

ELECTROSTATIC POTENTIAL AND TRAJECTORY OF AN ELECTRON IN
SINGLE ELECTRON TRANSISTOR

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ELECTROSTATIC POTENTIAL AND TRAJECTORY OF AN ELECTRON IN
SINGLE ELECTRON TRANSISTOR

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Specially dedicated to my beloved parents for setting me on the path towards intellectual pursuit. My sisters, brother and friends for their continuing support along the way

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ABSTRACT

Tunneling of an electron from the electrode towards the island in single electron transistor (SET) is a quantum mechanical phenomenon. This means, that electron can either tunnels to the island or not depending on the probability. Therefore, the study on how the electron interacts with a quantum dot should give the needed information in advancing the development of SET. With several assumptions, the electron trajectory from the electrode towards the island is studied in this research using classical approaches. The island is first developed by optimizing gallium arsenide (GaAs) cluster using the parallel version of GAMESS package. With the information from the optimized cluster, GaAs quantum dot is built as an island for the SET. The dot has a square bipyramidal shape with total 84 atoms in 1.6 nm^3 volume. Then the external electric field is applied towards the dot to study the potential distribution in the vicinity of the dot. Using this potential distribution, the electron trajectory is mapped and plotted using MacMolPlt and GnuPlot programs. The plotted result shows how the electron moves towards the dot and sticks in a loop. It is found that the loop is caused by the attraction of atomic nucleus of one of the atom in the dot. As the conclusion, the electron trajectory is discovered and plotted from the source electrode to the island. On the other hand, the electron does not pass through the island to the drain because of nuclear attraction which can be improved in future simulation.

ABSTRAK

Penerowongan elektron dari elektrod menuju ke pulau dalam transistor electron tunggal (SET) adalah satu fenomena kuantum mekanik. Ini bermakna elektron sama ada akan menerowong menuju ke pulau atau tidak bergantung kepada kebarangkalian. Oleh sebab itu kajian tentang bagaimana elektron berinteraksi dengan kuantum dot/pulau akan memberikan maklumat yang penting kepada pembangunan SET. Dengan membuat beberapa anggapan, trajektori elektron boleh dikaji dengan menggunakan pendekatan teori klasik. Pertama, suatu pulau mula dibina dengan mengoptimumkan struktur gugusan gallium arsenida (GaAs). Langkah pengiraan ini dilaksanakan dengan menggunakan perisian GAMESS dengan sistem pengkomputeran selari. Berdasarkan maklumat dari gugusan GaAs tersebut, kuantum dot galium arsenida dibina sebagai pulau untuk SET. Kuantum dot tersebut mempunyai bentuk gabungan dua-piramid berdasarkan segiempat sama yang mempunyai sejumlah 84 atom dan berisipadu sebanyak 1.6 nm^3 . Selanjutnya, medan elektrik luar dikenakan kepada kuantum dot tersebut untuk mengkaji taburan keupayaan di sekitar dot tersebut. Dengan menggunakan taburan keupayaan tadi trajektori elektron diplotkan menggunakan perisian MacMolPlt dan GnuPlot. Keputusan kajian menunjukkan pergerakan elektron tersangkut dalam lintasan berbentuk gelung. Ia dijumpai bahawa lintasan berbentuk gelung tersebut adalah disebabkan daya tarikan nukleus dari salah satu atom dalam dot tersebut. Sebagai kesimpulan, trajektori elektron ditemui dan diplot dari elektrod sumber ke pulau. Sebaliknya, elektron yang bergerak ke pulau tidak melepasi pulau tersebut untuk ke elektrod seterusnya disebabkan tarikan nukleus yang kuat dan model ini boleh dibaiki untuk simulasi selanjutnya.

TABLE OF CONTENTS

CHAPTER	TITLE	PAGE
	DECLARATION	ii
	DEDICATION	iii
	ACKNOWLEDGEMENTS	iv
	ABSTRACT	v
	ABSTRAK	vi
	TABLE OF CONTENTS	vii
	LIST OF FIGURES	xi
	LIST OF SYMBOLS	xiv
	LIST OF ABBREVIATIONS	xvi
	LIST OF APPENDICES	xix
1	INTRODUCTION	1
	1.1 Background of Research	1
	1.1.1 The Needs for Nanodevices	1
	1.1.2 Nanotechnology and Nanodevices	2
	1.1.3 Quantum Dot Nanodevices	3
	1.2 Introduction to Modeling and Simulation	4
	1.2.1 Modeling and Simulation Approach Used in This Research	5

1.3	Statement of Problems	6
1.4	Objective of Study	7
1.5	Scope of Study	7
1.6	Thesis Review	7
2	LITERATURE REVIEW	9
2.1	Introduction	9
2.2	Review of Quantum Mechanics	10
2.3	Bulk, Quantum Well and Quantum Wire	14
2.3.1	Bulk Solid	14
2.3.2	Quantum Well	16
2.3.3	Quantum Wire	18
2.4	Quantum Dot	21
2.4.1	GaAs Quantum Dot	23
2.4.2	GaAs Cluster	24
2.5	Single Electron Transistor (SET)	25
2.5.1	Coulomb Blokade	26
2.5.2	Quantum Tunneling	28
2.5.3	Single Electron Tunneling	29
2.6	Chapter Summary	31
3	COMPUTATIONAL METHOD	32
3.1	Introduction	32
3.2	Electronic Structure Method	33
3.3	Self-Consistent Field Theory (SCF)	35
3.4	Hartree-Fock Method	36
3.5	Density Functional Theory (DFT)	42
3.5.1	Basic of Density Functional Theory	44
3.5.2	Hohenberg Kohn Theorems	45
3.5.3	Kohn Sham Theory	47

3.5.4	Exchange Correlation Functional	50
3.5.4.1	Local Density Approximation (LDA)	50
3.5.4.2	Generaliz Gradient Approximation (GGA)	52
3.5.4.3	Hybrid Method	53
3.6	Basis Sets	55
3.6.1	Pseudopotential	56
3.7	Optimization Technique	58
3.8	Chapter Summary	59
4	METHODOLOGY	60
4.1	Introduction	60
4.2	GAMESS	61
4.2.1	GAMESS Input File	62
4.3	JAVA Program	65
4.4	Simulation Process	66
4.4.1	Geometry Optimization of GaAs	66
4.4.1.1	GaAs Clusters	67
4.4.1.1	GaAs Quantum Dot	68
4.4.2	Applies Electric Field on GaAs Dot	69
4.4.3	Potential Calculation of GaAs Dot	70
4.4.4	Geometry Configuration and Simulation Mechanism of SET	71
4.4.5	Determination of Electron Trajectory	73
4.4.5.1	The S-D-G Program	75
4.5	Plotting Program (MacMolPlt and GNUPlot)	76
4.6	Flow Chart of Simulation Process	79
4.7	Parallel Computing System	80
4.7.1	Performance of Parallelization	82
4.8	Assumption and Limmitation	84

5	RESULTS AND DISCUSSION	86
	5.1 Introduction	86
	5.2 Simulation of Gallium Arsenide Clusters	86
	5.3 Simulation of Gallium Arsenide Quantum Dot	89
	5.3.1 Electron Density of Gallium Arsenide Quantum Dot	92
	5.3.2 Potential Plot Around Gallium Arsenide Quantum Dot	95
	5.4 Electric Field Effect	98
	5.4.1 Electron Density with External Electric Field	98
	5.4.2 Potential Plot with External Electric Field	99
	5.5 Electron Trajectory	102
6	SUMMARY AND CONCLUSION	108
	6.1 Summary and Conclusion	108
	6.2 Sugestion	110
	6.2.1 Quantum Dot	110
	6.2.2 Simulation of SET	111
	REFERENCES	112
	APPENDICES	119

LIST OF FIGURES

FIGURE NO	TITLE	PAGE
2.1	Energy, E versus wave vector k for free electron	12
2.2	The density of states for free electron gas and the occupation probability for an electron in bulk solid.	15
2.3	Density of states for quantum well in comparison with bulk solid.	18
2.4	Density of state of quantum wire shows high peak in each energy level	20
2.5	The confinement sketch for material (a)Bulk GaAs, (b) GaAs Quantum Well, (c) GaAs Quantum Wire.	20
2.6	DOS for (a) bulk material, (b) quantum well and (c) quantum wire.	21
2.7	Square potential well in one dimension	21
2.8	The density of states of quantum dot from Dirac delta function shows discreteness of the energy due to zero dimension structure.	22
2.9	Schematic structure of SET	25
2.10	Transfer of electrons in (a) Single Electron Transistor, (b) MOSFET	25
2.11	A tunnel junction arrangement as it represents capacitor.	25
2.12	Diagram shows the classically forbidden region and the continuous wavefunction in the barrier.	28
2.13	Equivalent circuit of SET	29
3.1	Orbital energy level diagram for ground electronic configuration of (a) Close-shell system, (b) Open-shell system	37
3.2	Schematic illustration of pseudopotential	57

4.1	An overview of the software development process	65
4.2	The API and Java Virtual Machine insulate the program from the underlying hardware	66
4.3	Optimization process for Ga_nAs_n cluster	68
4.4	Side view for SET model used in this study.	71
4.5	Top view for SET model used in this study	71
4.6	Flow chart of the main program to study electron moving path around GaAs quantum dot	74
4.7	S-D-G program algorithm used to merge the electrodes potential with GAMESS potential	76
4.8	GUI for MacMolPlt program for (a) opening files and (b) plotting surface.	77
4.9	Picture of terminal and Gnu plot windows for plotting the 2D surface	78
4.10	Simulation Process	79
4.11	Schematic of parallel computing cluster illustrated a master-server distributes a job to 3 client nodes and communication between them is showed.	81
4.12	Graph of time versus number of CPUs for GAMESS parallel job using MPI and DDI	82
4.13	Graph of time versus number of CPUs for GAMESS parallel job with X(GUI) and without X	83
4.14	Graph of time versus number of CPUs for GAMESS parallel job using local installation and network (nfs)	83
4.15	Graph of time versus number of CPUs for GAMESS parallel job on Fedora 10 and Ubuntu 9.10	84
5.1	Lowest energy structure for Ga_nAs_n ($n=2-8$)	88
5.2	The optimized GaAs quantum dot	89
5.3	The optimized GaAs quantum dot with three different angle (a) side, (b) front, and (c) top view of the dot.	91
5.4	(a) Top view of SET and (b) side view of SET configuration equivalent with figure 4.4 and 4.5 respectively.	91
5.5	Electron density plot with its contour value (a) 0.100, (b) 0.050 and (c) 0.010 a.u	93

5.6	Electron density plot for Ga ₂ As ₂ cluster with pseudopotential basis sets, SBKJC (left) and with complete basis set, 6-31G (right).	94
5.7	Electrostatic potential surface with value 1.000 Hartree	95
5.8	Electrostatic potential surface with value 0.100 Hartree	95
5.9	Electrostatic potential surface with value 0.010 Hartree	96
5.10	Electrostatic potential surface with value 0.001 Hartree	96
5.11	(a) Electron density plot with contour value 0.100 and (b) Electron density plot with contour value 0.010	99
5.12	Electrostatic potential surface with value 1.000 Hartree.	100
5.13	Electrostatic potential surface with value 0.100 Hartree.	100
5.14	Electrostatic potential surface with value 0.010 Hartree	100
5.15	Electrostatic potential surface with value 0.001 Hartree	101
5.16	Electrostatic potential surface with value 0.0001 Hartree	101
5.17	Electron movement path (green line) with starting position (a)x=25, (b)x=50 , (c)x=75 and a layer of 2D electrostatic potential plot.	103
5.18	Electron movement path (blue line) with starting position x=25 and a layer of 2D electrostatic potential plot with contour.	104
5.19	Zoom in for electron movement path (blue line) with starting position x=25 and a layer of 2D electrostatic potential plot with contour.	105
5.20	Zoom in for electron movement path (blue line) with starting position x=25 and a layer of 2D electrostatic potential plot with contour from top view.	106
5.21	Zoom in for electron movement path (blue line) with starting position x=25 and a layer of 2D electrostatic potential plot with contour. This layer was the same level as the end of the electron movement	117

LIST OF SYMBOLS

E	-	Energy
λ	-	Wavelength
h	-	Plank constant
p	-	Momentum
k	-	Wave number
\hbar	-	Reduced Plank constant
Ψ	-	Wavefunction
i,j,k	-	Three coordinate vector
A	-	Amplitude
ρ	-	Density
T	-	Kinetic energy
V	-	Potential energy
m	-	Mass
v	-	Linear velocity
g	-	Density of states
ϕ	-	Wavefunction
u_k	-	Bloch function
N	-	Total number of states
L	-	Length
Θ	-	Unit step function
T	-	Temperature
e	-	electron
C	-	Capacitance

Σ	-	Summation
Q	-	Charge
V	-	Voltage
R	-	Nuclear position
r	-	Electronic position
H	-	Hamiltonian operator
t	-	time
α	-	Alpha-spin
β	-	Beta-spin
Π	-	Permutation operator
J		Coulomb integral
K		Exchange integral
$Y_l^m(\theta, \varphi)$	-	Spherical harmonic
Z_A	-	Nuclei charge
F	-	Fock operator
ε		Lagrange multipliers
v	-	Velocity
ω	-	Angular frequency
ν	-	Frequency
ε_i	-	Single-particle energy level
μ	-	Chemical potential
∇	-	Laplacian operator
ξ	-	Spin-polarization
Ga	-	Gallium
As	-	Arsenide
Ga _n As _n	-	Gallium arsenide cluster with n atom

LIST OF ABBREVIATIONS

ATLAS	-	Automatically Tuned Linear Algebra Software
API	-	Application Program Interface
B3LYP	-	Bake 3 Lee Yang Parr Basis
BLAS	-	Basic Linear Algebra Subprograms
BO	-	Born Oppenheimer
BP	-	Becke-Perdew
CC	-	Coupled cluster theory
CG	-	Conjugate gradient
CI	-	Configuration Interaction
CPU	-	Central Processing Unit
DDI	-	Data Distribution Interface
DFT	-	Density functional theory
DOS	-	Density of states
EC	-	Electron Correlation
EMA	-	Effective mass approximation
GAMESS	-	General Atomic and Molecular Electronic Structure System
GGA	-	Generalized gradient approximation
GTO	-	Gaussian-type orbital
GUI	-	Graphical User Interface
GVB	-	Generalized valence bond
HF	-	Hartree Fock theorem
HK	-	Hohenberg-Kohn

HOMO	-	Highest Occupied Molecular Orbital
JVM	-	Java Virtual Machine
KS	-	Kohn-Sham theorem
LAN	-	Local Area Network
LCAO	-	Linear combination of atomic orbitals
LD	-	Laser Diod
LDA	-	Local density approximation
LSDA	-	Local spin density approximation
LUMO	-	Lowest Unoccupied Molecular Orbital
LYP	-	Lee-Yang-Parr
MCSCF	-	Multi-Configurations Self Consistent Field
MD	-	Molecular dynamics
MO	-	Molecular Orbitals
MOSFET	-	Metal Oxide Semiconductor Field Effect Transistor
MPI	-	Message Passing Interface
MP2	-	Moller Plesset Pertubation Theory 2
NFS	-	Network file system
NRCC	-	National Resource for Computing in Chemistry
OS	-	Operating System
PAW	-	Projected Augmented Wave
PBE	-	Perdew-Burke-Ernzernhof
PES	-	Potential energy surfaces
PP	-	Pseudopotential
PW91	-	Perdew-Wang 1991
QD	-	Quantum Dot
rPBE	-	Revised-Perdew-Burke-Ernzernhof
RHF	-	Restrict Hartree Fock
ROHF	-	Restrict Open-shell Hartree Fock
RPA	-	Random phase approximation
SCF	-	Self-consistent functional

SD	-	Slater Determinant
S-D-G	-	Source-Drain-Gate
SSH	-	Secure Shell
SET	-	Single-electron transistor
SOA	-	Semiconductor optical amplifiers
STO	-	Slater-type orbitals
UHF	-	Unrestrict Hartree Fock
VWN	-	Vosko-Wilk-Nusair
xc	-	Exchange-correlation

LIST OF APPENDICES

APPENDIX	TITLE	PAGE
A	Parallel Computing System (SETPAR)	123
B1	GAMESS input file for geometry optimization	124
B2	GAMESS input file for geometry optimization of GaAs dot under external electric field.	125
B3	JAVA program used for mapping electron trajectory	126
C1	Electron movement path plotted from different starting position	137
C2	Electron movement path plotted with different level of potential surface	139

CHAPTER 1

INTRODUCTION

1.1 Background of the Research

The principal idea of this research is to study the movement of an electron in Single Electron Transistor (SET) from classical point of view. Thus, the main interest is to assess how the electron would move around the quantum dot with an applied external electric field. Ultimately this research hopefully gives the insight towards the new way to the simulation of Single Electron Transistor. In this first chapter of the thesis, the problem from the general idea is introduced and later converges towards the main interest of the research.

1.1.1 The Needs for Nanodevices

Almost all of our daily activities were carried out using the aid of electrical and electronic equipment. The used of electronics equipment are not only facilitated and accelerated a job, but also do the works that a man alone cannot do. Computers are a good example, almost every office and home and in fact in the developed country computer are personal property. A lot of calculation can be solve faster and beyond the limit of any human brain could do. In the mean time, the increased number of computers demanded higher electrical power to bear the needs of all the computers. According to a report from Energy Commission of Malaysia, electricity consumption in 2009 was 14 245 MW, an increase of 1.7 percent from the previous

year (Dept. of Statistic Malaysia, 2010). This report also showed that the increasing trend of electricity usage was constant every year. The trend is not only encountered in Malaysia but also involves the entire world. Thus there is a serious need in developing the electronic devices that works in low power consumption yet same or maybe speedy in performance. In this case, nanodevice is the answer to those problems.

Another reason to the development of nanodevices is miniaturization trend. Miniaturization is a continuing process in the creation and production of the ever-smaller scale for electronic, optical and mechanical product and devices. Products that take less space are more desirable than the larger items because it is more convenient to use, easier to carry and easier to kept. This gives human the morale to build smaller devices that features size efficiency. In electronics, miniaturization is explained by an empirical observation called Moore's law. In 1965, Gordon E. Moore predicted the number of transistor in an integrated circuit will be doubled periodically every 1.5 years (Moore, 1965). After 45 years introduction of Moore's law, the development of semiconductor technology nowadays is still following this law.

1.1.2 Nanotechnology and Nanodevices

One of the most advance and interesting idea is to control the electrical devices with its fundamental operator which is charge carrier (in this case an electron) so that the energy to operate the devices is not wasted. The technology needed to develop a device which is enabling the control of one electron is called nanotechnology.

Nanotechnology has emerged as a very popular and important issue in every field including science (physics, chemistry and biology) and engineering over the decade. Nanotechnology deals with natural and artificial structure on the nanoscale in the range from 1 μm down to 10 \AA (Bruus, 2004). One nanometer is roughly the distance of five neighboring atoms in an ordinary solid or about ten hydrogen atoms lined up together. It is very exciting area of study as the technology involves the

manipulation of the ultimate building blocks of ordinary matter which is single electron and molecule.

Although it is not referred to nanotechnology at the time, the emergence of nanotechnology already happened in the late nineteenth century when colloidal science started. In year 1959, Richard Feynman in his talk “There’s Plenty of Room at the Bottom” had firstly mentioned some of the nanotechnology concepts (William *et al.*, 2003). He described a process by which the ability to manipulate individual atoms and molecules might be developed. In 1974, the term “nanotechnology” was defined by Professor Norio Taniguchi from Tokyo Science University (Taniguchi, 1974).

When dealing with nano-size materials, quantum effects come into play in which classical theory is unable to explain what happens in these extremely small size systems. The properties of nanoscale particles are in the range between atom and bulk materials. These properties were proved to vary by size which leads to the establishment of material behavior engineering. This variation have made nanotechnology a very exotic field which still need a lot more efforts in research to open up and reveal its under covered ability.

The advancements from micro to nano-technology have allowed the miniaturization of amazingly complex devices. A lot of nano-devices are being researched widely and intensively, hence its market potential is bright. Although a portion of it is as yet conceptual, the realization of it is not an impossible matter. As nanotechnology is dealing with the fundamental building element of materials, it is worth to point out that the technology has remarkably brought together technologies from physics, biology and chemistry.

1.1.3 Quantum Dot Nanodevices

It has been a decade since scientist had done theoretical study of the properties of quantum dot to be effectively used as nanodevices, for example, single electron transistor (SET) (Kastner, 2000) semiconductor laser diode (LDs)

(Kirstaedter *et al.*, 1994; Huffaker *et al.*, 1998), semiconductor optical amplifiers (SOA) (Akiyama *et al.*, 2003; Sugawara *et al.*, 2004) and photodetector (Liu, 2003). Now, the demand in the usage of nanodevices is to produce nanosize-devices with low power consumption yet better performance. Although it has recently been possible to produce the quantum dot nanodevices, the study on properties of the devices is experimentally expensive because of the size. Thus the study of properties of the nanodevice via simulation is the most cost effective method. With the simulation is expected to be close to the real dot, the study of applied electric field on the dot is expected to yeild valuable knowledges for the future development of nanodevices.

1.2 Introduction to Modeling and Simulation

The introduction to modeling and simulation is an important part of this writing because the system that being studied were made via modeling and simulations. Modeling is a technique of representing a real world system via physics model and mathematical functions. Simulation on the other hand is an attempts to use the model on a computer so that it can be studied on how the system work.

Simulation is an important part of modeling nanostructure, in which, to obtain information about the behavior or properties of a structure or a system. This is a method which predicts the properties transformation for the variable before doing the actual experiment and the result can then be proved by the experiment. This approach is very helpful to select the most optimal and the best performance of a device which is build from those nanostructures before the real fabrication.

In the mean time, simulation can explain theoretical details that could not be explained by experiment solely, for example the occupation of electrons and reconstruction of nanostructure. We can view atomic structure model and the process of structure transformation via 3D graphical view and animation. With the simulation done before the experiment, the mastering of the nanostructures principles is improved and thus reducing unneeded steps during the experiment.

An importance things should be noted here is that, in doing the modeling and simulation there must be some approximation used based on assumption made to model the system. There is no simulation software which can take into account every detail that would contribute to system changes. Many of them simply adopt the approximation which is the most optimal and closest to the real system for the representation. First principle calculation for example is sufficient simulation approach in order to study electronic structures and properties of the nanostructures. The advantage is that, this calculation can be done without the need for experimental data.

However, the calculation could be massive and consumes a very long period to be done. Thus, to improve the performance and speed of large computation, one of the improvement approaches that very helpful is parallel computing. Parallel computing can reduce the computing time of computational costly calculation such as first principle calculation mentioned above, where it distributes the calculation to two or more processors or computers.

1.2.1 Modeling and Simulation Approach Used in This Research

In this research, there are two parts of modeling and simulation involved which is the optimization of the cluster and quantum dot, and another part is applied external electric field program. The cluster and dot are first build and optimized via GAMESS software and then the information from the calculation is used as an input to another computer program for the evaluation of the electric field effect around the cluster/dot.

General Atomic and Molecular Electronic Structure System (GAMESS-US) (Schmidt *et al.*, 1993; Gordon, 2005) is used as the simulation tools for electronic structures optimization of gallium arsenide clusters and quantum dot. Developed by M. S. Gordon group GAMESS is a program for ab-initio molecular quantum chemistry. Briefly, GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wavefunctions include Configuration Interaction, second order perturbation Theory,

and Coupled-Cluster approaches, as well as the Density Functional Theory approximation.

The electric field calculation part in this study is calculated using a program written in Java and developed during this study. Java is a programming language originally developed by James Gosling at Sun Microsystems (which is now a subsidiary of Oracle Corporation) and released in 1995 as a core component of Sun Microsystems' Java platform. The language derives much of its syntax from C and C++ but has a simpler object model and fewer low-level facilities. Steepest decent method is the principal method used in this program. The detail of the program algorithm is discussed in the methodology chapter.

1.3 Statement of Problem

As the research in development of SET is experimentally aggressive, the theoretical part on how exactly the electron moving around an island in SET is still not conclusive. This involves of how the electron ejected from the electrode to where the electron go and finally how the interaction with the island/dot. The study on how the electron interacts with the quantum dot should give very much needed information in advancing the development in SET. Although the problem is, the tunneling of electron from the electrode to the island was quantum effect, thus projection of the electron movement is simply does not exist. So, one way to look on the phenomena is from the classical point of view and this is the main ideas which this study will be working on. Rather than doing a very expensive in terms of technology and high sensitive measurement experimentally, simulation is one of the best tools nowadays to study operation of SET.

1.4 Objective of the Study

The main interest of this research is in the interaction of an electron with Gallium Arsenide quantum dot in an applied external electric field. The objectives of this study can be summarized as the following:

1. To construct a virtual quantum dot from a selected optimized GaAs cluster.
2. To determine charge distribution and electrostatic potential plot around the optimized quantum dot.
3. To calculate classically the path of electron movement around the GaAs quantum dot in SET simulation.

1.5 Scope of study

The area of this field of study are very large and it is decided to focus on the crucial part that are expected. This research will cover the installation of software that will be used, parallel system computing, construction of virtual GaAs cluster and quantum dot, and finally studying the movement of electron with external electric field in the vicinity of a quantum dot. This study is hoped to improve the modeling and thus will result in parameters that could be experimentally measured.

1.6 Thesis Review

In this chapter the general introduction and brief description to the whole study is discussed; from the need of background, nanotechnology, and simulation, towards research objective and scope of the study. In the next chapter, the literature review on operational principle of Single Electron Transistor (SET) is discussed and it is included with the effect of confinement. In chapter three, the computational method of developing virtual quantum dot is discussed. The quantum theory used in the calculation which includes Hartree-Fock Method (HF) and Density functional Theory (DFT) is explained in this chapter. In chapter four, the methodology of the

whole research is explained and a flow chart is presented to simplify the work process. Limitations and assumption used in this theoretical study are also included as to show the scope of the study. Chapter five present the result and the discussion analysis. Chapter six which is the last chapter concludes the study by summarizing the theory and result of the analysis. Suggestions for future work are also given in this chapter.

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