Characteristics Study of Heterojunction Nanoelectronic Device (HEMT) using Quantum Transport Model through an Indigenous Program.

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by

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CERTIFICATE

*This is to certify that the work contained in this thesis entitled "**Characteristics Study of Heterojunction Nanoelectronic Device (HEMT) using Quantum Transport Model through an Indigenous Program.**" is a bonafide work of **Sourjya Mukherjee (2014182)**,**Kurumoju Deepak (2014189)**, and **Pankaj Gupta (2014038)** , carried out in the Department of Electronics and Communications Engineering, National Institute of Technology Silcahr under my supervision and that it has not been submitted elsewhere for a degree.*

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Contents

Abstract

This report offers an extensive exploration of High Electron Mobility Transistors (HEMTs) with a particular focus on the fundamental principle governing their operation—the formation of a two-dimensional electron gas (2DEG). HEMTs, composed of Group III-nitride materials, play a pivotal role in high-power RF and microwave applications. The unique characteristic of HEMTs lies in the creation of a 2DEG at the heterointerface, which is accomplished by strategically designing the semiconductor layers with varying bandgaps. By engineering the layers to have distinct bandgap energies, a potential energy step is established at the heterointerface. This energy discontinuity confines electrons within a two-dimensional plane, creating the 2DEG. The report introduces an innovative simulation system employing Kronecker matrices with convolution-based interpolation to solve the Poisson and Schrödinger equations self-consistently. This system offers comprehensive insights into electron wave functions, electric potential distribution, electron density, Fermi surface energy, and current density distribution throughout the HEMT device. This research significantly advances our understanding and optimization of HEMTs for advanced nanoscale electronic applications.

Chapter 1

Introduction

In the rapidly evolving landscape of electronic devices and power conversion technologies, High Electron Mobility Transistors (HEMTs) have emerged as pivotal components, offering exceptional high-frequency performance and power handling capabilities. Unlike traditional Metal-Oxide-Semiconductor Field-Effect Transistors (MOSFETs), HEMTs rely on a fundamentally different operational principle—the creation of a two-dimensional electron gas (2DEG) at a heterojunction interface. This unique feature, enabled by carefully engineered material combinations and energy band alignments, empowers HEMTs with unparalleled electron mobility and makes them well-suited for high-power Radio Frequency (RF) and microwave applications.

While MOSFETs have been the cornerstone of silicon technology, their application in high-performance transistors is limited in the context of Group III-nitride materials, such as Gallium Nitride (GaN). The absence of a high-quality gate dielectric comparable to silicon's native oxide (SiO2) has posed a significant challenge. In response, researchers have explored alternative transistor structures like the Metal-Semiconductor Field-Effect Transistor (MESFET) in GaN technology. However, achieving the required doping levels and gate-channel proximity for high-performance, short-channel devices has proven to be a formidable task.

Enter the HEMT—a transformative structure that overcomes these challenges. HEMTs offer a unique blend of attributes, including close gate proximity to the conducting channel, high transconductance, and high drain efficiency. Additionally, their superior characteristics, such as high low-field mobility, maximum drift velocity, and electron sheet densities, render them exceptionally well-suited for demanding high-power RF and microwave applications. The inherent high power per device width of GaN HEMTs translates into smaller, more manufacturable devices with enhanced impedance characteristics, simplifying impedance matching in complex systems.

Furthermore, the emergence of HEMTs owes its inspiration to the exploration of AlGaAs/GaAs quantum wells and superlattices, where the confinement and high concentration of carriers at heterointerfaces were discovered. The HEMT structure effectively harnesses this principle by burying the 2DEG at the heterojunction interface, isolating it from the rough surface, and controlling it through gate-induced band bending.

In addition to exploring the principles and applications of High Electron Mobility Transistors (HEMTs), this paper aims to achieve the following objectives:

- To develop a comprehensive, indigenous simulation software tailored for nanoelectronic devices, particularly HEMTs.
- To Iteratively solve the Poisson and Schrödinger equations to attain a self-consistent solution, crucial for accurate device modeling.
- To Obtain the electric potential profile across the HEMT device, revealing the electrostatics and potential energy landscape.
- To Calculate electron probability densities ($|\psi|^2$) and energy eigenvalues, providing insights into electron behavior and energy levels.
- To Determine the electron concentration distribution within the device.
- To Analyze the current density distribution across the device, shedding light on electron flow and device performance.
- To Extend the model to incorporate quantum transport effects, enhancing simulation accuracy.

By addressing these objectives, this research advances our understanding of HEMTs and contributes valuable simulation tools for nanoelectronic device analysis.

Chapter 2

Literature Review

In the realm of semiconductor physics and nanoelectronic device modeling, Schrödinger's equation elucidates the quantum behavior of electrons within the material, determining energy levels and electron wave functions. Poisson's equation, on the other hand, characterizes electric potential and charge distribution, crucial for understanding the electrostatics within devices. [1] by Neaman et al. provides a foundational understanding of these equations, enabling us to grasp how quantum mechanics and electrostatics influence the behavior of electrons and charge carriers in semiconductor materials. [2] by Morkoç et al is a comprehensive reference work that focuses on Gallium Nitride (GaN)-based semiconductor materials and their applications in electronic and optical devices. The book covers a wide range of topics related to GaN, including electronic and optical processes, device physics, material parameters and practical applications. It served as a valuable resource to this work as it helped understand the intrinsic band properties of the materials that were used in this work.($Al_xGa_{(1-x)}N$ and GaN).

Zarak et al.[3] proposed a physics-based analytical model for p-GaN/AlGaN/GaN High Electron Mobility Transistors (HEMTs) at the 2022 IEEE 19th India Council International Conference (INDICON). This model leverages MATLAB with FlexPDE to efficiently solve the Schrödinger's equation and Poisson's equation, to arrive at a self consistent solution which are fundamental in understanding the quantum behavior of electrons and electrostatics within the semiconductor material. However the proposed work does not take into account the polarization effect of the materials involved.In contrast to previous papers, the study proposed by Singh et al.[4] utilizes ATLAS, a semiconductor device simulation software, to delve into a comprehensive analysis of the current-voltage (I-V) characteristics in AlN/-Ga2O3 High Electron Mobility Transistors (HEMTs). One noteworthy aspect of this research is its in-depth exploration of Dirichlet and Neumann boundary conditions, shedding light on their intricate roles and implications within the

context of semiconductor device modeling.The Ph.D. thesis by G. Leuzzi[5] holds significance in the context of simulating High Electron Mobility Transistor (HEMT) characteristics for AlGaN materials. Notably, the author modified a MATLAB library called "AQUILA" to facilitate the simulation of HEMT device characteristics, particularly in the AlGaN semiconductor material. This thesis is of particular relevance to our work as it provides a clear and detailed explanation of how to solve the Schrödinger's equation through discretization and matrix-based methods.

In conclusion, the reviewed papers, books, and theses have collectively provided valuable insights into the intricate realm of semiconductor physics and the modeling of High Electron Mobility Transistors (HEMTs). These resources have shed light on fundamental equations, such as Schrödinger's equation and Poisson's equation, which govern the behavior of electrons and electrostatics within semiconductor materials. Notably, the proposed methods in these works have been implemented using licensed software tools, highlighting the importance of developing an indigenous and freely accessible program for simulating and modeling HEMT characteristics.

The primary aim of our project is to comprehensively understand the underlying principles of HEMTs, leveraging the knowledge gleaned from these valuable resources. Moreover, we aspire to bridge the gap by creating an indigenous software solution that stands on par with established models while remaining cost-free. This software will be a valuable asset for researchers and engineers, facilitating the simulation and modeling of HEMT characteristics with ease and accessibility, ultimately advancing the field of semiconductor device research and design.

Chapter 3

Materials and Methodology

3.1 Theory:

3.1.1 Heterojunction Structure:

HEMTs are typically built using semiconductor materials with different bandgap energies, creating what is known as a heterojunction structure. Common material combinations include Gallium Nitride (GaN) or Indium Phosphide (InP) for the channel region and Aluminum Gallium Nitride ($Al_xGa_{(1-x)}As$)) or other materials for the barrier layer. The heterojunction interface plays a crucial role in forming a two-dimensional electron gas (2DEG), which is a key feature of HEMTs. 1st Section

3.1.2 Formation of 2DEG Electron Gas:

The formation of a two-dimensional electron gas (2DEG) in a High Electron Mobility Transistor (HEMT) is a key principle that underlies its high electron mobility and exceptional performance. The formation of the 2DEG is primarily dependent on the energy band alignment at the heterojunction interface between the channel and barrier materials. Here's a detailed explanation of how the 2DEG is formed and its relationship to electron mobility:

In a HEMT, two different semiconductor materials are used, typically with different bandgap energies. For example, Gallium Nitride (GaN) is often used as the channel material, and Aluminum Gallium Nitride ($Al_xGa_{(1-x)}As$) or similar materials are used as the barrier material. The key to forming a 2DEG lies in creating a conduction band discontinuity (energy step) at the heterojunction interface between these materials.

- The conduction band of the barrier material should be lower in energy than the conduction band of the channel material. This energy difference is the key factor. (*Here we are con-*

sidering all bound electron energy levels to be negative i.e E_c values are negative as they are compared to the energy of an electron in free space)

- This means that the energy difference (ΔE_c) between the conduction band edges of the two materials must be sufficient to create an energy step that confines electrons to the interface. ($\Delta E_c > 0$)
- The result is that electrons accumulate at the heterojunction interface, forming a 2DEG within a narrow region at the interface.

2nd Section

3.1.3 High Electron Mobility:

The high electron mobility associated with the 2DEG in HEMTs arises from the fact that electrons in the 2DEG experience minimal scattering and resistive losses. This is due to:

- The 2DEG's confinement to a narrow interface region, which reduces scattering events and electron-phonon interactions.
- The absence of impurities in the channel region, which further minimizes scattering.
- The relatively high electron mobility of the materials used in the channel region of HEMTs, such as GaN, which inherently supports high electron mobility.

3.2 Material Parameters

BandGap

The ternary alloy of GaN and AlN, $Al_xGa_{(1-x)}$, provides a wide continuous range of bandgap values with a small associated change in the lattice constant. The energy bandgap of $Al_xGa_{(1-x)}As$ is modelled with both a temperature and a compositional dependence. The compositional dependence of the principal bandgap of $Al_xGa_{(1-x)}As$ shows a nonlinear increase of the bandgap with increasing Al-content. It is modelled by the empirical equation 3.1

$$E_g(x) = xE_g(\mathrm{AlN}) + (1-x)E_g(\mathrm{GaN}) - bx(1-x)\,\mathrm{eV} \tag{3.1}$$

with x and b representing the mole-fraction of Al and the bowing parameter, respectively. The values of the bowing parameter still show big inconsistencies in the literature. The temperature dependence of the bandgap is modelled by the empirical Varshni equation 3.2

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{\beta + T}\,\mathrm{eV} \tag{3.2}$$

with α and β being empirical parameters which are given along with other parameters in table 3.1

Table 3.1 Energy bandgaps of AlN and GaN and empirical fitting parameters

Parameter	Value
Bandgap E_g(AlN) [eV]	6.1
Bandgap E_g(GaN) [eV]	3.42
Bowing parameter b	-1
Fitting parameter α	2.15×10^{-3}
Fitting parameter β	1561
EV discontinuity [eV]	$0.85x$

Effective carrier masses

The effective mass for $Al_xGa_{(1-x)}As$ is once again a linear interpolation between the values of AlN and GaN given by eqn 3.3

$$m^*(Al_xGa_{1-x}N) = (1-x)m^*(GaN) + xm^*(AlN) \tag{3.3}$$

effective m* values have been tabulated in table 3.2

Table 3.2 Effective masses of carriers in AlN and GaN (expressed in units of free electron mass m_0)

Carrier	Mass in AlN	Mass in GaN
$m_{\perp,e^-}$ $(=m_{\|\|,e^-})$	0.27 m_0	0.18 m_0

Dielectric constant

The relative dielectric constant of the $Al_xGa_{(1-x)}$ alloy is a linear interpolation between the dielectric constants of the binary alloys GaN and AlN for Al mole fraction x given by eqn 3.4

$$\varepsilon_{Al_xGa_{1-x}N} = 10.28 + 0.03x \tag{3.4}$$

Schottky Barrier

The electron affinity of GaN and AlN are approximately 4.2 eV and 2.05 eV, respectively.By using a linear interpolation between the electron affinities of GaN and AlN the barrier height between an arbitrary metal and the alloy $Al_xGa_{(1-x)}As$ can be calculated with eqns 3.5

$$\phi_{B(\text{metal}-Al_xGa_{1-x}N)} = \phi_m - \chi_{Al_xGa_{1-x}N} \tag{3.5}$$

$$\chi_{Al_xGa_{1-x}N} = \chi_{GaN} + (1-x)\chi_{AlN} \tag{3.6}$$

3.3 Algorithm

The quantum-mechanical Schrödinger equation, which describes the distribution of electric charges, is intricately linked with the Poisson equation and the equations governing charge conservation. These equations, in turn, rely on probabilistic wave functions. Therefore, to accurately simulate HEMT devices, it is imperative to solve this system of equations in a self-consistent manner. Solving the Schrödinger equation yields energy eigenvalues and electron wave functions, enabling the determination of electron density. Subsequently, the electric field and potential distribution are extracted from the Poisson equation solution. When the charge conservation law is applied, it allows for the determination of Fermi surface distribution and current density within the device.The proposed algorithm is depicted in fig3.1 The algorithm must be executed adhering to the Dirichilet

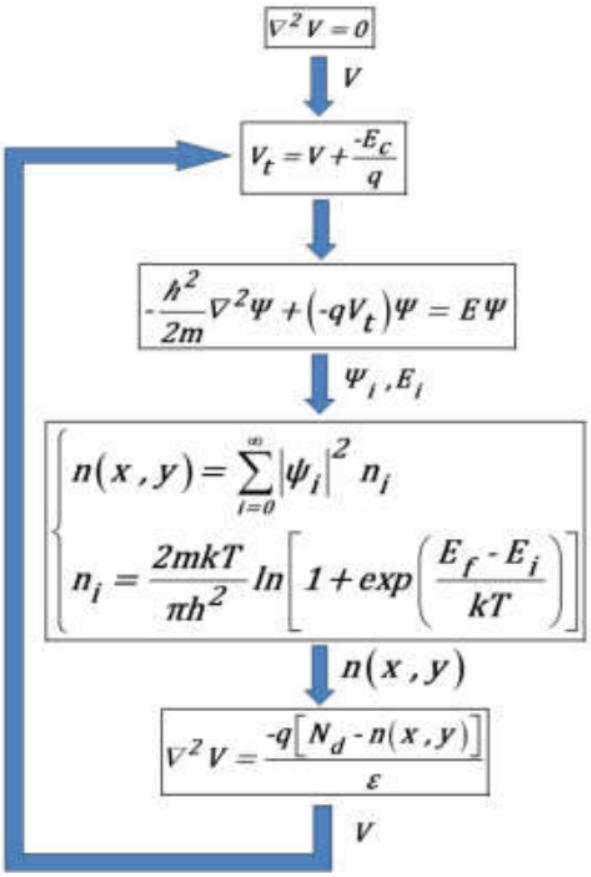


Fig. 3.1 Proposed algorithm for simulation

and Neumann boundary conditions enlisted in Fig 3.2. The proposed experimental structure on which the simulation was conducted is shown in Fig 3.4 and the dimensions have been enlisted in Fig 3.2

Number	Details
1 (Drain)	$V = V_d, \psi = 0, E_f = -qV_d + \varphi_{ms}$
2 (Gate)	$V = V_g, \psi = 0, E_f = -qV_g + \varphi_{ms}, \frac{d}{dn} E_f = 0$
3 (Source)	$V = V_s, \psi = 0, E_f = -qV_s + \varphi_{ms}$
4	$\frac{d}{dn} V = 0, \psi = 0, \frac{d}{dn} E_f = 0$

Fig. 3.2 Boundary Conditions

W_1	W_2	W_3	W_4	l_D	l_G	l_{SU}	l_{SD}
20nm	28nm	15nm	10nm	30nm	20nm	5nm	5nm

Fig. 3.3 Dimensions of the experimental structure

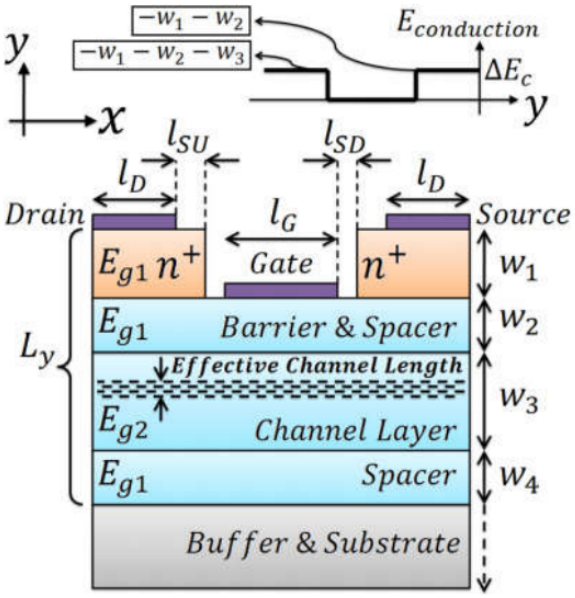


Fig. 3.4 Experimental 2D HEMT structure

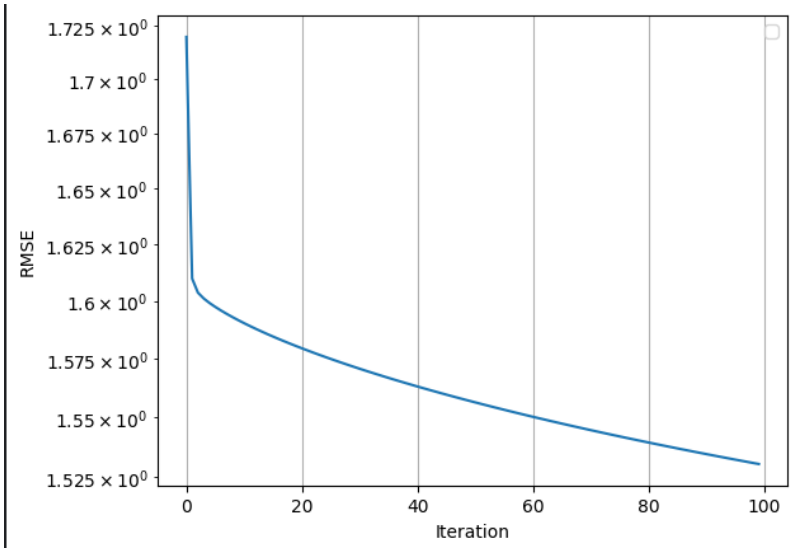


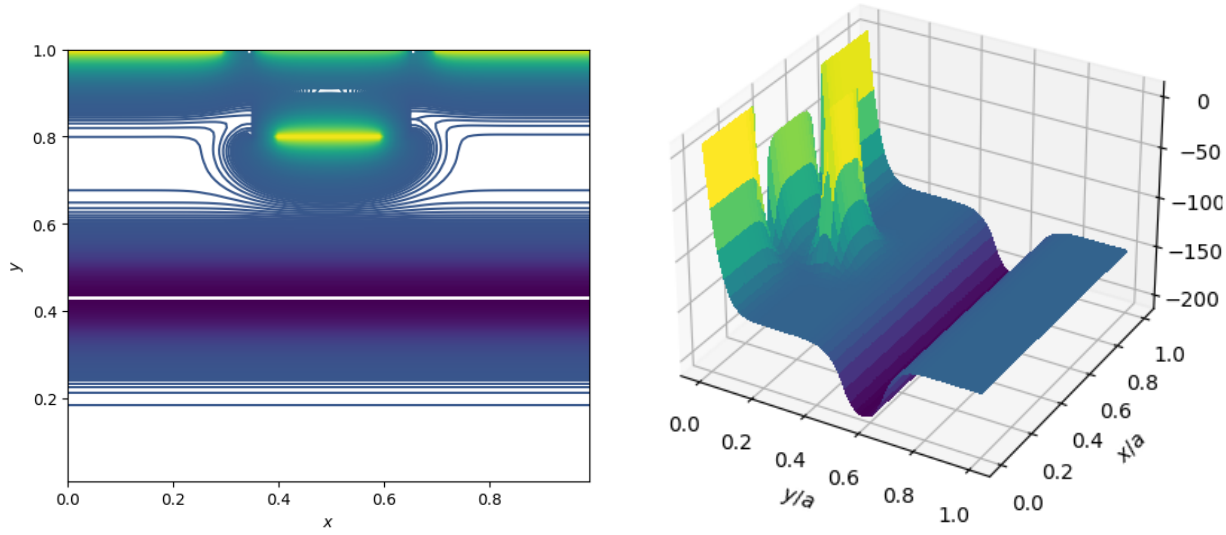
Fig. 3.2 loss curve for convergence

Chapter 4

Results and Discussions

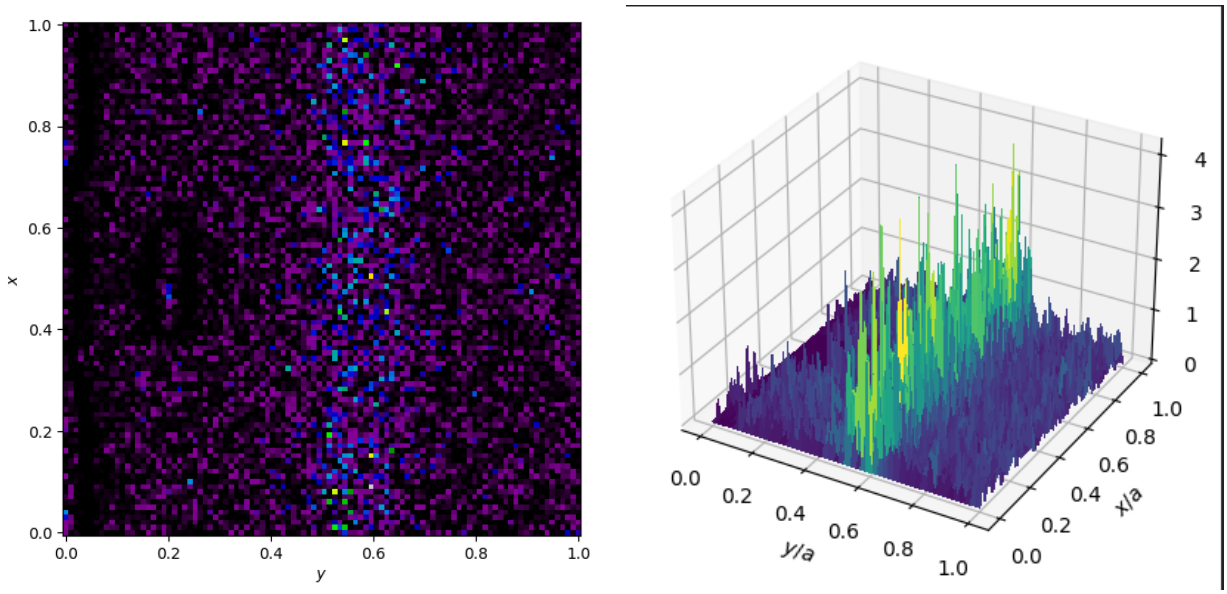
After running the algorithm, we have obtained crucial results that shed light on the behavior of High Electron Mobility Transistors (HEMTs). These results include the potential profiles across the device, the electron probability density distribution, and the electron density distribution across the device. The potential profiles provide insights into the electrostatics within the HEMT structure, revealing how the electric potential varies throughout the device. The electron probability density distribution offers information about the spatial distribution of electrons within the device, highlighting regions of higher and lower electron concentrations. Finally, the electron density distribution provides quantitative data on the number of electrons present at different positions within the HEMT, which is essential for understanding the device's electrical characteristics. These results serve as a foundation for further analysis and optimization of HEMT devices, contributing to advancements in high-frequency and high-power electronic applications. Additionally, they validate the accuracy and effectiveness of our simulation approach in capturing the intricate physics governing HEMT operation. The output graphs are as follows:

- fig4.1 represents the potential variation across the device
- fig4.2 represents the electron probability density across the device
- fig4.3 represents the electron density across the device



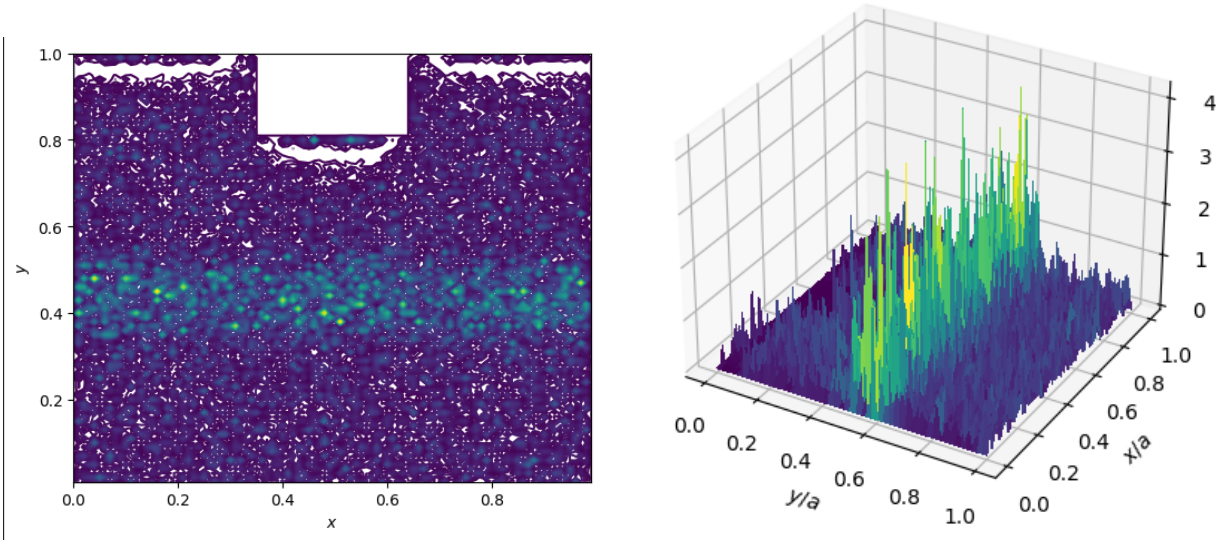
(a) 2D plot (b) 3D surface plot

Fig. 4.1 potential plots



(a) 2D plot (b) 3D surface plot

Fig. 4.2 Probability density plots for electrons



(a) 2D plot (b) 3D surface plot

Fig. 4.3 Electron density plots

Chapter 5

Conclusion and Future Work

For future work, there are several avenues of research and development that we would like to explore to further enhance our understanding of High Electron Mobility Transistors (HEMTs) and their performance. First, we aim to analyze the current density distribution across the device in more detail. This analysis will provide valuable insights into the flow of electrons within the device, allowing us to gain a deeper understanding of its overall performance and efficiency.

Additionally, we plan to extend our model to incorporate quantum transport effects. By doing so, we can enhance the accuracy of our simulations, especially in scenarios where quantum mechanical phenomena play a significant role. This expansion of our model will enable us to better capture the intricate quantum behaviors that occur within HEMTs.

Furthermore, as part of our future research, we are interested in experimenting with the characteristics of novel Heterostructure Field-Effect Transistor (HFET) structures. Investigating these innovative structures will not only contribute to the advancement of HEMT technology but also open up new possibilities for device design and optimization.

In conclusion, our future work will focus on refining our understanding of current density distribution, incorporating quantum transport effects for improved simulation accuracy, and exploring the potential of novel HFET structures. These endeavors will contribute to the ongoing development and innovation in the field of nanoelectronics and semiconductor devices.

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