 & 0 & 1 & -2 & 1 & \dots \\ 0 & 0 & 0 & 1 & -2 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix},\quad B = \frac{1}{12}\begin{pmatrix} 10 & 1 & 0 & 0 & 0 & \dots \\ 1 & 10 & 1 & 0 & 0 & \dots \\ 0 & 1 & 10 & 1 & 0 & \dots \\ 0 & 0 & 1 & 10 & 1 & \dots \\ 0 & 0 & 0 & 1 & 10 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \tag{2.20}$$

$$V = \begin{pmatrix} F_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & F_2 & 0 & 0 & 0 & \dots \\ 0 & 0 & F_3 & 0 & 0 & \dots \\ 0 & 0 & 0 & F_4 & 0 & \dots \\ 0 & 0 & 0 & 0 & F_5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix},\quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \vdots \end{pmatrix} \tag{2.21}$$

Multiplying both sides of Eq. (2.19) by B^{-1},we get

$$-\frac{\hbar^2}{2m}B^{-1}A\psi + V\psi = E\psi \tag{2.22}$$

$$H\psi = E\psi, H = -\frac{\hbar^2}{2m}B^{-1}A + V \tag{2.23}$$

The square matrix H which is the sum of the kinetic energy matrix and the potential energy matrix F. The stationary states of the time-independent Schrodinger equation are represented by the eigenvectors of H, and their corresponding energies are represented by the eigenvalues.

Numerov process has many advantages as it can be applied to existing solution techniques without significantly altering the way the software is organized or increasing the computational cost; for this reason, as well as the improvement in accuracy, it is worthwhile to take into account the application of Numerov process to the semiconductor equation.

B. Finite Difference method (FDM)

The Schrodinger equation for a one-dimension quantum system [1] is given in Eq. (1.1)

Using the second order centered derivative formula; we can discretise Eq. (1.1) as follows

$$-\frac{\hbar}{2m}\left(\frac{\psi_{j+1}-2\psi_j+\psi_{j-1}}{h^2}\right)+V_j\psi_j = E\psi_j \tag{2.24}$$

Where h is the step size

Let's suppose we want to solve this equation in the region $x\in[a,b]$.then we can create N+1 grid points such that $x_0 = a$ and $x_N = b$ since the particle is confined in the region $x\in[a,b]$.this leads to the following boundary conditions:

$$\psi_0 = 0,\quad \psi_N = 0 \tag{2.25}$$

Asmaa A. Salama,Mohamed S. Abdel-wahed, D. A. Hammad, Mourad S. Semary, "Review of numerical solutions of differential equations applied to semiconductor materials," *International Journal of Multidisciplinary Research and Publications (IJMRAP)*, Volume 5, Issue 12, pp. 88-96, 2023.

This means we need to compute ψ_j for $j = 1,2,3,\cdots,N-1$.

We obtain the following linear system

$$\frac{-1}{2h^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & 0 & \dots \\ 0 & 1 & -2 & 1 & 0 & \dots \\ 0 & 0 & 1 & -2 & 1 & \dots \\ 0 & 0 & 0 & 1 & -2 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \vdots \end{pmatrix} + \begin{pmatrix} V_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & V_2 & 0 & 0 & 0 & \dots \\ 0 & 0 & V_3 & 0 & 0 & \dots \\ 0 & 0 & 0 & V_4 & 0 & \dots \\ 0 & 0 & 0 & 0 & V_5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \vdots \end{pmatrix} = E\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \vdots \end{pmatrix} \quad (2.26)$$

Construct the kinetic energy matrix

$$T = \frac{-1}{2h^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & 0 & \dots \\ 0 & 1 & -2 & 1 & 0 & \dots \\ 0 & 0 & 1 & -2 & 1 & \dots \\ 0 & 0 & 0 & 1 & -2 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \quad (2.27)$$

Construct the potential energy matrix

$$V = \begin{pmatrix} V_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & V_2 & 0 & 0 & 0 & \dots \\ 0 & 0 & V_3 & 0 & 0 & \dots \\ 0 & 0 & 0 & V_4 & 0 & \dots \\ 0 & 0 & 0 & 0 & V_5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \quad (2.28)$$

Construct the Hamiltonian matrix

$$H = T + V \quad (2.29)$$

Diagonalize H to obtain the eigenvalues (energies) and eigenvectors (wavefunction).

CASE STUDY

For the infinite square well, consider a particle whose mass 0.5g is only found in the infinite interval [0,1], such that

$$V(x) = \begin{cases} 0 & x \in [0,1] \\ \infty & \text{otherwise} \end{cases}$$

And the boundary conditions are $\psi(0) = 0$, $\psi(1) = 0$ and using N = 1000.

The exact solution to Schrodinger equation and the numerical solution using Finite Difference method and Numerov method is shown in TABLE I.

TABLE I. Comparison between exact and numerical solution of Schrodinger equation for first ten values

N	Exact solution	Numerov method	Finite Difference method
1	9.8696044	9.869604	9.869596
2	39.4784176	39.478418	39.478288
3	88.826439	88.826439	88.825783
4	157.913670	157.913670	157.911596
5	246.740110	246.740109	246.735047
6	355.305758	355.305758	355.295259
7	483.610616	483.610615	483.591165
8	631.654682	631.654680	631.621499
9	799.437956	799.437954	799.384805
10	986.960440	986.960436	986.879431

From Table I. Numerov method is more accurate than Finite Difference method compared to exact solution.

III. POISSON EQUATION IN 1-D

Poison equation can be linear equation or non-linear equation. It will be shown each one and presents method which be used to solve. Linear Poison equation will be solved at different boundary condition using finite difference method. Non-linear Poison equation will be solved using Newton Raphson method

A. Linear form of Poisson equation

Paper presents solving Poison equation using finite difference method [6, 7, 20, 21] at different boundary condition (Dirichlet-Dirichlet boundary conditions, Neumann-Dirichlet and Dirichlet-Neumann boundary conditions).

1) Finite Difference Method with Dirichlet-Dirichlet boundary conditions

Consider a function $u(x)$ that satisfies the Poisson equation Eq. (1.2) where $g(x)$ is given function on the interval $]a,b[$. We need to the function $u(x)$ satisfy the Dirichlet–Dirichlet boundary conditions. $Au = G$ with boundary condition $u(a) = \alpha, u(b) = \beta, u_i = u(x_i)$ and $g_i = g(x_i)$ for $i = 0,\dots,N+1$ the values of the function and the approximation solution on the right. We derive the following system for internal nodes by substituting symmetric difference equations for the second derivative.

On the considered interval $]a,b[$ we specify a one-dimensional grid $x_i = a + i \cdot \Delta x, i = 0,\dots,N+1$ where the uniform step of the grid is calculated as $\Delta x = \frac{b-a}{N} = h$

$$-u_1 + u_2 = h^2 \frac{g_i}{2} + hu_a', \quad i = 1,\dots,N \quad (3.1)$$

Asmaa A. Salama,Mohamed S. Abdel-wahed, D. A. Hammad, Mourad S. Semary, "Review of numerical solutions of differential equations applied to semiconductor materials," *International Journal of Multidisciplinary Research and Publications (IJMRAP)*, Volume 5, Issue 12, pp. 88-96, 2023.

The system of linear algebraic equations Eq. (3.1) can be represented in matrix form as follows:

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & \ddots & \cdots & 0 \\ 0 & 0 & 0 & 1 & -2 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix}$$

$$= \begin{pmatrix} h^2 g_1 - u_a \\ h^2 g_2 \\ h^2 g_3 \\ h^2 g_4 \\ h^2 g_5 \\ \vdots \\ h^2 g_{N-1} \\ h^2 g_N - u_b \end{pmatrix} \quad (3.2)$$

Poisson equation can be solved by the above system of matrices

CASE STUDY

At N=500 points, a= -1, b = 1, Dirichlet-Dirichlet boundary condition $u(a) = -.2$, $u(b) = .1$ and $g = \cos(\pi(x-.5))^2$.

The output results of poison equation are shown in Fig. 1 and the absolute error between exact and numerical results is shown in Fig. 2.

2) FDM with Neumann-Dirichlet and Dirichlet-Neumann boundary conditions.

Using Eq. (1.2) with The Neumann-Dirichlet boundary conditions satisfied by $u'(a) = u_a^{'}$ and $u(b) = u_b$. Consider a specific uniform grid for the step-by-step finite difference approach $\Delta x = \frac{b-a}{N} = h$ consisting of $N+1$ points.

The coordinates of the grid nodes x_i are calculated by:

$$\mathrm{x_i} = \mathrm{a} + (\mathrm{i}-1)\cdot \mathrm{h}, \mathrm{i} = 0,1,\ldots \mathrm{N}+1 \quad (3.3)$$

We denote by u_i at point $x_i : u_i = u(x_i)$ and at the same point fi is the value of the given function in the right hand side. We denote by $u_i^{'} = u'(x_i)$ and $u_i^{''} = u''(x_i)$ for the boundary conditions.

By substituting symmetric finite-difference expressions for the derivatives, we arrive at the approximation formulas of the second order of accuracy for the first derivatives

$$u_{i-1} - 2u_i + u_{i+1} = h^2 g_i, \quad i = 1,\ldots,N \quad (3.4)$$

a) The Neumann–Dirichlet boundary conditions

We will consider the boundary conditions at the left and right ends of the interval. This will delete u_{-1} from the system.

$$-u_1 + u_2 = h^2 \frac{g_i}{2} + h u_a^{'}, \quad i = 1,\ldots,N \quad (3.5)$$

By considering $x_0 = a - h$, it is possible to use the central differences to find the desired solution even at the interval's border point with an approximate precision of $o(h^2)$.

We present the vector G, which has components that are represented as

$$G_1 = h^2 \frac{g_i}{2} + h u_a^{'}, \quad G_N = h^2 g_N - u_b, \quad G_i = h^2 g_i, \quad i = 2,3,\ldots,N-1 \quad (3.6)$$

Consequently, the equations that determine the elements of the solution decrease to the form

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & \ddots & \cdots & 0 \\ 0 & 0 & 0 & 1 & -2 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix}$$

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix} = \begin{pmatrix} \frac{h^2}{2} g_1 + h u_a^{'} \\ h^2 g_2 \\ h^2 g_3 \\ h^2 g_4 \\ h^2 g_5 \\ \vdots \\ h^2 g_{N-1} \\ h^2 g_N - u_b \end{pmatrix} \quad (3.7)$$

We can solve this system of matrices and produce the results.

CASE STUDY

At N=500 points, a = -1, b = 1, $u'(a)$ = .25, $u(b)$ = -.5 and $g = \cos(\pi(x-.5))^2$. The output results after solving Poisson equation with Neumann–Dirichlet boundary conditions is shown in Fig. 3 and the absolute error between exact and numerical solution is shown in Fig. 4.

Dirichlet–Neumann boundary conditions

We take into account the symmetric case with the Dirichlet-Neumann boundary conditions by analogy with the case of the Neumann-Dirichlet boundary conditions. First, let's establish a suitable sampling grid for the interval [a, b]. Grid

Asmaa A. Salama,Mohamed S. Abdel-wahed, D. A. Hammad, Mourad S. Semary, "Review of numerical solutions of differential equations applied to semiconductor materials," *International Journal of Multidisciplinary Research and Publications (IJMRAP)*, Volume 5, Issue 12, pp. 88-96, 2023.

points $\{x_i, i = 0, 1, \ldots, N+1\}$ are specified as $xi = a + ih$. The boundary conditions used are u_a and u_b', the system of finite difference equations is redefined in addition to the Poisson equation. The solution value u_{N+1} at the 'virtual' point x_{N+1} is represented using the derivative's boundary condition, with symmetric central differences used to approximate it. Grouping all, we get.

$$u_{N-1} - u_N = h^2 \frac{g_N}{2} - hu_b' \tag{3.8}$$

$$G_N = h^2 \frac{g_N}{2} - hu_b', \quad G_1 = h^2 g_1 - u_a, \tag{3.9}$$

$$G_i = h^2 g_i, \quad i = 2, \ldots, N-1$$

Resulting matrix of the equation

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & \ddots & \cdots & 0 \\ 0 & 0 & 0 & 1 & -2 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix}$$

$$= \begin{pmatrix} h^2 g_1 - u_a \\ h^2 g_2 \\ h^2 g_3 \\ h^2 g_4 \\ h^2 g_5 \\ \vdots \\ h^2 g_{N-1} \\ h^2 \frac{g_N}{2} - hu_b' \end{pmatrix} \tag{3.10}$$

CASE STUDY

At N=500 points, a= -1 ,b = 1, $u(a)$ = .5 and $u'(b)$ = -.25 and $f = \cos(\pi(x-.5))^2$ .results of solving Poisson equation using Dirichlet–Neumann boundary conditions is shown in Fig. 5 and absolute error between exact and numerical solution for N=300,500 and 700 is shown in Fig. 6.

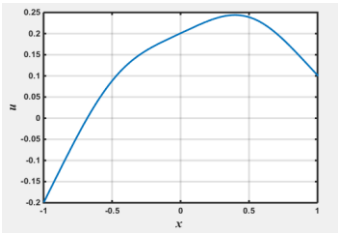

Fig. 1. Results of Poisson equation at Dirichlet-Dirichlet boundary condition at N=500.

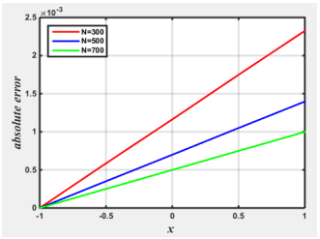

Fig. 2. Absolute error between exact and Finite Difference solutions at Dirichlet-Dirichlet boundary condition at various values of N.

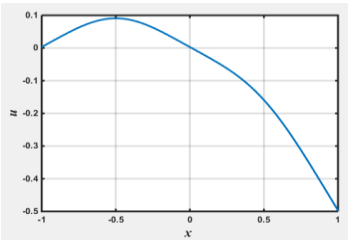

Fig. 3. Poisson equation results at Neumann-Dirichlet boundary conditions at N=500.

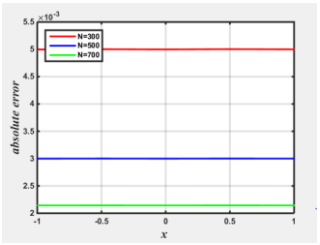

Fig. 4. Absolute error between exact and Finite Difference solutions at Neumann- Dirichlet boundary conditions at various values of N.

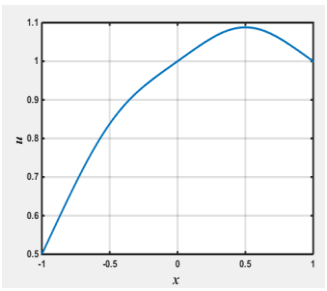

Fig. 5. Poisson equation results with Dirichlet–Neumann boundary conditions at N=500.

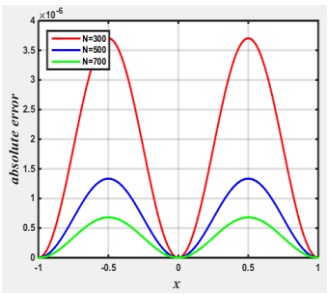

Fig. 6.Absolute error between exact solution and finite difference Dirichlet–Neumann boundary conditions solution at various values of N.

From the output figures we note that the output results become more accurate for larger N and the error decrease.

IV. NUMERICAL SOLUTION OF CONTINUITY EQUATION

In this section, the procedure for the numerical solution of continuity equation is explained. The method used is called Scharfetter-Gummel method [22-24]. In this method we need to find n (electron concentration) at each node in the interval.

A. Scharfetter-Gummel

We start with continuity equation for electrons and solution is shown step by step.

$$\frac{\partial n}{\partial t} = +\frac{1}{q}\frac{\partial J_n}{\partial x} + G - R \tag{4.1}$$

$$\frac{\partial n}{\partial t} = +\frac{1}{q}\frac{\partial J_n}{\partial x} - R_{net} \tag{4.2}$$

Where, $R_{net} = G - R$. At steady state $\frac{\partial n}{\partial t} = 0$

Asmaa A. Salama,Mohamed S. Abdel-wahed, D. A. Hammad, Mourad S. Semary, "Review of numerical solutions of differential equations applied to semiconductor materials," *International Journal of Multidisciplinary Research and Publications (IJMRAP)*, Volume 5, Issue 12, pp. 88-96, 2023.

$$\frac{dJ_n}{dx} = qR_{net} \tag{4.3}$$

$$\frac{d}{dx}\left[qn\mu_n\varepsilon + qD_n \frac{dn}{dx} \right] = qR_{net} \tag{4.4}$$

The interval has been divided into subintervals (mesh elements) with equal space.

We need to calculate n at each node taking into consider two assumptions at each node

J is constant at each node, and V is linear at each node

For the subinterval from i to $i+1$ the value of J will be equal to $J_{i+\frac{1}{2}}$

$$J_{i+\frac{1}{2}} = qn\mu_n\varepsilon + qD_n \frac{dn}{dx} \tag{4.5}$$

$$\frac{dn}{dx} + \frac{\varepsilon}{V_T} n = \frac{J_{i+\frac{1}{2}}}{qD_n} \tag{4.6}$$

Where $\frac{KT}{q} = V_T = \frac{D_n}{\mu_n}$ from Eq. (4.6) is first order linear differential equation after solving it will be

$$e^{\varepsilon x/V_T} n(x) = \int e^{\varepsilon x/V_T} \frac{J_{i+1/2}}{qD_n} dx + c_1 \tag{4.7}$$

We need solution at each node using values of n at boundary of nodes n_i, n_{i+1}

At $x = x_i \Rightarrow n = n_i$ (4.8)

At $x = x_{i+1} \Rightarrow n = n_{i+1}$ (4.9)

By substitution in equation (4.7)

$$n_i = \frac{J_{i+1/2}}{qD_n}\frac{V_T}{\varepsilon} + c_1 e^{-\varepsilon x_i/V_T} \tag{4.10}$$

$$n_{i+1} = \frac{J_{i+1/2}}{qD_n}\frac{V_T}{\varepsilon} + c_1 e^{-\varepsilon x_{i+1}/V_T} \tag{4.11}$$

Subtract equation (4.10) from equation (4.11)

$$n_{i+1} - n_i = c_1 e^{-\varepsilon x_i/V_T}\left(e^{-\varepsilon \Delta x V_T} - 1\right) \tag{4.12}$$

$$c_1 = \frac{n_{i+1} - n_i}{e^{-\varepsilon x_i/V_T}\left(e^{-\varepsilon \Delta x/V_T} - 1\right)} \tag{4.13}$$

By substitution in equation (4.11)

$$n_i = \frac{J_{i+1/2}}{qD_n}\frac{V_T}{\varepsilon} + \frac{\eta_{i+1} - \eta_1}{e^{-\varepsilon \Delta x/V_T} - 1} \tag{4.14}$$

$$J_{i+1/2} = \frac{qD_n\varepsilon}{V_T}\left[n_i - \frac{n_{i+1} - n_i}{e^{-\varepsilon \Delta x/V_T} - 1} \right] \tag{4.15}$$

$$J_{i+1/2} = \frac{qD_n}{\Delta x}\left[\frac{-\left(\varepsilon \Delta x/V_T\right)}{e^{\varepsilon \Delta x/V_T} - 1} n_i + \frac{\left(-\varepsilon \Delta x/V_T\right)}{e^{-\varepsilon \Delta x/V_T} - 1} n_{i+1} \right] \tag{4.16}$$

Define Bernoulli function

$$B(x) = \frac{x}{e^x - 1} \tag{4.17}$$

$$J_{i+\frac{1}{2}} = \frac{qD_n}{\Delta x}\left[-B\left(\frac{\varepsilon \Delta x}{V_T}\right) n_i + B\left(\frac{-\varepsilon \Delta x}{V_T}\right) n_{i+1} \right] \tag{4.18}$$

$$J_{i-\frac{1}{2}} = \frac{qD_n}{\Delta x}\left[-B\left(\frac{-\Delta V_{i-1}}{V_T}\right) n_{i-1} + B\left(\frac{\Delta V_{j-1}}{V_T}\right) n_i \right] \tag{4.19}$$

Using continuity equation in discretized form

$$\frac{dJ}{dx} = qR_{net} \tag{4.20}$$

$$\frac{J_{i+1} - J_{i-1}}{\Delta x} = qR_{net} \tag{4.21}$$

From equation (4.18) and (4.19) we can write system of linear equations from $i = 1$ to $i = N$

$$\frac{qD_n}{(\Delta x)^2}\left(B\left(\frac{-\Delta V_{i-1}}{V_T}\right) n_{i-1} - \left(B\left(\frac{-\Delta V_i}{V_T}\right) + B\left(\frac{\Delta V_{i-1}}{V_T}\right)\right) n_i \right. \tag{4.22}$$
$$\left. + B\left(\frac{-\Delta V_i}{V_T}\right) n_{i+1}\right) = qR_{net}$$

This system can be solved by putting it in matrix form $An = B$ where

$$A = \frac{qD_n}{\Delta x^2}\begin{pmatrix} M_1 & M_2 & 0 & 0 & \cdots & 0 \\ M_3 & M_4 & M_5 & 0 & \cdots & 0 \\ 0 & M_6 & M_7 & M_8 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ & 0 & 0 & 0 & M_{N-1} & M_N \end{pmatrix} \tag{1.23}$$

Where

$$M_1 = -\left(B\left(\frac{-(V_3 - V_2)}{V_T}\right) + B\left(\frac{V_2 - V_1}{V_T}\right)\right) \tag{1.24}$$

$$M_2 = M_3 = B\left(\frac{-(V_3 - V_2)}{V_T}\right) \tag{1.25}$$

$$M_4 = -\left(B\left(\frac{-(V_4 - V_3)}{V_T}\right) + B\left(\frac{V_3 - V_2}{V_T}\right)\right) \tag{1.26}$$

$$M_5 = M_6 = B\left(\frac{-(V_4 - V_3)}{V_T}\right) \tag{1.27}$$

$$M_7 = -\left(B\left(\frac{-(V_5 - V_4)}{V_T}\right) + B\left(\frac{V_4 - V_3}{V_T}\right)\right) \tag{1.28}$$

$$M_8 = B\left(\frac{-(V_5 - V_4)}{V_T}\right) \tag{1.29}$$

Asmaa A. Salama,Mohamed S. Abdel-wahed, D. A. Hammad, Mourad S. Semary, "Review of numerical solutions of differential equations applied to semiconductor materials," *International Journal of Multidisciplinary Research and Publications (IJMRAP)*, Volume 5, Issue 12, pp. 88-96, 2023.

$$M_{N-1} = B\left(\frac{-(V_{N-1}-V_{N-2})}{V_T}\right) \quad (1.30)$$

$$M_N = -\left(B\left(\frac{-(V_N-V_{N-1})}{V_T}\right)+B\left(\frac{V_{N-1}-V_{N-2}}{V_T}\right)\right) \quad (1.31)$$

$$B = \begin{pmatrix} qR_{net} - \frac{qD_n}{(\Delta x)^2}B\left(\frac{-(V_2-V_1)}{V_T}\right) \\ qR_{net} \\ \vdots \\ qR_{net} \\ qR_{net} - \frac{qD_n}{(\Delta x)^2}B\left(\frac{-(V_N-V_{N-1})}{V_T}\right) \end{pmatrix} \quad (4.32)$$

CASE STUDY

Scharfetter-Gummel Method was used to produce numerical solution of continuity equation. The output results were compared with exact results in the case of linear potential. The electron continuity equation is solved for the electron concentration n at N mesh points. n is shown versus distance x where: the starting point (a) is at x=0 nm, the ending point(b) is at x=L=40 nm ,$\Delta x = 1$nm, the number of points $N = \frac{b-a}{\Delta x}+1$=41 points ,the recombination-generation rate R_i is assumed to be zero, the electron mobility μ_n =1500 (cm2/(V-s))($D_n = \mu_n v_t$)(where v_t is thermal voltage) V is linear vector of N element from $V = 0$ to $V = 0.1, 0.2 and 0.3$, boundary condition n(1)=10 and n(N) = 20.

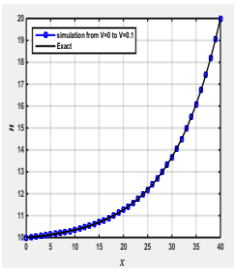

Fig. 7. Scharfetter-Gummel results compared with exact solution at V change from 0 to 0.1

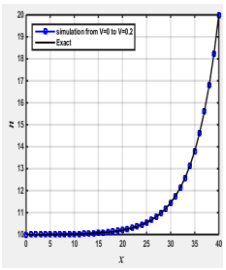

Fig. 8. Scharfetter-Gummel results compared with exact solution at V change from 0 to 0.2

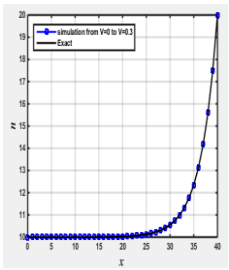

Fig. 9. Scharfetter-Gummel results compared with exact solution at V change from 0 to 0.3

Calculating norm error between exact solution and scharfetter-Gummel outcomes at various values of linear potential from $V = 0$ to $V = 0.1, 0.2, 0.3, ..., 0.8$ the results was shown in Fig. 10.

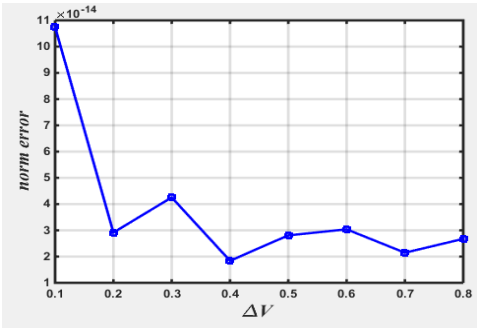

Fig. 10.Norm error between exact and Schrafetter-Gummel outcomes with various range of linear potential.

For the same case study above if we take $V = 0$ to $V = 0.1$ at $\Delta x = 0.5 and 2$.

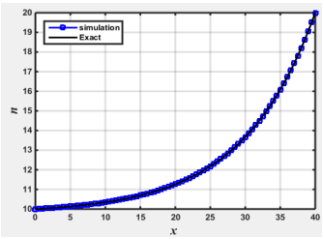

Fig. 11.Scharfetter-Gummel outcomes and exact solution at V change from 0 to 0.1 and Δx =0.5nm

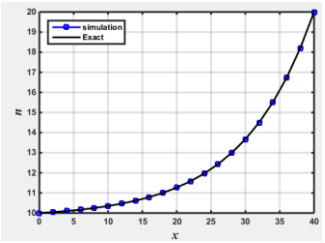

Fig. 12.Scharfetter-Gummel outcomes and exact solution at V change from 0 to 0.1 and Δx =2nm

Calculating norm error between exact solution and scharfetter-Gummel outcomes at various values of Δx (Δx=0.5 nm, 1nm and 2nm) from $V = 0$ to $V = 0.1$ the results was shown in Fig. 12.

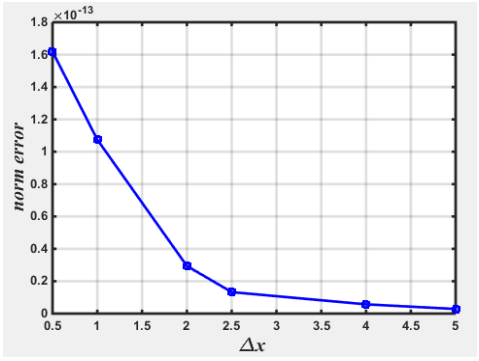

Fig. 13.Norm error between exact and Scharfetter-Gummel outcomes with various Δx.

From the norm error above, we can deduce that the error shown is the round-off error not the discretization error. Round-off error is the variance between a particular algorithm's output produced using exact arithmetic and a similar algorithm's output produced using finite-precision, rounded arithmetic. Round-off errors accumulates with increase the number of calculations.

For the same case study, we changed potential from linear potential to function $V = 10^{10} x^2$ .At various values of Δx, the output results are more accurate for smaller of Δx and this implies that the output error in this case is the discretization error. Discretization error can usually be reduced by using a more finely spaced mesh on the expense of increased computational cost.

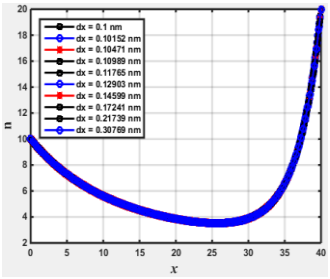

Fig. 14. Scharfetter-Gummel outcomes and exact solution at various values of Δx

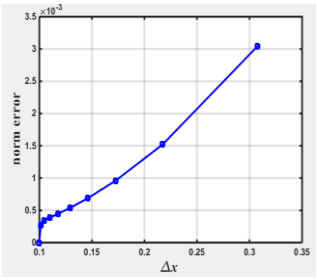

Fig. 15.Norm error between exact and Scharfetter-Gummel outcomes with various values of Δx

V. CONCLUSION

This paper presents several numerical methods of solving semiconductor equations. Schrodinger equation is solved using Numerov Method and Finite Difference Method. Numerov Method produces more accurate results than Finite Difference Method compared to exact results. Poisson equation is solved using Finite difference method and output results are compared to exact results. Also absolute error is shown using Matlab. We can see that absolute error between exact and numerical outcomes of Poisson equation is very small. Continuity equation is solved using Scharfetter-Gummel Mehtod. The paper presents derivation of Scharfetter-Gummel Method. Output results from Scharfetter-Gummel Mehtod is compared with exact solution and the output graph is shown using Matlab.

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