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Computational Technique for Coupled Poisson-Schrödinger Equation With Mixed Boundary Conditions in Nano Scale Semiconductor Devices Using Iterative Finite Difference Schemes

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Abstract: Accurate and effective solutions of coupled Poisson-Schrödinger equations are sought to enable higher degree of accuracy in nanoscale semiconductor device simulations. This is due to the fact that the system accounts for quantum confinement effects that surface in nanoscale devices and induces significant alterations in the device characteristics. In this article, we formulate and analyze a novel and efficient computational technique which besides deriving self-consistent solutions also attends to the singularly perturbed nature of the Schrödinger equation. The coupled system with appropriate boundary conditions is investigated using singular perturbation approach applying iterative finite difference schemes on various layer adapted meshes. A meticulous convergence analysis of an iterative scheme on the coupled system comprising of singularly perturbed reaction diffusion equation subjected to Robin boundary conditions is the first of its kind. The desired efficacy of the proposed numerical technique is confirmed by presenting computational findings.

Key Words: Poisson-Schrödinger equation, singular perturbation, Shishkin and B-Shishkin meshes, finite difference method.

Contents

1. Introduction

The past few decades witnessed an outbreak in technological innovations and significant advances in all fields of our day today lives. Effective tools that aid in better understanding and implementation of the underlying theories has played a crucial role in the path towards groundbreaking innovations. Mathematical modeling which creates representations of the real world phenomena has always served as a key tool to gain insights and predict various physical, biological and economic systems. Differential equations have been an integral part of mathematical modeling as they provide a strong framework to comprehend the understanding of many dynamical systems [7,6,5,11]. Of these are systems with multiscale behavior which are modeled by a particular class of differential equations termed 'Singularly Perturbed Differential

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Equations (SP Diff Eqs).

The class of differential equations characterized by the presence of a small parameter multiplying the highest order derivative terms are categorized into SP Diff Eqs. The solutions to such differential equations exhibit a varied behavior of rapid change towards the boundary (or interior). The occurrence of such regions termed 'layers' (boundary/interior) pose a challenge as the exact solutions either fail to exist or are hard to be approximated with good precision using numerical techniques.

A considerable literature [14,10,17,15,4,3,16]can be found on the studies of SP Diff Eqs. Aerodynamics, plasmadynamics, hydrodynamics, oceanography, meteorology, the mathematical modeling of ecology [8], physiological processes [1], control theory, digital electronics [21], immune responses [2] and modeling of semiconductor devices [13] are few realms in which studies on SP Diff Eqs are of great significance. The few recent works of Sridevi et. al [19,18] studied about the quantum confinement effects in MoS_2 based transistors using the coupled Poisson-Schrödinger system given below:

$$-\phi^{''}(x) = \frac{q}{\varepsilon_p}[N(x) - P(x) + N_A - N_D] \tag{1.1}$$

$$-\frac{\hbar^2}{2m^*}\psi^{''}(x) + q\phi(x) = E\psi(x), \qquad x \in \Omega \tag{1.2}$$

subject to

$$\phi(0) = \phi(a) = 0, \tag{1.3}$$

$$\psi(0) - \psi^{'}(0) = \alpha, \psi(a) + \psi^{'}(a) = \beta \tag{1.4}$$

where $\Omega = (0, a), a \in t_{ch}$ where t_{ch} is the device channel length (in nano meters). Here, $P(x)$ and $N(x)$ are hole and electron concentrations respectively, $N(D)$ the donor concentration and $N(A)$ the acceptor concentrations, E energy of the system, $\hbar$ Planck's constant $(6.626 \times 10^{-34} J.s)$ and m^* electron effective mass.

The small parameter $\frac{\hbar^2}{2m^*}$ that multiplies the highest order term in Schrödinger equation categorizes it into the class of SP Diff Eqs. The estimation of accurate solutions to this system is crucial due to the fact that it aids in comprehending the varied device characteristics due to quantum effects in semiconductor devices of nano scale dimensions. Various studies on deriving the solution to (1.1)-(1.2) subject to (1.3)-(1.4) has been carried out. But, a numerical technique that accounts to its Singularly Perturbed (SP) nature is yet to be done. Hence, we set forth a study to bridge the gap and propose an effective numerical technique followed by a meticulous analysis using SP approach.
The proposed finite difference scheme is applied on various layer adapted meshes to enhance increased understanding of layers. The technique is implemented in an iterative fashion starting off with initial electron density approximation, plug it into the Poisson equations solving which gives the surface potential. This is then input into the Schrödinger equation to solve for wave equations which finally derive a new improved electron density. The Poisson equation is again solved using the newly derived electron density and the process is repeated until a desirable convergence is obtained. The framing of a numerical technique that accounts the SP nature of the system and an analysis of an iterative framework using SP methods is first of its kind. The flow chart of the algorithm used is depicted in figure (1).

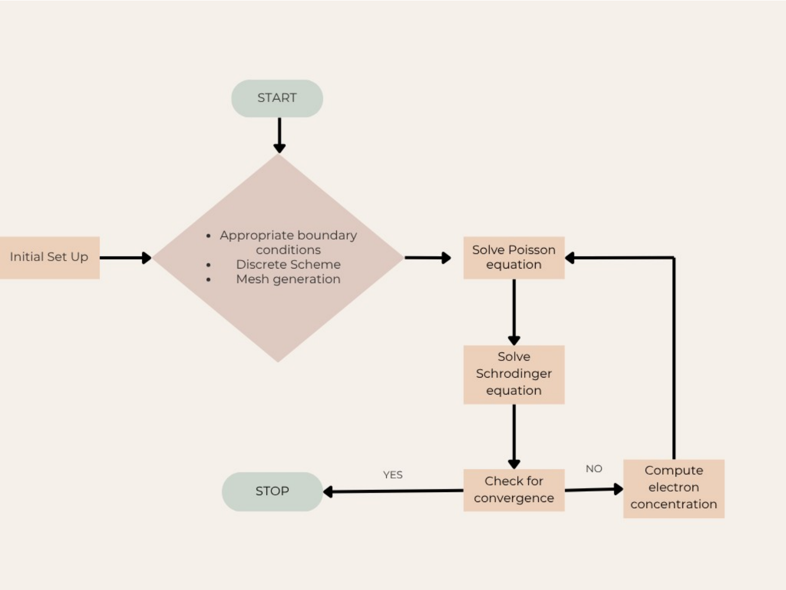

Figure 1: Iterative Algorithm

Remark: Throughout this article, C denotes a generic constant n and N the number of iterations and number of mesh intervals respectively and we assume $\sqrt{\varepsilon} leq C N^{-1}$. $||.||$ represents maximum norm which is defined as

$$||u_i|| = \max_{x\in\Omega} |u_i(x)| \qquad \textit{and} \qquad ||\mathbf{u}|| = \max_{i=1,2} ||u_i||,$$

where, $\Omega = (0, a)$, $\mathbf{u} = (u_1, u_2)$

2. The Iterative Problem

We formulate an iterative procedure to solve the coupled Poisson-Schrödinger equation (1.1)-(1.2) subject to (1.3)-(1.4) as follows:

The initial electron concentration be n_1.
Find $(u_{p,n}, u_{s,n}) \in C^2(\Omega) \times C^2(\Omega)$ such that :

$$\begin{cases} \left.\begin{array}{l} L_1 u_{p,n} \equiv -u''_{p,n} = \frac{q}{\varepsilon_p}\left[n_n(x) - p(x) + N_A - N_D\right] \\ u_{p,n}(0) = u_{p,n}(a) = 0 \end{array}\right\} n = 1, 2, \cdots & \text{(2.1a)} \\ \left.\begin{array}{l} L_2 u_{s,n} \equiv -\varepsilon u''_{s,n} + \left[q u_{p,n} - E\right] u_{s,n} = 0 \\ B_L u_{s,n}(0) = \alpha, B_R u_{s,n}(a) = \beta \end{array}\right\} n = 1, 2, \cdots & \text{(2.1b)} \\ n_n(x) = DOS.f(E)|u_{s,n-1}(x)|^2, \qquad n = 2, 3, \cdots & \text{(2.1c)} \end{cases}$$

where, $\varepsilon = \frac{\hbar^2}{2m^*}$, $B_L u_{s,n} \equiv u_{s,n} - u'_{s,n}$, $B_R u_{s,n} \equiv u_{s,n} + u'_{s,n}$, $q u_{p,n} - E \geq \gamma_n > 0$ and DOS is density of states and $f(E)$ denotes Fermi Dirac distribution.

3. Analytical Properties of the solution

3.1. Maximum Principle

Theorem 3.1.1. *Let L_1 be the differential operator defined above in (2.1a) and $u(x) \in C^2(\Omega)$. Suppose $u(0) \geq 0$, $u(a) \geq 0$ and $L_1 u(x) \geq 0, \forall x \in \Omega$. Then, $u(x) \geq 0, \forall x \in \bar{\Omega}$.*

Proof. The theorem can be proved using the test function $p(x) = \frac{x+a}{x+b}$, $b > a$, $x \in (0, a)$ and proceeding as in [20]. □

Theorem 3.1.2. *Let L_2 be the differential operator defined above in (2.1b) and $u(x) \in C^2(\Omega)$. Suppose $B_L u(0) \geq 0, B_R u(a) \geq 0$ and $L_2 u(x) \geq 0, \forall x \in \Omega$. Then, $u(x) \geq 0, \forall x \in \bar{\Omega}$.*

Proof. If the statement is false, we find x^* such that

$$u(x^*) = \min_{x \in \bar{\Omega}} u(x)$$

Then, if $x^* \in \Omega$, then, $L_2 u(x^*) = -\varepsilon u^{''}(x^*) + b(x^*)u(x^*) < 0$ a contradiction. Whereas, if $x^* = 0$, gives $B_L(u(0)) < 0$ and $x^* = a$ gives $B_R(u(0)) < 0$ posing a contradiction. □

3.2. Stability and Derivative Estimates

Theorem 3.2.1. *If problem (2.1a) has a solution $u_{p,n}(x)$, then,*

$$|u_{p,n}(x)| \leq C \max\{|u_{p,n}(0)|, |u_{p,n}(a)|, ||L_1 u_{p,n}(x)||\}, \quad \forall x \in \bar{\Omega}$$

Proof. Considering the barrier function

$$B_1{}^{\pm}(x) = M_1 p(x) \pm u_{p,n}(x)$$

where, $M_1 = \max\{|u_{p,n}(0)|, |u_{p,n}(a)|, ||L_1 u_{p,n}(x)||\}$ and $p(x)$ as defined in the proof of Theorem 3.1.1. Applying Theorem 3.1.1 on $B_1{}^{\pm}(x)$ derives the required result.
□

Theorem 3.2.2. *Let $v(x) \in C^2(\Omega)$ be the solution of the problem class:*

$$\begin{cases} L_2 v \equiv -\varepsilon v^{''}(x) + (q u_{p,n}(x) - E)v(x) = f(x) \\ B_L v(0) = \alpha \\ B_R v(a) = \beta \end{cases}$$

where, $f \in C^2(\Omega)$. Then,

1. $||v(x)|| \leq \max\{||B_L v(0)||, ||B_R v(a)||\} + \frac{||L_2 v(x)||}{\gamma}$
2. $|v^{(k)}(x)| \leq C\left(1 + \varepsilon^{\frac{-k}{2}}\right)$, $k = 1, 2, 3, 4$ *where, $v^{(k)}$ denotes the k^{th} derivative of v.*

Proof. Construct barrier functions $B_2^{\pm}(x) = M_2 \pm v(x)$, where,
$M_2 = \max\{||B_L v(0)||, ||B_R v(a)||\} + \frac{||L_2 v(x)||}{\gamma}$. Then it easily follows that $B_2^{\pm}(x)$ satisfies Theorem 3.1.2 deriving the desired stability. Whereas, the derivative estimate can be formulated by proceeding as in [12], and combining the stability result. □

3.2.1. Solution Decomposition. Due to the singularly perturbed nature of (2.1b), we decompose the solution $u_{s,n}(x)$ to facilitate an efficient analysis.

Theorem 3.2.3. *Let $u_{s,n}(x) = u_{s,n}^L(x) + u_{s,n}^S(x)$ be the decomposition of the solution where, $u_{s,n}^L(x)$ and $u_{s,n}^S(x)$ corresponds to the layer component and the smooth component respectively. Then, for $k = 1, 2, 3, 4$,*

$$(u_{s,n}^S)^{(k)}(x) \leq C(1 + \varepsilon^{1-\frac{k}{2}} e_n(x)) \tag{3.1}$$

$$(u_{s,n}^L)^{(k)} \leq C\varepsilon^{\frac{-k}{2}} e_n(x) \tag{3.2}$$

where, $e_n(x) = e^{-x\sqrt{\frac{\gamma_n}{\varepsilon}}} + e^{-(a-x)\sqrt{\frac{\gamma_n}{\varepsilon}}}$,$q u_{p,n} - E \geq \gamma_n > 0$, for each $n = 1, 2, \cdots$

4. The Discrete Problem

4.1. Layer Adapted Mesh

To effectively capture the boundary layers, the domain Ω is subdivided as $\Omega = \Omega_L \cup \Omega_S \cup \Omega_R$ where, $\Omega_L = (0,\sigma), \Omega_S = (\sigma, a-\sigma)$and $\Omega_R = (a-\sigma, a)$ where, σ is the transition point defined as $\sigma = 2\sqrt{\frac{\varepsilon}{\gamma}}\ln N$. Two mesh generating functions $g_1(x)$ and $g_2(x)$ monotonically increasing and decreasing respectively are chosen such that

$$g_1(0) = 0, \quad g_2(1) = 0$$

$$g_1(\frac{1}{4}) = \ln N, \quad g_2(\frac{3}{4}) = \ln N.$$

The mesh points x_j's, $j = 0, 1, \cdots, N$ are described as

$$x_j = \begin{cases} 2\sqrt{\frac{\varepsilon}{\gamma}} g_1(t_j), & 0(1)\frac{N}{4} \\ \frac{2}{N}\left(ai - N\frac{a}{4} - \sigma\frac{N}{2}\right), & \frac{N}{4}+1(1)\frac{3N}{4} \\ a - 2\sqrt{\frac{\varepsilon}{\gamma}} g_2(t_j), & \frac{3N}{4}+1(1)N \end{cases}$$

where, $t_j = \frac{j}{N}$ and we define new functions as $g_j = -\ln f_j, j = 1, 2.$

The mesh characterizing functions f_j's are of various types [9] namely Shishkin mesh (Sh-mesh), Bakhvalov Shishkin mesh (B-Sh mesh), Modified Bakhvalov Shishkin mesh (with $q = \frac{1}{2} + \frac{1}{2\ln N}$) (Mod B-Sh mesh), Polynomial Shishkin mesh (with $m > 1$) (P-Sh mesh) are presented in Table (1) below.

	Sh-mesh	B-Sh mesh	Mod B-Sh mesh	P-Sh mesh
$f_1(t)$	$e^{-4t\ln N}$	$1 - 4\frac{N-1}{N}t$	$e^{\frac{-2t}{q-2t}}$	$N^{-(4t)^m}$
$f_2(t)$	$e^{-4(1-t)\ln N}$	$1 - 4\frac{N-1}{N}(1-t)$	$e^{\frac{-2(1-t)}{q-2+2t}}$	$N^{-(4(1-t))^m}$

Table 1: Mesh characterizing functions

5. Iterative Finite Difference Scheme (IFDS)

An iterative numerical scheme using finite differences are proposed in this section to derive the approximate solutions of (2.1a)-(2.1b).

Using standard central finite difference scheme on $\Omega^N = \{x_j, j = 0, 1, 2, \cdots, N\}$, we derive the following finite difference scheme for (2.1a)-(2.1b).

Find $(U^N_{p,n}, U^N_{s,n})$ such that,

$$\begin{cases} \left.\begin{aligned} & L_1^N U^N_{n,p,j} \equiv -\delta^2 U^N_{p,n,j} = \frac{q}{\varepsilon_p}\left[n^N_n(x_j) - p + N_A - N_D\right] \\ & U^N_{p,n,0} = U^N_{p,n,a} = 0 \end{aligned}\right\} n = 1,2,3,\cdots & \text{(5.1a)} \\ \left.\begin{aligned} & L_2^N U^N_{s,n,j} \equiv -\varepsilon\delta^2 U^N_{s,n,j} + \left[qU^N_{p,n,j} - E\right] U^N_{s,n,j} = o, \\ & B_L^N U^N_{s,n,0} = \alpha \ \ B_R^N U^N_{s,n,N} = \beta \end{aligned}\right\} n = 1,2,\cdots & \text{(5.1b)} \\ n^N_n(x_j) = DOS.f(E)|U^N_{s,n-1,j}|^2, \qquad n = 2,3,\cdots & \text{(5.1c)} \end{cases}$$

where, $U^N_{p,n,j} = \{U^N_{p,n}(x_j)\}^N_{j=0}$, $U^N_{s,n,j} = \{U^N_{s,n}(x_j)\}^N_{j=0}$ and $\{n^N_1(x_j)\}^N_{j=0}$ is the initial electron concentration approximation.

Here,

$$\delta^2 v_{n,j}^N = \frac{2}{x_{j+1} - x_{j-1}} \left(\frac{v_{n,j+1}^N - v_{n,j}^N}{x_{j+1} - x_j} - \frac{v_{n,j}^N - v_{n,j-1}^N}{x_j - x_{j-1}} \right)$$

$$B_L^N v_{n,j}^N = v_{n,j}^N - \frac{v_{n,j+1}^N - v_{n,j}^N}{x_{j+1} - x_j}$$

and

$$B_R^N v_{n,j}^N = v_{n,j}^N + \frac{v_{n,j}^N - v_{n,j-1}^N}{x_j - x_{j-1}}$$

Now, we proceed to the discrete analytical properties of the solution.

Theorem 5.0.1. *Let L_1^N be the differential operator defined above in (5.1a). Suppose $U(x_0) \geq 0$, $U(x_N) \geq 0$ and $L_1^N U(x_j) \geq 0, \;\; j = 1, 2, \cdots, N-1$. Then, $U(x_j) \geq 0, \forall x_j \in \Omega^N$.*

Proof. Choosing a discrete test function $p(x_j) = \frac{x_j + x_0}{x_j + b}, \quad x_j \in \Omega^N, b > x_N$ and adopting the idea from [20] we deduce the property. □

Lemma 5.0.2. *For any $U_{p,n}^N$ that satisfies (5.1a) we have,*

$$|U_{p,n,j}^N| \leq C \max\left\{|U_{p,n,0}^N|, |U_{p,n,N}^N|, ||L_1^N U_{p,n,j}^N||\right\}, \quad \forall x_j \in \Omega^N, \;\; n = 1, 2, \cdots$$

Proof. The proof is similar to the derivation of Theorem (3.2.1) using the same discrete test function $p(x_j)$ as above and constructing the following barrier function

$$B_{1,j}^{N\,\pm} = M_1^N p(x_j)(x_0 + b)^2 \pm U_{p,j}^N$$

where, $M_1^N = \max\left\{|U_{p,n,0}^N|, |U_{p,n,N}^N|, ||L_1^N U_{p,n,j}^N||\right\}$ □

Theorem 5.0.3. *If $U_{s,j}^N$ is the solution of (5.1b) and suppose $B_L^N U_{s,n,0}^N \geq 0, B_R^N U_{s,n,N}^N \geq 0$ and $L_2^N U_{s,n,j}^N \geq 0, \;\; j = 1, 2, \cdots, N-1$. Then, $U_{s,n,j}^N \geq 0, \forall x_j \in \Omega^N$.*

Proof. The proof is carried out using method of contradiction as in the continuous case above.

□

Lemma 5.0.4. *Let V_j be the solution of the problem class:*

$$\begin{cases} L_2^N V_j \equiv -\varepsilon \delta^2 V_j + (q U_{p,n,j}^N - E) V_j = f_j \\ B_L^N V_0 = \alpha \\ B_R^N V_{n,N} = \beta \end{cases}$$

Then,

$$||V_j|| \leq \max\left\{\left|B_L^N V_0\right|, \left|B_L^N V_N\right|\right\} + \frac{||f||}{\gamma} \tag{5.2}$$

Proof. Proceeding as in Theorem 3.2.2 by choosing a barrier function $B_2^N(x_j) = M_2^N \pm V(x_j)$ where $M_2^N = \max\left\{\left|B_L^N V_0\right|, \left|B_L^N V_N\right|\right\} + \frac{||f||}{\gamma}$ and using Theorem 5.0.3 the stability can be established. □

We now proceed to the error estimation.

6. Error Estimation

In this section, we derive the error generated in the proposed IFDS. The analysis is carried out in Shishkin meshes.

We initiate the analysis by deriving the associated truncation errors.

Let the operator L_2^{*N} be as defined below:

$$\begin{cases} \left.\begin{array}{l} L_1^N U_{p,n,j}^{*N} \equiv -\delta^2 U_{p,n,j}^{*N} = \frac{q}{\varepsilon_p}\left[n_n^{*N} - p + N_A - N_D\right] \\ U_{p,n}^{*N}(x_0) = U_{p,n}^{*N}(x_N) = 0 \end{array}\right\} n = 1, 2, 3, \cdots & (6.1a) \\ \left.\begin{array}{l} L_2^{*N} U_{s,n,j}^{*N} \equiv -\varepsilon\delta^2 U_{s,n,j}^{*N} + \left[q u_{p,n,j}(x) - E\right] U_{s,n,j}^{*N} = 0, \\ B_L^N U_{s,n}^{*N}(x_0) = \alpha, \quad B_R^N U_{s,n}^{*N}(x_N) = \beta \end{array}\right\} n = 1, 2, \cdots & (6.1b) \\ n_n^{*N}(x_j) = DOS.f(E)|U_{s,n-1}^{*N}(x_j)|^2, \qquad n = 2, 3, \cdots & (6.1c) \end{cases}$$

The truncation error $TE_{n,j}^p = \delta^2 U_{p,n,j}^N - u''_{p,n,j}$ is computed using Taylor series expansions and we derive,

$$TE_{n,j}^p = \begin{cases} \mathcal{O}(h) & x_j \in \{\sigma, a - \sigma\} \\ \mathcal{O}(h^2) & x_j \in \Omega^N \setminus \{\sigma, a - \sigma\} \end{cases}$$

which derives,

$$|TE_{n,j}^p| = |L_1^N(U_{p,n}^{*N} - u_{p,n})(x_j)| \le CN^{-1}, \quad x_j \in \Omega^N \tag{6.2}$$

Now, the truncation error for the second order singularly perturbed equation is obtained as follows:

$$TE_{n,j}^S = L_2^{*N}(U_{s,n}^{*N} - u_{s,n})(x_j) = \varepsilon\left(\frac{d^2}{dx^2} - \delta^2\right)u_{s,n}(x_j) = \begin{cases} Ch_0|u''_{s,n}|, & x_j = 0 \\ Ch_{N-1}|u''_{s,n}|, & x_j = a \\ C\varepsilon(h_i + h_{i-1})|u_{s,n}^{(3)}|, & x_j \in \{\sigma, a - \sigma\} \\ C\varepsilon h_{i-1}^2|u_{s,n}^{(4)}| & otherwise \end{cases}$$

Consider the decomposition $u_{s,n}(x) = u_{s,n}^L(x) + u_{s,n}^S(x)$. Using the classical estimates from [12] and Theorem 3.2.3 above,

$$|L_2^{*N}(U_{s,n}^{S^{*N}} - u_{s,n}^S)(x_j)| \le \begin{cases} CN^{-1}, & x_j \in \{0, a\} \\ CN^{-2}, & x_j \in \Omega^N \setminus \{0, a\} \end{cases} \tag{6.3}$$

Whereas for the layer component, we consider the different cases as below.

1. when $\sigma = \frac{1}{4}$, we have $h_i = \frac{1}{N}$ and hence $\frac{1}{\sqrt{\varepsilon}} \le C \ln N$.
   From [12] and Theorem 3.2.3, we derive

   $$|L_2^{*N}(U_{s,n}^{L^{*N}} - u_{s,n}^L)(x_j)| \le C(N^{-1}\ln N)^2, \quad x_j \in \Omega^N \setminus \{0, a\}.$$

   whereas for $x_j \in \{0, a\}$,

   $$|L_2^{*N}(U_{s,n}^{L^{*N}} - u_{s,n}^L)(x_j)| \le h_i|(u_{s,n}^L)''| \le C(N^{-1}\ln N).$$

2. $\sigma < \frac{1}{4}$, the mesh is piecewise uniform with $h_i = \frac{4\sigma}{N}$ and $\frac{2(1-2\sigma)}{N}$ in layer and regular region respectively. Then by [12] and Theorem 3.2.3,

$$|L_2^{*N}(U_{s,n}^{L^{*N}} - u_{s,n}^L)(x_j)| \quad \leq \quad C(N^{-1}\ln N)^2, \quad x_j \in \Omega^N \setminus \{0, a\}.$$

Further, when $x_j \in \{0, a\}$,

$$|L_2^{*N}(U_{s,n}^{L^{*N}} - u_{s,n}^L)(x_j)| \leq h_i|(u_{s,n}^L)^{''}| = h_i|(u_{s,n}^L)^{'}| \leq C(N^{-1}\ln N)$$

Hence,

$$|L_2^{*N}(U_{s,n}^{L^{*N}} - u_{s,n}^L)(x_j)| \leq CN^{-1}\ln N, \ \ \forall x_j \in \Omega^N. \tag{6.4}$$

Finally combining (6.3) and (6.4), we derive

$$|TE_{n,j}^S| = |L_2^{*N}(U_{s,n}^N - u_{s,n})(x_j)| \leq CN^{-1}\ln N, \quad \forall x_j \in \Omega^N \tag{6.5}$$

□

Theorem 6.0.1. *Let $(u_{p,n}, u_{s,n})$ and $(U_{p,n}^{*N}, U_{s,n}^{*N})$ be the solutions of (2.1a)-(2.1b) and (6.1a)-(6.1b) respectively. Then,*

$$||u_{p,n} - U_{p,n}^{*N}|| \leq CN^{-1} \tag{6.6}$$

$$||\left(u_{s,n} - U_{s,n}^{*N}\right)|| \leq C\left(N^{-1}\ln N\right), \qquad n \in \mathbb{N} \tag{6.7}$$

Proof. For $x_j \in \Omega^N$, consider the mesh function

$$f_p^{\pm}(x_j) = CN^{-1}(a+b)^2\left(\frac{x_j + a}{x_j + b}\right) \pm e_n^p(x_j).$$

where, $e_n^p(x_j) = (u_{p,n} - U_{p,n}^{*N})(x_j)$ and $b > a$. Then, using (6.2) we get $f_p^{\pm}(x_j)$ satisfies Theorem 5.0.1 by proper choice of C and hence,

$$||u_{p,n} - U_{p,n}^{*N}|| \leq CN^{-1}$$

Now construct the mesh function

$$f_s^{\pm}(x_j) = \frac{\left(CN^{-1}\ln N\right)}{\gamma_n} \pm e_n^s(x_j)$$

where, $e_n^s(x_j) = \left(u_{s,n} - U_{s,n}^{*N}\right)(x_j)$. Then, we observe $B_L^N f_s^{\pm}(x_0), B_R^N f_s^{\pm}(x_N) \geq 0$, and also using (6.5) that, $L_2^{*N} e_n^s(x_j) \geq 0$, $\forall x_j \in \Omega^N$. Thus from Theorem 5.0.3, it follows that

$$|e_n^s(x_j)| \quad \leq \quad C\left(N^{-1}\ln N\right)$$

This completes the proof of the theorem.

□

Theorem 6.0.2. *Let $(U_{p,n}^{*N}, U_{s,n}^{*N})$ and $(U_{p,n}^N, U_{s,n}^N)$ be the solutions of (6.1a)-(6.1b) and (5.1a)-(5.1b) respectively. Then, for n=2,3,4 $\cdots$ we have*

$$||U_{p,n}^{*N} - U_{p,n}^N|| \leq qC_1||u_{s,n-1} - U_{s,n-1}^N|| \tag{6.8}$$

$$||U_{s,n}^{*N} - U_{s,n}^N|| \leq qC_2||u_{p,n} - U_{p,n}^N||, \qquad 0, 1, 2, \cdots, N \tag{6.9}$$

Proof. Let $e^{p,N}_{n,j} = U^{*N}_{p,n}(x_j) - U^N_{p,n}(x_j)$. Then it can be seen that $e^{p,N}_{n,j}$ satisfies the discrete problem

$$\begin{cases} L^N_1(e^{p,N}_{n,j}) = \frac{q}{\varepsilon_p}(DOS.F(E))(|u_{s,n-1,j}|^2 - U^N_{s,n-1,j}|^2), \\ e^{p,N}_{n,0} = 0, e^{p,N}_{n,N} = 0. \end{cases} \tag{6.10}$$

Therefore, by Lemma 5.0.2,

$$|e^{p,N}_{n,j}| \leq C\frac{q}{\varepsilon_p}|u_{s,n-1,j} - U^N_{s,n-1,j}| = qC_1|u_{s,n-1,j} - U^N_{n-1,j}|$$

Similarly, $e^{s,N}_{n,j} = U^{*N}_{s,n}(x_j) - U^N_{s,n}(x_j)$ satisfies the discrete problem

$$\begin{cases} L^N_2(e^{s,N}_{n,j}) = q\Psi^N_{n,j}(U^N_{p,n,j} - u_{p,n,j}), \\ B^N_L(e^{s,N}_{n,0}) = 0; B^N_R(e^{s,N}_{n,N}) = 0. \end{cases} \tag{6.11}$$

Applying Lemma 5.0.4,

$$|e^{s,N}_{n,j}| \leq qC_2|u_{p,n,j} - U^N_{p,n,j}| \tag{6.12}$$

□

Now, we derive the final error estimate using the following triangle inequality.

Let $(u_{p,n}, u_{s,n})$, $(U^{*N}_{p,n}, U^{*N}_{s,n})$ and $(U^N_{p,n}, U^N_{s,n})$ be the solutions of (2.1a)-(2.1b), (6.1a)-(6.1b) and (5.1a)-(5.1b) respectively. Then,

$$||u_{p,n} - U^N_{P,n}|| \leq ||(u_{p,n}) - U^{*N}_{P,n}|| + ||U^{*N}_{p,n} - U^N_{P,n}|| \tag{6.13}$$

$$||u_{s,n} - U^N_{s,n}|| \leq ||(u_{s,n}) - U^{*N}_{s,n}|| + ||U^{*N}_{s,n} - U^N_{s,n}|| \tag{6.14}$$

Theorem 6.0.3. *Let $(u_{p,n}, u_{s,n})$ and $(U^N_{p,n}, U^N_{s,n})$ be the solutions of (2.1a)- (2.1b) and (5.1a)-(5.1b) respectively. Then,*

$$||(u_{p,n} - U^N_{p,n})|| \leq CN^{-1}$$
$$||(u_{s,n} - U^N_{s,n})|| \leq CN^{-1}\ln N$$

Proof. From (6.6) in Theorem 6.0.1,

$$|(u_{p,1,j} - U^N_{p,1,j})| \leq C_P N^{-1}$$

Next using (6.7) in Theorem 6.0.1 and (6.9) from Theorem 6.0.2 derives,

$$\begin{aligned} |(u_{s,1,j} - U^N_{s,1,j})| &\leq |(u_{s,1,j} - U^{*N}_{s,1,j})| + |(U^{*N}_{s,1,j} - U^N_{s,1,j})| \\ &\leq C(N^{-1}\ln N) + qC_P N^{-1} \\ &\leq C_S(N^{-1}\ln N) \end{aligned}$$

Similarly, using (6.6) in Theorem 6.0.1 and (6.8) in Theorem 6.0.2 we obtain,

$$\begin{aligned} |(u_{p,2,j} - U^N_{p,2,j})| &\leq |(u_{p,2,j} - U^{*N}_{p,2,j})| + |(U^{*N}_{p,2,j} - u^N_{p,2,j})| \\ &\leq CN^{-1} + qC_S N^{-1}\ln N \\ &\leq C_P N^{-1} \end{aligned}$$

Following the same procedure in an iterative fashion, for $n = 2, \cdots$ we estimate,

$$\begin{aligned} ||(u_{p,n} - U^N_{p,n})|| &\leq C_P N^{-1} \\ ||(u^N_{s,n} - U^N_{s,n})|| &\leq C_S(N^{-1}\ln N) \end{aligned}$$

□

7. Computational Results

In this section, the theoretical results are validated by carrying out few computations. The obtained order of convergence assures the accuracy of the proposed IFDS. Double mesh principle was imposed to compute order of convergence ORD_n^N as shown below:

$$ORD_{p,n}^N = log_2\left(\frac{ERR_{p,n}^N}{ERR_{p,n}^{2N}}\right) \qquad ORD_{s,n}^N = log_2\left(\frac{ERR_{s,n}^N}{ERR_{s,n}^{2N}}\right)$$

where

$$ERR_{p,n}^N = ||U_{p,n}^N - U_{p,n}^{2N}||, \qquad ERR_{s,n}^N = ||U_{s,n}^N - U_{s,n}^{2N}||$$

Computations are carried out for channel length of $5nm$ using parameters from [19]. Table 2 and Table 3 presents the error obtained in Sh-mesh and B-Sh mesh respectively. Whereas, the order of convergence for Sh-mesh and B-Sh mesh are given in in Table 4 and Table 5 respectively. Also, figure (2) shows the error in Shrodinger equation when $N = 1024$ and $n = 4$ in Sh-meshes.

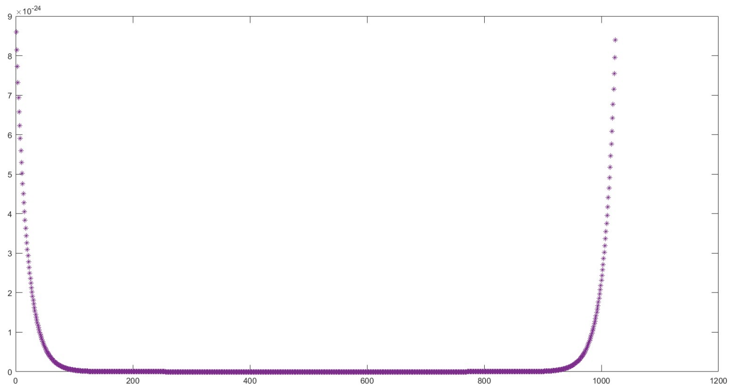

Figure 2: **Error graph (Shcrodinger equation)**

Table 2: **Values on $ERR_{p,n}^N$ and $ERR_{s,n}^N$ in maximum norm in Sh-mesh**

N \ n		2	3	4
16	$ERR_{p,n}^N$	3.177795409490151e-22	3.177795409490151e-22	3.177795409490151e-22
	$ERR_{s,n}^N$	2.801653240021689e-21	2.801653240021783e-21	2.801653240021783e-21
32	$ERR_{p,n}^N$	1.641860960953611e-22	1.641860960953611e-22	1.641860960953611e-22
	$ERR_{s,n}^N$	1.763110920514982e-21	1.763110920514878e-21	1.763110920514878e-21
64	$ERR_{p,n}^N$	8.341712940316192e-23	8.341712940316192e-23	8.341712940316192e-23
	$ERR_{s,n}^N$	9.635713317671357e-22	9.635713317670800e-22	9.635713317670800e-22
128	$ERR_{p,n}^N$	4.203958498195839e-23	4.203958498195839e-23	4.203958498195839e-23
	$ERR_{s,n}^N$	5.252431055172272e-22	5.252431055171971e-22	5.252431055171971e-22
256	$ERR_{p,n}^N$	2.110254749553466e-23	2.110254749553466e-23	2.110254749553466e-23
	$ERR_{s,n}^N$	2.871719369959479e-22	2.871719369959314e-22	2.871719369959314e-22
512	$ERR_{p,n}^N$	1.057196242632051e-23	1.057196242632051e-23	1.057196242632051e-23
	$ERR_{s,n}^N$	1.572403448750841e-22	1.572403448750698e-22	1.572403448750698e-22
1024	$ERR_{p,n}^N$	5.291153303112054e-24	5.291153303112054e-24	5.291153303112054e-24
	$ERR_{s,n}^N$	8.598849792957172e-23	8.598849792953786e-23	8.598849792953786e-23

Table 3: **Values of $ERR_{p,n}^N$ and $ERR_{s,n}^N$ in maximum norm in B-Sh mesh**

N \ n		2	3	4
16	$ERR_{p,n}^N$	2.444458007756365e-21	2.444458007756365e-21	2.444458007756365e-21
	$ERR_{s,n}^N$	3.142212272849887e-22	3.142212272850075e-22	3.142212272849887e-22
32	$ERR_{p,n}^N$	1.262969970632269e-21	1.262969970632269e-21	1.262969970632269e-21
	$ERR_{s,n}^N$	1.763110920514879e-22	1.763110920514985e-22	1.763110920514879e-22
64	$ERR_{p,n}^N$	6.416702269651688e-22	6.416702269651688e-22	6.416702269651688e-22
	$ERR_{s,n}^N$	9.635713317670815e-23	9.635713317671370e-23	9.635713317670815e-23
128	$ERR_{p,n}^N$	3.233814238498219e-22	3.233814238498219e-22	3.233814238498219e-22
	$ERR_{s,n}^N$	5.252431055171894e-23	5.252431055172185e-23	5.252431055171894e-23
256	$ERR_{p,n}^N$	1.623272894662017e-22	1.623272894662017e-22	1.623272894662017e-22
	$ERR_{s,n}^N$	2.871719369959133e-23	2.871719369959293e-23	2.871719369959133e-23
512	$ERR_{p,n}^N$	8.132278906231591e-23	8.132278906231591e-23	8.132278906231591e-23
	$ERR_{s,n}^N$	1.572403448750958e-23	1.572403448751136e-23	1.572403448750958e-23
1024	$ERR_{p,n}^N$	4.070118055133412e-23	4.070118055133412e-23	4.070118055133412e-23
	$ERR_{s,n}^N$	8.598849792953598e-24	8.598849792964225e-24	8.598849792953598e-24

Table 4: **Values on $ORD_{p,n}^N$ and $ORD_{s,n}^N$in maximum norm in Sh-mesh**

N \ n		2	3	4
16	$ORD_{p,n}^N$	9.526942856997385e-01	9.526942857631834e-01	9.526942857631834e-01
	$ORD_{s,n}^N$	6.681551647016998e-01	6.681551647018336e-01	6.681551647018336e-01
32	$ORD_{p,n}^N$	9.769163880025247e-01	9.769163880049477e-01	9.769163880049477e-01
	$ORD_{s,n}^N$	8.716598639054773e-01	8.716598639054757e-01	8.716598639054757e-01
64	$ORD_{p,n}^N$	9.885952392779257e-01	9.885952392808733e-01	9.885952392808733e-01
	$ORD_{s,n}^N$	8.754061512462008e-01	8.754061512462001e-01	8.754061512462001e-01
128	$ORD_{p,n}^N$	9.943312556519077e-01	9.943312556554772e-01	9.943312556554772e-01
	$ORD_{s,n}^N$	8.710705467536424e-01	8.710705467536429e-01	8.710705467536429e-01
256	$ORD_{p,n}^N$	9.971739686767292e-01	9.971739686808180e-01	9.971739686808180e-01
	$ORD_{s,n}^N$	8.689433399248164e-01	8.689433399248645e-01	8.689433399248645e-01
512	$ORD_{p,n}^N$	9.985890792763537e-01	9.985890792808323e-01	9.985890792808323e-01
	$ORD_{s,n}^N$	8.707558343721130e-01	8.707558343725499e-01	8.707558343725499e-01

Table 5: **Values of $ORD_{p,n}^N$ and $ORD_{s,n}^N$ in maximum norm in B-Sh mesh**

N \ n		2	3	4
16	$ORD_{p,n}^N$	9.526942852694527e-01	9.526942852694520e-01	9.526942852694520e-01
	$ORD_{s,n}^N$	8.336574054267325e-01	8.336574054267327e-01	8.336574054267325e-01
32	$ORD_{p,n}^N$	9.769163869985052e-01	9.769163869985062e-01	9.769163869985062e-01
	$ORD_{s,n}^N$	8.716598639054741e-01	8.716598639054773e-01	8.716598639054741e-01
64	$ORD_{p,n}^N$	9.885952369830563e-01	9.885952369830581e-01	9.885952369830581e-01
	$ORD_{s,n}^N$	8.754061512462237e-01	8.754061512462267e-01	8.754061512462237e-01
128	$ORD_{p,n}^N$	9.943312504884493e-01	9.943312504884475e-01	9.943312504884475e-01
	$ORD_{s,n}^N$	8.710705467537125e-01	8.710705467537121e-01	8.710705467537125e-01
256	$ORD_{p,n}^N$	9.971739572024862e-01	9.971739572024877e-01	9.971739572024877e-01
	$ORD_{s,n}^N$	8.689433399245357e-01	8.689433399244522e-01	8.689433399245357e-01
512	$ORD_{p,n}^N$	9.985890540332142e-01	9.985890540332157e-01	9.985890540332157e-01
	$ORD_{s,n}^N$	8.707558343728196e-01	8.707558343712007e-01	8.707558343728196e-01

8. Conclusion

Nano scale semiconductor technology is a recent area of immense research interest. The numerical modeling of device properties plays a vital role in the simulation of nano semiconductor devices. In this article, we proposed an iterative finite difference scheme on layer adapted meshes to account for the SP nature of the Schrödinger equation in the Coupled Poisson-Schrödinger system that defines the quantum confinement effects in device of nano scale dimensions. Error estimates are derived theoretically in maximum norm and verified by numerical computations. The order of convergence obtained for various layer adapted meshes are also presented. □

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