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An analytical approach to quantum mechanical tunneling time in electronic devices

Thanikasalam, Prabhaharan, M.S.

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University of Nevada, Las Vegas, 1992



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AN ANALYTICAL APPROACH TO QUANTUM MECHANICAL TUNNELING TIME IN ELECTRONIC DEVICES

by

Prabhaharan Thanikasalam

A thesis submitted in partial fulfillment

of the requirements for the degree of

Master of Science in Electrical and Computer Engineering

••

Department of Electrical and Computer Engineering University of Nevada, Las Vegas August, 1992

The thesis of Prabhaharan Thanikasalam for the degree of Master of Science in Electrical and Computer Engineering is approved.

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ABSTRACT

Starting from the analytical solution to the Time-Independent Schrödinger Equation, and exploiting the analogy between the transmission line equations and the time-independent Schrödinger wave equation, an analytical expression for the Average Particle Traversal (APT) time, τ_{APT} , through a rectangular potential barrier region. under no bias. is derived, in terms of the barrier width, potential, and the incident energy of the electron. This approach is extended to derive an analytical expression for the APT time through a resonant tunneling structure, two symmetrical rectangular potential barriers sandwiching a potential well, under no bias. The results of the single potential barrier traversal time are compared with that of other approaches. The APT time is inversely proportional to the transmission coefficient, and satisfies physically intuitive energy limits. For the resonant tunneling structure, the APT time is minimum at resonant energies, and the τ_{APT} is inversely proportional to the transmission coefficient. The maximum frequency of oscillation is estimated and compared for some of the experimentally studied resonant tunneling structures based on the APT time. The agreement is excellent.

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Chapter 1

INTRODUCTION

1.1 Quantum Mechanics and Schrödinger's Wave Equation

The Schrödinger Equation is analogous to a classical energy conservation equation, and describes the dynamics of a quantum particle. A quantum particle is one whose wavelength is very small compared to the dimensions of the system. When the dimensions of the dynamic system of the particle are extremely small, the classical mechanics does not explain many of the experimental observations, such as diffraction and tunneling. The Schrödinger equation was developed to explain these physical phenomena. The timedependent Schrödinger equation in one-dimension for a quantum particle subjected to a potential, V(x), is given by:

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\Psi(x)}{\partial x^2}\Xi(t)+V(x)\Psi(x)\Xi(t)=-\frac{\hbar}{j}\Psi(x)\frac{\partial\Xi(t)}{\partial t}$$

where m^* is the effective mass of the particle, \hbar is the modified Planck's constant, $\frac{\hbar}{2\pi}$, and E is the energy of the particle. The time-independent Schrödinger equation which holds good when the total energy of the particle is independent of time, is given by:

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m^*}{\hbar^2} [E - V(x)]\Psi(x) = 0$$

The boundary conditions are: $\Psi_n(x - \pm \infty) = 0$ and $\Psi_n(x)$ and $\Psi'_n(x)$ are continuous everywhere, $-\infty < x < \infty$. The number of solutions to this equation are infinite. The eigen values and functions are denoted with n as the index - E_n and $\Psi_n(x)$. The physical meaning of $\Psi_n(x)$ is that $|\Psi_n(x)|^2 dx$ provides the probability of finding the quantum particle between x and x + dx with unity probability of finding the particle in $-\infty < x < \infty$.

1.2 **Tunneling Phenomena**

In a single potential barrier comprising of GaAs/AlAs/GaAs, conduction band edge profile shown in Figure[1.1], as the height of the potential barrier is finite, Ψ_n is now zero at the AlAs/GaAs barrier interface. Ψ_n and Ψ'_n are continuous and non-zero at each boundary of the barrier, and Ψ_n and Ψ'_n are non-zero within and beyond the potential barrier. Since Ψ_n has a non-zero value to the right side of the barrier as shown in Figure[1.1], $\Psi_n^*\Psi_n$ is nonzero, implying that the probability of finding the particle with $E < V_o$ beyond the barrier region is finite. According to classical mechanics, the probability of finding the particle with $E < V_o$ beyond the first AlGaAs/GaAs interface is zero, since such a real space transfer of the particle through a potential barrier region is prohibitted classically. The physical mechanism by which the particle, with $E < V_o$, penetrating a finite potential barrier is called quantum mechanical tunneling through the barrier. The tunneling probability is directly related to the energy of the particle, E, relative to V_o and the barrier width, d.

The first device proposed, based on the tunneling phenomena, was the tunnel diode. The Tunnel diode is often called the Esaki diode after L. Esaki [20, 23], who in 1973 received the Nobel prize for his work on this effect. The basic structure is a p^+n^+ diode with p and n regions are degenerately doped so that the depletion layer region is very thin. Due to thin depletion layer, electrons in the conduction band can tunnel through the thin depletion region to the valence band electrons. A tunnel diode exhibits the critical feature of negative differential resistance (NDR), over a portion of it's I - V characteristics, as shown in Figure[1.2]. In NDR region, the I - V characteristics exhibits a negative slope. i.e., the quantity $\frac{dI}{dV}$ is negative.



Figure 1.1: Quantum mechanical tunneling: (a) potential barrier of height V_o and thickness W; (b) wave function Ψ for an electron with energy $E < V_o$, indicating a non zero value of the wave function beyond the barrier



Figure 1.2: The I-V characteristics of a tunnel diode. **a-b** is the linear resistance region; **b-c** is the negative differential resistance, (NDR), region; and **c-d** is the exponential region. I_p and I_v are the peak and valley current. V_p and V_f are the peak and forward voltage, respectively.



Figure 1.3: Quantum mechanical tunneling in a resonant tunneling structure with a barrier width of b and well width of w.

1.3 Resonant Tunneling Phenomena

With the advent of Molecular Beam Epitaxy (MBE), it is possible to grow thin layers of AlAs sandwiched between GaAs, thus creating a potential barrier in the conduction band edge profile, as shown in Figure[1.1]. The thickness of the AlAs layers can be as small as 10\AA , which is 4 mono layers of AlAs. Double barrier structures as shown in Figure[1.3], successfully grown by MBE, in which a GaAs layer (well) is sandwiched between two AlAs barrier layers, quantized energy levels, dictated by quantum mechanics, exist within the well region. When the incident energy of the particle in the free propagating region out side the potential barrier equals one of the quantized energies, the transmission probability is unity, i.e., resonant tunneling results. For energy values other than the resonant ones, the transmission probability is less than unity. This is referred to as non-resonant tunneling phenomena.

R. Tsu and L. Esaki[20] proposed a superlattice structure in 1969 for application in negative differential resistance (NDR) devices. In 1972, L.Esaki *et. al.* reported for the first time, the observation of NDR in a GaAs/AlGaAs superlattice[22]. Two years later L.L. Chang *et. al.*, observed NDR at temperature below $77^{\circ}K$ in a double barrier resonant tunneling diode, i.e. two periods of a GaAs/AlGaAs superlattice.

In 1983, Sollner et. al.[48] reported a large NDR region in the I - V characteristics of GaAs/AlGaAs double barrier resonant tunneling device, with a peak-to-valley ratio of 6:1 at 25°K. Moreover, the current response measured at a driving frequency of 2.5 THz was remarkably similar to the response expected from DC measurements, indicating the potential for high frequency applications[25]. A year later, Sollner et. al. reported the first high frequency oscillations generated by a resonant tunneling device at frequencies up to 18 GHz[47]. In 1985, Shewchuk et. al. reported the first room temperature observation of the NDR in a GaAs/AlGaAs system[43, 44].

The demonstration of resonant tunneling phenomena has led to a number of proposals for devices with a third terminal to control the NDR characteristics. Capasso *et. al.* proposed a heterojunction bipolar transistor with a single quantum well in the base region [13, 14, 15]. There are other resonant tunneling devices proposed by Luryi *et. al.*[34], Ray *et. al.*[42] using MOCVD at 300° K. Tsuchiya *et. al.*[49] reported room-temperature observations of negative differential resistance in 1985.

Bonnefoi et. al. [5, 6], proposed a device; Negative Resistance Stark Effect Transistor (NERSET). This is a double barrier resonant tunneling device with an extra (base) contact. Since this base is shielded by a thick 1000 - 1500Å potential barrier, the base current is negligible. Nakata et. al. proposed a triode with a metal-insulator superlattice in the base, acting as an artificial semiconductor [35]. This device, called resonant electron transfer triode (RETT), is exceed to perform well in high-speed applications because of low resistivity of metal contacts. Due to the periodicity of the metal-insulator superlattice, an artificial conduction band in the base region is formed. When the device is biased such that emitter Fermi level is aligned with the artificial conduction band in the base, electrons resonantly tunnel from emitter to collector.

Magnetic-field-induced resonant tunneling was discussed by Ramaglia *et. al.*[39]. Recent paper by Glazer *et. al.* discusses the case of tunneling through highly transparent double barriers[24]. Ranfagni *et. al.* reported delay-time measurements in narrow wave guides as a test of tunneling through single barrier[40, 41]. A thorough recount of the history of resonant tunneling can be found in Reference[21].

In the context of tunneling devices, the two physical quantities of interest to device physicists and engineers are the tunneling current and the tunneling time. The subject of this thesis is the latter quantity, the tunneling time. Specifically, based on average particle velocity during tunneling, the tunneling time for a single and double barrier are studied. Henceforth, this tunneling time is called the Average Particle Traversal time or APT time.

1.4 Overview of the Thesis

A brief literature survey, discussing various theoretical approaches to tunneling times is presented in Chapter 2. The analogy between the solutions to the one-dimensional timeindependent Schrödinger equation and transmission line equations is exploited and the derivation of APT time based on the analogy are discussed in Chapter 3. Analytical expressions for APT time for the case of a single potential barrier and a symmetrical double barrier under no bias are derived in Chapters 4 and 5, respectively. Results and discussion are presented in Chapter 6. Conclusions along with the proposal for future work are presented in Chapter 7.

Chapter 2

LITERATURE OVERVIEW

The prospect of high-speed devices based on resonant tunneling structures has brought new urgency to understand every aspect of tunneling phenomena for the formulation of the theory of dynamics of such systems. The question which is relevant to the dynamics of such a system and that has resulted in a wealth of literature is "How long does it take for a particle to tunnel?".

The recent theoretical work on the tunneling times has centered around one-dimensional models. Within this limited area of research, there are atleast six different approaches suggested in the literature. These approaches are : the dwell time[45], the phase-delay time[26, 50], the Buttiker-Landauer traversal time[7, 8, 9, 10], the complex traversal time[37, 38, 46], the Collins-Barker Monte-Carlo simulation time[16, 17, 18], and the Average Particle Traversal (APT) time. No two of these approaches agree[27, 28, 29, 32, 33]. In this chapter, five approaches are reviewed and contrasted.

2.1 Dwell Time

The dwell time [45] is, in the context of the scattering of particles with fixed energy, the time spent in any finite region of space, averaged over all the incoming particles. Thus, the dwell

time can serve as a reference point in any discussion on tunneling times. This describes the average time a particle dwells within the barrier irrespective of it either reflects or transmits at the end of it's stay. The dwell time, τ_{dwell} , is defined as:

$$\tau_{dwell} = \frac{N}{J}$$

where N is the number of particles within the barrier region and J is the incident flux of the particles. The τ_{dwell} for a single rectangular barrier can be shown to be equal to[7]:

$$\tau_{dwell} = \left(\frac{m^*k}{\hbar\alpha}\right) \frac{2\alpha d(\alpha^2 - k^2) + k_o^2 \sinh(2\alpha d)}{4k^2\alpha^2 + k_o^4 \sinh^2(\alpha d)}$$

where m^* is the effective mass, \hbar is the modified Planck's constant, $\frac{\hbar}{2\pi}$, $k = \sqrt{\frac{2m^*E}{\hbar^2}}$, $\alpha = \sqrt{\frac{2m^*(V_o - E)}{\hbar^2}}$ and $k_o = \sqrt{\frac{2m^*V_o}{\hbar^2}}$ with E being the energy of the incident electrons. V_o and d are the barrier height and width, respectively. The dwell time in a resonant tunneling structure is discussed by Pandey *et. al.* [36].

2.2 Phase-delay Time

The other well established tunneling time concept is the phase-delay time[26, 50]. A time delay for the scattering process can be calculated by following the peak of a wave packet via. the method of stationary phase[26]. Phase-delay time is the time interval between the time the peak of the incident wave enters the barrier and the time the peak of the transmitted wave appears beyond the barrier. The expression for the phase-delay time for single rectangular barrier is given by[7]:

$$\tau_{phase} = \left(\frac{m^*}{\hbar k \alpha}\right) \frac{2\alpha dk^2(\alpha^2 - k^2) + k_o^4 \sinh(2\alpha d)}{4k^2 \alpha^2 + k_o^4 \sinh^2(\alpha d)}$$

A strong deformation of the wave packet will result when the wave packet interacts with a thick barrier. This deformation may shift the peak of the wave from k in the incident wave to k' in the transmitted wave, with $k \neq k'$. Thus, the traversal time calculated by this method of following the peak of the wave packet becomes meaningless, as the same particle is not used for the time delay measurement.

2.3 Buttiker-Landauer Time

Buttiker and Landauer[7, 8, 9, 10] considered tunneling through time-dependent rectangular barrier with a small oscillating component added to the static barrier height. For a slowly varying potential, the additional time dependence of the transmitted wave is caused by the variation of the transmission probability with the height of the barrier. If the potential oscillates fast compared to the traversal time ($\omega >> 1/\tau$), then the particles see a timeindependent barrier of average height V_o . For slowly varying potential ($\omega << 1/\tau$), the tunneling particles see an effective time-dependent static barrier of height V(t). Identifying the transition frequency at which the static barrier becomes an oscillating barrier for the particles, provides one with the inverse of a traversal time. The expression for Buttiker-Landauer traversal time for a single rectangular barrier is given as:

$$\tau_{B-L} = (\tau_{dwell}^2 + \tau_z^2)^{\frac{1}{2}}$$

where τ_z is given by:

$$\tau_{z} = (\frac{m^{*}k_{o}^{2}}{\hbar\alpha^{2}})\frac{(\alpha^{2} - k^{2})\sinh^{2}(\alpha d) + (k_{o}^{2}d\alpha/2)\sinh(2\alpha d)}{4k^{2}\alpha^{2} + k_{o}^{4}\sinh^{2}(\alpha d)}$$

In this approach, the particles that are tunneling and those which are reflected are differentiated.

2.4 Collins-Barker Monte-Carlo Simulation Time

In this approach, a Gaussian wave packet with a particular standard deviation k, is made to impinge on a potential barrier and the time delay associated between the entrance of the peak of the incident wave and the appearance of the peak of the transmitted wave beyond the potential barrier, is computed numerically [16, 17], using the conventional Monte-Carlo approach. Based on excellent agreement of Monte-Carlo time and phase-delay time. it was concluded that the phase-delay time result originally obtained by Wigner[50] and Hartman[26] is the best expression to use for a wide parameter range of barriers, energies and wave packets.

2.5 Average Particle Traversal (APT) Time

In this approach, an average tunneling velocity at steady state is defined as $v_{av}(x) = \frac{J}{|\Psi(x)|^2}$, with J being independent of x, and $|\Psi(x)|^2$ is the probability density function at any point x along the barrier[31]. The analogy between the solution to the time-independent Schrödinger equation and the steady state transmission line equation for a loss-less homogeneous transmission line with a load, is exploited. A quantity analogous to the characteristic impedance of the transmission line called, Quantum Mechanical Wave Impedance (QMWI), Z(x), is derived in terms of the complex coefficients of the solutions to the wave function as a function of x[3, 31]. The $v_{av}(x)$ is then related to Z(x) and the APT time, τ_{APT} , is obtained as:

$$\tau_{APT} = \int_0^d \frac{dx}{v_{av}(x)} \tag{2.1}$$

where d is the width of the barrier.

The integral expression given by Eq.[2.1] was used to obtain the tunneling time through a delta function by Anwar *et. al.*[4] numerically. The tunneling through an emitter-base junction of a Heterojunction Bipolar Transistor was investigated by Cahay *et. al.* using numerical integration of the Eq.[2.1][11, 12].

Chapter 3

THEORETICAL FORMULATION

3.1 Introduction

In this chapter, a discussion of the analogy between the the solution to the time-independent Schrödinger equation and transmission line equations in one-dimension are presented. Exploiting this analogy, a quantity called the Quantum Mechanical Wave Impedance (QMWI) is derived in terms of the wave function solutions. Using QMWI, the average tunneling velocity is derived and is used to derive the APT time, τ_{APT} .

3.2 Formalism

Let a flux of electrons, with energy E, be incident on the potential barrier, as shown in Figure [3.1]. The dynamic equation governing the electron system is the time-dependent Schrödinger equation. The Schrödinger equation at steady state is given by:

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m^*}{\hbar^2} [E - V(x)]\Psi(x) = 0$$
(3.1)



Figure 3.1: Transmission line analogy: (a) transmission line circuit equivalent with a load impedance of Z_L , (b) quantum mechanical system with a potential step barrier configuration.

The solution to this time-independent Schrödinger equation in region 1 with conduction band edge potential profile, as shown in Figure[3.1], can be written as:

$$\Psi(x) = A^+ (e^{\alpha x} - \rho e^{-\alpha x}) \tag{3.2}$$

where $\alpha = \gamma + j\beta = j\sqrt{\frac{2m^{*}(x)}{\hbar^{2}}(E - V_{o})}$

 ρ is the wave amplitude reflection coefficient, α is the propagation constant, and E is the energy of the incident electrons. γ and β are the real and imaginary parts of the propagation constant α , respectively.

In particular, the wave equation for regions 1 and 2 can be written as:

$$\Psi_1(x) = A_1^+ (e^{\alpha_1 x} - \rho e^{-\alpha_1 x}) \cdots x < 0$$
(3.3)

$$\Psi_2(x) = A_2^+ e^{\alpha_2 x} \cdots x > 0 \tag{3.4}$$

respectively,

where $\alpha_i = j \sqrt{\frac{2m_i^*}{\hbar^2}(E - V_i)} = \gamma_i + j\beta_i$

 $m_i^*(x), V_i, (i = 1, 2)$ are the effective mass, and the potential, respectively, for the i^{th} region. Here, γ_i and β_i are the real and imaginary parts of the propagation constant α_i for the i^{th} region.

There is no reflection of the wave in region x > 0, because the region is homogeneous and of infinite extent. Applying the boundary conditions at x = 0, $\Psi_1(x = 0) = \Psi_2(x = 0)$ and $\Psi'_1(x = 0)/m_1^* = \Psi'_2(x = 0)/m_2^*$, an expression for ρ is obtained as:

$$\rho = \frac{\left[\alpha_2/m_2^* - \alpha_1/m_1^*\right]}{\left[\alpha_2/m_2^* + \alpha_1/m_1^*\right]} \tag{3.5}$$

Differentiating Eq.[3.2] with respect to x and multiplying both sides of the equation by a factor $\frac{\hbar}{jm^*}$, an expression for $\Phi(x)$ is obtained as:

$$\Phi(x) = \frac{\hbar}{jm^*} \frac{d\Psi(x)}{dx} = A^+ Z_0(e^{\alpha x} + \rho e^{-\alpha x})$$
(3.6)

where $Z_0 = \frac{\alpha \hbar}{jm^*}$

3.3 Transmission Line Analogy

The expressions for voltage, V(x), and current, I(x), along the homogeneous lossless transmission line with generalized distributed impedance, are given by:

$$I(x) = I^+ (e^{\alpha x} - \Gamma_t e^{-\alpha x}) \tag{3.7}$$

$$V(x) = I^+ Z_0(e^{\alpha x} + \Gamma_t e^{-\alpha x})$$
(3.8)

where

$$\Gamma_t = \left[\frac{Z_L - Z_O}{Z_L + Z_O}\right]$$

where Γ_t is the wave amplitude reflection coefficient.

 Z_L and Z_O are the load and characteristic impedance of the transmission line, respectively. Comparing the expressions for $\Psi(x)$ and $\Phi(x)$ given by Eqs.[3.2] and [3.6] respectively, with the expressions for I(x) and V(x) for transmission line given by Eqs.[3.7] and [3.8], respectively, it is observed that they are analogous. Z_0 in Eq.[3.2] and [3.6] is the quantum mechanical analog of the characteristic impedance of the transmission line, Z_O given by, $-\sqrt{Z/Y}$ where Z and Y are the series impedance and the shunt admittance, per unit length of the transmission line, respectively.

3.3.1 The Quantum Mechanical Wave Impedance

At any plane x, the Quantum Mechanical Wave Impedance (QMWI) [31] can be obtained from Eq.[3.2] and [3.6] as:

$$Z(x) = \frac{\Phi(x)}{\Psi(x)}$$
(3.9)

Z(x) can be re-written as:

$$\frac{2\hbar}{jm^*(x)}\frac{\Psi'(x)}{\Psi(x)} = Z(x) = R(x) + jX(x)$$
(3.10)

where R(x) and X(x) are the real and imaginary parts of Z(x) at any point x, looking in the positive x direction.

Multiplying both sides of Eq.[3.10] by $\frac{jm^{\bullet}(x)}{2\hbar}$, Eq.[3.10] modifies to:

$$\frac{\Psi'(x)}{\Psi(x)} = j\kappa(x) + \eta(x) \tag{3.11}$$

where $\kappa(x) = \frac{m^*(x)R(x)}{2\hbar}$ and $\eta(x) = \frac{m^*(x)X(x)}{2\hbar}$ are the propagation and attenuation constants of the wave function, respectively.

Integrating Eq.[3.11] from x = 0 to any $x, \Psi(x)$ can be written as:

$$\Psi(x) = \Psi_0 e^{\int_0^x \eta(x) dx} e^{j \int_0^x \kappa(x) dx}$$
(3.12)

where $\Psi(x)$ is the wave function at any point x, and Ψ_0 is the incident wave function at the x = 0 boundary.

3.3.2 Steady State Probability Current Density

The wave function, $\Psi(x)$, can be used to express the probability current density, J(x) as follows. Using Eq.[3.12], the steady state probability current density, J(x), at any point x can be written in terms of R(x) and $\eta(x)$ as:

$$J = \frac{1}{2} Re[\frac{2\hbar}{jm^{*}(x)}\Psi^{*}(x)\Phi(x)] = \frac{1}{2}|\Psi_{0}|^{2}R(x)e^{2\int_{0}^{x}\eta(x)dx}$$
(3.13)

where $\Psi^*(x)$ is the complex conjugate of the wave function, $\Psi(x)$. At steady state, the current continuity equation necessitates that the probability current density everywhere along the barrier be equal in the absence of any generation or recombination mechanisms.

Using Eqs.[3.12] and [3.13], J(x) can be written as:

$$J = \frac{1}{2}R(x)|\Psi(x)|^2$$
(3.14)

The current density, J(x), can be defined in terms of an average steady state velocity, $v_{av}(x)$, and probability density as:

$$J = v_{av}(x)|\Psi(x)|^2$$
(3.15)

This equation is similar to the drift current density equation in terms of the drift velocity, and charge density. Considering the probability current density again:

$$J(x) = \left(\frac{\hbar}{2jm^{*}(x)}\right) \left[\Psi^{*}(x)\frac{d\Psi(x)}{dx} - \frac{d\Psi^{*}(x)}{dx}\Psi(x)\right]$$
(3.16)

J(x) can be modified to:

$$J(x) = \frac{1}{2}Re[\Phi(x)\Psi^*(x)] = \frac{1}{2}Re[V(x)I^*(x)]$$
(3.17)

Thus, J(x) is analogous to the average power in the transmission line. V(x) is the

voltage, $I^*(x)$ is the complex conjugate of the current at any x along the transmission line.

3.3.3 Average Particle Traversal Time

Comparing Eqs.[3.14] and [3.15], $v_{av}(x)$ can be written as :

$$\nu_{av}(x) = \frac{1}{2}R(x)$$
(3.18)

In other words, the average velocity of the particle at any x is one half the real part of the QMWI. The τ_{APT} required for a particle to move an elemental distance, dx, at any point x is given by[3]:

$$d\tau_{APT} = \frac{dx}{v_{av}(x)} \tag{3.19}$$

Using Eqs.[3.16] and [3.19], an integral expression for the time required to traverse a distance L can be obtained as[3]:

$$\tau_{APT} = \int_0^L d\tau = 2 \int_0^L \frac{dx}{R(x)}$$
(3.20)

where R(x) is the real part of the Quantum Mechanical Wave Impedance, Z(x). It is noted that using Eq.[3.10], Z(x) can be obtained from the wave function solution to the Schrödinger equation, given by Eq.[3.3]. Identifying the real part, R(x), and using Eq.[3.20], τ_{APT} can be obtained for any structure.

Chapter 4

SINGLE BARRIER

In this chapter, the APT time, τ_{APT} , through a single rectangular potential barrier is considered. Based on the theoretical formulation, discussed in Chapter 3, an analytical expression for the τ_{APT} is derived. In order to calculate the τ_{APT} for the barrier region, the real part of the QMWI should be known. The real part of the quantum mechanical wave impedance can be obtained from the wave solution to the Schrödinger equation in that particular region. By knowing the real part of the QMWI, and using Eq.[3.20], an analytical expression for the τ_{APT} is derived in terms of the incident energy, barrier height and width.

4.1 Calculation of the Complex Coefficients of Wave Func-

tion Solutions

The solutions to the time-independent Schrödinger equation for a rectangular potential barrier structure shown in Figure[4.1] is given by:

$$\Psi_1(x) = e^{ikx} + Ae^{-ikx} \cdots x < \frac{-d}{2}$$
(4.1)



Figure 4.1: Conduction band edge profile for a single rectangular potential barrier with the corresponding wave function solution for different regions.

$$\Psi_2(x) = Be^{\alpha x} + Ce^{-\alpha x} \cdots \cdots \frac{-d}{2} < x < \frac{d}{2}$$
(4.2)

$$\Psi_3(x) = De^{ikx} \cdots x > \frac{d}{2}$$
(4.3)

where A, B, C, and D are the complex coefficients, α is the attenuation constant given by $\sqrt{\frac{2m^*(V_o-E)}{\hbar^2}}$, k is the propagation constant given by $\sqrt{\frac{2m^*E}{\hbar^2}}$, V_o and d are the height and width of the potential barrier, respectively, and E is the incident energy of the particle.

Boundary Conditions

The boundary conditions at $x = \frac{-d}{2}$ and $x = \frac{d}{2}$ are that the wave function, $\Psi(x)$, and the derivative of the wave function, $\Psi'(x)$ be continuous, which are given by:

$$\Psi_1(x = -d/2) = \Psi_2(x = -d/2) \cdots x = -\frac{d}{2}$$
(4.4)

$$\Psi_2(x = d/2) = \Psi_3(x = d/2) \cdots x = \frac{d}{2}$$
 (4.5)

$$\Psi'_{1}(x = -d/2) = \Psi'_{2}(x = -d/2) \cdots x = -\frac{d}{2}$$
 (4.6)

$$\Psi'_2(x = d/2) = \Psi'_3(x = d/2) \cdots x = \frac{d}{2}$$
 (4.7)

Substituting the respective wave function solutions from Eqs.[4.2] and [4.3] in Eqs.[4.4] - [4.7], at the interface $x = \frac{d}{2}$, an analytical expression for B and C can be obtained as:

-

$$B = \frac{De^{ikd/2}(\alpha + ik)}{2\alpha e^{\alpha d/2}}$$
(4.8)

$$C = \frac{De^{ikd/2}(\alpha - ik)}{2\alpha e^{-\alpha d/2}}$$
(4.9)

An expression for the complex coefficient A can be obtained by using the continuity condition on $\Psi(x)$ and $\Psi'(x)$ at the interface $x = -\frac{d}{2}$ as follows:

$$e^{-ikd/2} + Ae^{ikd/2} = Be^{-\alpha d/2} + Ce^{\alpha d/2}$$
(4.10)

$$ike^{-ikd/2} - ikAe^{ikd/2} = \alpha Be^{-\alpha d/2} - \alpha Ce^{\alpha d/2}$$

$$\tag{4.11}$$

Solving Eqs.[4.10] and [4.11] simultaneously and using Eqs.[4.8] and [4.9], the complex coefficient A can be obtained in terms of the the complex coefficient D as:

$$A = \frac{D(\alpha^2 + k^2)\sinh(\alpha d)}{i2k\alpha}$$
(4.12)

Using Eqs.[4.8],[4.9], and [4.12] in Eq.[4.10], an analytical expression for the complex constant D can be written as:

$$D = \frac{2ik\alpha e^{-ikd}}{(k^2 - \alpha^2)\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)}$$
(4.13)

4.2 APT Time Expression for the Single Barrier

The solution to the Schrödinger equation in the potential barrier region is given by:

$$\Psi_2(x) = Be^{\alpha x} + Ce^{-\alpha x} \tag{4.14}$$

Reiterating the definition of Quantum Mechanical Wave Impedance (QMWI) given by Eq.[3.10]:

$$Z(x) = \frac{2\hbar}{jm^*} \frac{\Psi_2'(x)}{\Psi_2(x)}$$
(4.15)

Considering the fractional part of Z(x) and using Eq.[4.14] and [4.15], an analytical expression for $\frac{\Psi'_2(x)}{\Psi_2(x)}$ can be obtained as:

$$\frac{\Psi_2'(x)}{\Psi_2(x)} = \frac{\alpha [Be^{\alpha x} - Ce^{-\alpha x}]}{[Be^{\alpha x} + Ce^{-\alpha x}]}$$
(4.16)

Substituting for B and C in terms of D from Eqs.[4.8] and [4.9] an expression for the QMWI can be written in terms of the attenuation constant α and the propagation constant k as:

$$\frac{\Psi_2'(x)}{\Psi_2(x)} = \frac{\alpha[(\alpha+ik)e^{\alpha(x-d/2)} - (\alpha-ik)e^{-\alpha(x-d/2)}]}{[(\alpha+ik)e^{\alpha(x-d/2)} + (\alpha-ik)e^{-\alpha(x-d/2)}]}$$
(4.17)

Eq.[4.17] can be modified to:

$$\frac{\Psi_2'(x)}{\Psi_2(x)} = \frac{\alpha [\alpha \sinh(\alpha x') + ik \cosh(\alpha x')]}{[\alpha \cosh(\alpha x') + ik \sinh(\alpha x')]}$$
(4.18)

where $x' = x - \frac{d}{2}$

Eq.[4.18] can also be written as:

$$\frac{\Psi_2'(x)}{\Psi_2(x)} = \frac{\alpha[(\alpha^2 + k^2)\sinh(\alpha x')\cosh(\alpha x') + ik\alpha]}{[\alpha^2\cosh^2(\alpha x') + k^2\sinh^2(\alpha x')]}$$
(4.19)

Multiplying by $\frac{2\hbar}{jm^*}$, the real part of Z(x), R(x), can be obtained as:

$$Re[Z(x')] = \frac{2\hbar}{m^*} \left[\frac{\alpha^2 k}{\alpha^2 \cosh^2(\alpha x') + k^2 \sinh^2(\alpha x')} \right]$$
(4.20)

The τ_{APT} through the barrier can be obtained by substituting Eq.[4.20] into Eq.[3.20] as follows:

$$\tau_{APT} = 2 \int_{-d}^{0} \left[\frac{m^{*}}{2\hbar\alpha^{2}k}\right] [\alpha^{2}\cosh^{2}(\alpha x') + k^{2}\sinh^{2}(\alpha x')] dx'$$
(4.21)

The above expression for τ_{APT} is analytically integrable for all values of incident energy of the particle.

4.2.1 The APT Time for $E < V_o$.

When the energy of the incident electron, E, is less than the barrier height, V_o , the attenuation constant, α , is a real quantity, and the electron wave function is decaying in nature. Then, Eq.[4.21] can be integrated to obtain τ_{APT} given by:

$$\tau_{APT}^{below} = (\frac{m^*}{4\hbar\alpha^3 k})[(k^2 + \alpha^2)\sinh(2\alpha d) + 2\alpha d(\alpha^2 - k^2)]$$
(4.22)

4.2.2 The APT Time for $E > V_o$.

When the energy of the incident electron, E, is more than the barrier height, V_o , α is an imaginary quantity, and the electron wave function is propagating in nature. Then Eq.[4.21] can be analytically integrated to obtain the following expression for τ_{APT} :

$$\tau_{APT}^{above} = \left(\frac{m^*}{4\hbar k_B^3 k}\right) \left[2k_B d(k^2 + k_B^2) - (k^2 - k_B^2)\sin(2k_B d)\right]$$
(4.23)

where k_B is the propagation constant given by $\sqrt{\frac{2m^*(E-V_o)}{\hbar^2}}$.

4.3 Various energy limits of τ_{APT}

The limiting values for the τ_{APT} for three cases of the incident energy of the particle, viz. $E \to 0, E \to V_o$, and $E \to \infty$ can be computed analytically. The derivation of these limits are discussed in this section.

$\underline{E-0.}$

When the incident energy of the particle approaches zero, E - 0, from Eq.[4.22] the propagation constant k tends to zero, hence τ_{APT} given by Eq.[4.22], tends to the following limit:

$$\tau_{APT} - \infty$$
 (4.24)

$\underline{E \to \infty}$.

When the incident energy of the particle approaches infinity, $E \rightarrow \infty$, the propagation constant in the barrier, $k_B \rightarrow \infty$. The corresponding limit of τ_{APT} is:

$$\tau_{APT} \rightarrow \frac{m^*}{4\hbar k_B^4} [2k_B d(2k_B^2)] \tag{4.25}$$

$$\tau_{APT} \to \frac{m^* d}{\hbar k_B} = \tau_{classical} \tag{4.26}$$

The τ_{APT} tends to the classical time which is defined as the time it takes for a particle of same energy and effective mass to traverse a distance equal to the barrier width, d, in the absence of the barrier.

$E \rightarrow V_o$.

When the incident energy, E, of the particle tends to the barrier height, V_o , the limiting values for the τ_{APT} can be obtained from either Eqs.[4.22] or [4.23] as follows[19]:

$$\tau_{APT} \to \frac{m^*}{\hbar k \alpha^3} \left[\frac{(k^2 + \alpha^2)}{4} \left[2\alpha d + \frac{(2\alpha d)^3}{6} \right] + \frac{(\alpha^2 - k^2)}{4} 2\alpha d \right]$$
(4.27)
$$\tau_{APT} \to \frac{m^*}{\hbar \alpha^3 k} [\alpha^3 d + \frac{8\alpha^3 d^3}{6}] \tag{4.28}$$

$$\tau_{APT} - \frac{m^* d}{\hbar k} [1 + \frac{(kd)^2}{3}]$$
 (4.29)

From Eq.[4.29], the τ_{APT} is finite when $E \to V_o$ as k is finite. The limiting values of τ_{dwell} , $\tau_{phase-delay}$, τ_{B-L} and $\tau_{classical}$ were obtained for three cases of limiting energies, $E \to 0$, $E \to \infty$ and $E \to V_o$ and listed in Table I for comparison of these values. A detailed comparison is made in Chapter 6.

Table I. The limits for the traversal times; the dwell time, τ_{dwell} , the phase-delay time, $\tau_{phase-delay}$, the Buttiker-Landauer time, τ_{B-L} , the classical traversal time, $\tau_{classical}$, and the APT time, τ_{APT} , for various incident energy limits.

	$E \rightarrow 0$	$E \to \infty$	$E \rightarrow V_o$
Tdwell	0	$\frac{m^*d}{\hbar k}$	$\frac{m^*k_a}{\hbar} \left(\frac{4d^3 + 6d/k_a^2}{12 + 3k_a^2 d^2}\right)$
$ au_{phase-delay}$	œ	$\frac{m^*d}{\hbar k}$	$\frac{m^{\bullet}k_o}{\hbar} \left(\frac{4d^3 + 6d/k_o^2}{12 + 3k_o^2 d^2}\right)$
τ_{B-L}	$\Big(\frac{m^*k_o^2}{\hbar\alpha^2}\Big)\frac{(\alpha^2-k^2)\sinh^2(\alpha d)+(\alpha dk_o^2/2)\sinh(2\alpha d)}{4k^2\alpha^2+k_o^2\sinh^2(\alpha d)}$	$\frac{m^{\bullet}d}{\hbar k}$	$\sqrt{ au_x^2+ au_y^2}^{\ddagger}$
$ au_{classical}$	œ	$\frac{m^*d}{\hbar k}$	$\frac{m^{\bullet}d}{\hbar k}$
$ au_{APT}$	∞	<u>m[•]d</u> ħk	$\frac{m^{\bullet}d}{\hbar k} \left[1 + \frac{(kd)^2}{3}\right]$

[†] $\tau_x = (\frac{m^*}{\hbar})(\frac{3d^2+2d^4k_o^2}{12+3k_o^2d^2})$ and $\tau_y = (\frac{m^*k_o}{\hbar})(\frac{4d^3+6d/k_o^2}{12+3k_o^2d^2})$

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Chapter 5

DOUBLE BARRIER

In this chapter, an analytical expression for the τ_{APT} through a symmetrical double rectangular potential barrier structure is obtained by using an approach similar to that used for a single barrier case in Chapter 4.

The conduction band edge profile of a symmetrical double rectangular potential barrier is shown in Figure [5.1]. Firstly, the solution to the Schrödinger equation is obtained analytically. Then the solution is used to obtain the real part of the QMWI, which in turn is used to obtain $v_{av}(x)$. $v_{av}(x)$ is used to obtain an analytical expression for the τ_{APT} .

5.1 Calculation of the Complex Coefficients of Wave Function Solutions

The wave function solution to Schrödinger equation in the five regions shown in Figure[5.1] is given by:

$$\Psi_1(x) = e^{ikx} + Ae^{-ikx} \cdots x < 0 \tag{5.1}$$



Figure 5.1: Conduction band edge profile for a symmetrical double rectangular potential barrier with the wave function solutions for different regions.

$$\Psi_2(x) = Be^{\alpha x} + Ce^{-\alpha x} \dots 0 < x < d$$
(5.2)

$$\Psi_3(x) = De^{ikx} + Ee^{-ikx} \cdots d < x < (d+d_1)$$
(5.3)

$$\Psi_4(x) = Fe^{\alpha x} + Ge^{-\alpha x} \dots \dots \dots (d+d_1) < x < (d_1+2d)$$
(5.4)

$$\Psi_5(x) = He^{ikx} \cdots x > (d_1 + 2d) \tag{5.5}$$

where d and d_1 are the barrier and well widths, respectively, and V_o is the height of the barrier. Applying the boundary conditions viz. the wave function, $\Psi(x)$, and the derivative of the wave function, $\Psi'(x)$, are continuous at the interfaces x = 0, x = d, $x = d + d_1$, and at $x = 2d + d_1$, analytical expressions for the complex coefficients A, B, C, D, E, F, and G, can be obtained in terms of the complex constant H, which is the wave function transmission coefficient. The analytical solutions to the complex coefficients are:

$$A = \frac{e^{i2kd}}{i2k\alpha e^{\alpha d}} \left(\frac{\alpha + ik}{\alpha - ik}\right) \left[\left[(k^2 - \alpha^2) + (\alpha - ik)^2 e^{i2kd_1}\right] \sinh(\alpha d) + i2k\alpha \cosh(\alpha d)\right] - \left(\frac{\alpha + ik}{\alpha - ik}\right) (5.6)$$

$$B = \frac{He^{ik2d}(\alpha+ik)}{i4k\alpha^2 e^{\alpha d}} [[(k^2 - \alpha^2) + e^{i2kd_1}(\alpha-ik)^2]\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)]$$
(5.7)

$$C = \frac{He^{i2kd}(\alpha - ik)}{i4k\alpha^2 e^{-\alpha d}} [[(k^2 - \alpha^2) + e^{i2kd_1}(\alpha + ik)^2]\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)]$$
(5.8)

$$D = \frac{He^{ikd}}{i2k\alpha} [(k^2 - \alpha^2)\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)]$$
(5.9)

$$E = \frac{He^{ik(3d+2d_1)}}{i2k\alpha} (\alpha^2 + k^2) \sinh(\alpha d)$$
 (5.10)

$$F = \frac{He^{ik(2d+d_1)}(\alpha+ik)}{2\alpha e^{\alpha(2d+d_1)}}$$
(5.11)

$$G = \frac{He^{ik(2d+d_1)}(\alpha - ik)}{2\alpha e^{-\alpha(2d+d_1)}}$$
(5.12)

5.2 The τ_{APT} for a Resonant Tunneling Structure

In order to derive an analytical expression for the τ_{APT} , the Quantum Mechanical Wave Impedance (QMWI) should be computed. The QMWI can be obtained from the wave function solution involving the complex constants B, C, D, E, F, and G. The analytical expressions for the real and imaginary parts of the complex coefficients are given in Appendix A. The real parts are subscripted '1' and the

imaginary parts are subscripted '2'. In order to calculate the total τ_{APT} through the structure, the τ_{APT} 's for the two barriers and the well region are calculated individually and added up as follows:

$$\tau_{APT}^{total} = \tau_{APT}^{lb} + \tau_{APT}^{well} + \tau_{APT}^{rb}$$
(5.13)

where τ_{APT}^{lb} , τ_{APT}^{well} , and τ_{APT}^{rb} are the traversal times in the left barrier region, well region, and right barrier region, respectively. The τ_{APT} 's, τ_{APT}^{lb} , τ_{APT}^{well} and τ_{APT}^{rb} are calculated using the integral expression for τ_{APT} given by Eq.[3.20].

5.2.1 The τ_{APT} for the Left Barrier Region

In order to calculate the τ_{APT} time for the barrier region, the real part of the QMWI should be computed. Once the the real part of the QMWI, Re[Z(x)], is known, it can be substituted into Eq.[3.20] to obtain an integral expression for the τ_{APT} for the barrier region.

The solution to the time-independent Schrödinger equation for the left barrier region is given by:

$$\Psi(x) = (B_1 + iB_2)e^{\alpha x} + (C_1 + iC_2)e^{-\alpha x}$$
(5.14)

where B_1 , C_1 are the real parts and B_2 , C_2 are the imaginary parts of the complex constants B and C, respectively. The $\Psi'(x)$ can be obtained from Eq.[5.14] as:

$$\Psi'(x) = \alpha[(B_1 + iB_2)e^{\alpha x} - (C_1 + iC_2)e^{-\alpha x}]$$
(5.15)

Re[Z(x)] can be obtained from Eq.[5.14], Eq.[5.15] and Eq.[3.19] as:

$$Re[Z(x)] = \left(\frac{2\hbar\alpha}{m^*}\right) \left[\frac{2(B_2C_1 - B_1C_2)}{(B_1^2 + B_2^2)e^{2\alpha x} + (C_1^2 + C_2^2)e^{-2\alpha x} + 2(B_1C_1 + B_2C_2)}\right]$$
(5.16)

 τ^{lb}_{APT} can be obtained from Eq.[5.16] and Eq.[3.20] as:

$$\tau_{APT}^{lb} = 2 \int_0^d (\frac{m^* dx}{2\hbar\alpha}) \left[\frac{(B_1^2 + B_2^2)e^{2\alpha x} + (C_1^2 + C_2^2)e^{-2\alpha x} + 2(B_1C_1 + B_2C_2)}{2(B_2C_1 - B_1C_2)} \right]$$
(5.17)

Integrating Eq.[5.17]:

$$\tau_{APT}^{lb} = \left[\frac{m^{*}}{4\hbar\alpha(B_{2}C_{1} - B_{1}C_{2})}\right]\left[\left(\frac{B_{1}^{2} + B_{2}^{2}}{2\alpha}\right)\left[e^{2\alpha d} - 1\right] - \left[\frac{C_{1}^{2} + C_{2}^{2}}{2\alpha}\right]\left[e^{-2\alpha d} - 1\right] + 2d(B_{1}C_{1} + B_{2}C_{2})\right] (5.18)$$

5.2.2 The τ_{APT} for the Potential Well Region

The solution to the time-independent Schrödinger equation for the well region is given by:

$$\Psi(x) = (D_1 + iD_2)e^{ikx} + (E_1 + iE_2)e^{-ikx}$$
(5.19)

where D_1 , E_1 are the real parts and D_2 , E_2 are the imaginary parts of the complex constants Dand E, respectively. The expressions for all the coefficients are given in appendix A. The $\Psi'(x)$ is obtained from Eq.[5.19] as:

$$\Psi'(x) = ik[(D_1 + iD_2)e^{ikx} - (E_1 + iE_2)e^{-ikx}]$$
(5.20)

The τ_{APT} in the potential well region can be written as:

$$\tau_{APT}^{well} = 2 \int_{d}^{d+d_1} \frac{dx}{Re[Z(x)]}$$
(5.21)

Using Eq.[5.19] and Eq.[5.20] in Eq.[3.9], and writing the exponentials in terms of trignometric functions, multiplying by $\frac{2\hbar}{m^*}$, in the expression for Re[Z(x)] in terms of the complex coefficients, an expression for the τ_{APT} for the well region can be obtained as:

$$\tau_{APT}^{well} = \int_{d}^{d+d_1} [p + q\cos(2kx) + r\sin(2kx)] dx$$
(5.22)

where p, q, and r are given by:

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$$p = \frac{D_1^2 + D_2^2 + E_1^2 + E_2^2}{D_1^2 + D_2^2 - E_1^2 - E_2^2}$$
(5.23)

$$q = \frac{D_1 E_1 + D_2 E_2}{D_1^2 + D_2^2 - E_1^2 - E_2^2}$$
(5.24)

$$r = \frac{D_1 E_2 - D_2 E_1}{D_1^2 + D_2^2 - E_1^2 - E_2^2}$$
(5.25)

Integrating Eq.[5.22], an analytical expression for the τ_{APT} in the well region, τ_{APT}^{well} , is obtained as follows:

$$\tau_{APT}^{well} = \left(\frac{m^*}{2\hbar k}\right) \left[pd_1 + \left(\frac{q}{2k}\right) \left[\sin\left[2k(d+d_1)\right] - \sin(2kd)\right] - \left(\frac{r}{2k}\right) \left[\cos\left[2k(d+d_1)\right] - \cos(2kd)\right]\right]$$
(5.26)

5.2.3 The τ_{APT} for the Right Barrier Region

The solution to the time-independent Schrödinger equation in the baarrier region is given by:

$$\Psi(x) = (F_1 + iF_2)e^{\alpha x} + (G_1 + iG_2)e^{-\alpha x}$$
(5.27)

where F_1 , G_1 are the real parts and F_2 , G_2 are the imaginary parts of the complex constants F and G, respectively. $\Psi'(x)$ can be obtained from Eq.[5.27] as:

$$\Psi'(x) = \alpha[(F_1 + iF_2)e^{\alpha x} - (G_1 + iG_2)e^{-\alpha x}]$$
(5.28)

Re[Z(x)] can be obtained from Eq.[5.27] and Eq.[5.28] as follows:

$$Re[Z(x)] = \left(\frac{2\hbar\alpha}{m^*}\right) \left[\frac{2(F_2G_1 - F_1G_2)}{(F_1^2 + F_2^2)e^{2\alpha x} + (G_1^2 + G_2^2)e^{-2\alpha x} + 2(F_1G_1 + F_2G_2)}\right]$$
(5.29)

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and the τ^{rb}_{APT} can be obtained as follows:

$$\tau_{APT}^{rb} = 2 \int_{d+d_1}^{2d+d_1} \left(\frac{m^* dx}{2\hbar\alpha}\right) \left[\frac{(F_1^2 + F_2^2)e^{2\alpha x} + (G_1^2 + G_2^2)e^{-2\alpha x} + 2(F_1G_1 + F_2G_2)}{2(F_2G_1 - F_1G_2)}\right]$$
(5.30)

Integrating Eq.[5.30]:

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$$\tau_{APT}^{rb} = \left[\frac{m^{*}}{4\hbar\alpha(F_{2}G_{1} - F_{1}G_{2})}\right] \\ \left[\left[\frac{F_{1}^{2} + F_{2}^{2}}{2\alpha}\right]\left[e^{2\alpha(d_{1} + 2d)} - e^{2\alpha(d_{1} + d)}\right] - \left[\frac{G_{1}^{2} + G_{2}^{2}}{2\alpha}\right]\right] \\ \left[e^{-2\alpha(d_{1} + 2d)} - e^{-2\alpha(d + d_{1})}\right] + 2d(F_{1}G_{1} + F_{2}G_{2})\right]$$
(5.31)

Chapter 6

RESULTS, COMPARISONS and DISCUSSIONS

In this chapter, the τ_{APT} obtained from the analytical expressions are compared with previous work reported in the literature for the single and double barrier cases. The τ_{APT} for single barrier is compared with the dwell time[7, 45], the phase-delay time[7, 16, 26, 50], the Buttiker-Landauer traversal time[7, 8, 9], and the classical traversal time. The double barrier τ_{APT} is compared with the experimentally obtained maximum frequency of oscillation of some of the structures experimentally grown and tested by Sollner *et. al.* [25, 47, 48].

6.1 Single Barrier

A plot of τ_{APT} and transmission coefficient vs. the normalized incident energy for a rectangular potential barrier is shown in Figure[6.2] for a barrier of height 0.3eV and width of 200\AA as shown in Figure[6.1], for the case of incident energy of the particle less than the barrier height, i.e., $E < V_o$. The transmission coefficient increases with incident energy, E, as expected. The τ_{APT} decreases with increasing energy. It is noted that the τ_{APT} reaches infinity in the limit of zero energy like a classical particle. A plot of τ_{APT} and transmission coefficient vs. the normalized incident energy is shown in Figure[6.3] for the structure shown in Figure[6.1], where the incident energy of the particle is more than the barrier height, i.e., $E > V_o$. In the limit of incident energy of the particle tending to the barrier height, i.e. $E \to V_o$, the τ_{APT} is large but finite as given by Eq.[4.29]. The τ_{APT} decreases with the increasing incident energy. It is also noted that the τ_{APT} oscillates slightly for large barrier thicknesses. In the limit of $E \to \infty$, τ_{APT} reaches the classical limit as given by Eq.[4.26].

6.1.1 Comparison of Dwell time, Phase-delay time, Buttiker-Landauer time, τ_{APT} , and the Classical time for, $E < V_o$

A plot of the dwell time, the phase-delay time, the Buttiker-Landauer time, the τ_{APT} and the classical traversal time vs. normalized incident energy is shown in Figure[6.4], for a rectangular potential barrier with a barrier height of 0.3eV and a width of 200\AA as shown in Figure[6.1], when $E < V_o$.

 τ_{APT} is always greater than the classical time. τ_{APT} is infinity in the limit of no energy, E = 0, implying that the particle takes infinite time to traverse the distance when the particles possess no energy at all. For all incident energy values below the barrier height, V_o , the dwell time and the phase-delay time are less than the classical traversal time as shown in Figure[6.4]. Whereas, the Buttiker-Landauer time is below the classical time for a range of incident energy, and above the classical time for the rest of the incident energy interval.

6.1.2 Comparison of Dwell time, Phase-delay time, Buttiker-Landauer time, τ_{APT} , and the Classical time for $E > V_o$

A plot of the dwell time, the phase-delay time, the Buttiker-Landauer time, the τ_{APT} and the classical traversal time vs. normalized incident energy are shown in Figure[6.5], for a rectangular potential barrier with a barrier height of 0.3eV and a width of 200Å as shown in Figure[6.1], when $E > V_o$. In this case, all the traversal times are above the classical traversal time. A plot of the

dwell time, the phase-delay time, the Buttiker-Landauer time, the τ_{APT} , and the classical time with the transmission coefficient is shown in Figure[6.6]. The dwell time, the phase-delay time and the Buttiker-Landauer time attain a maximum value when the transmission coefficient is maximum, and reaches a minimum when the transmission is minimum. Whereas, the τ_{APT} attains a minimum when the transmission coefficient is maximum, and reaches a maximum when transmission is minimum. In other words, According to τ_{APT} , the particle travels fastest at resonant energies, whereas according to the approaches, the particle travels fastest at non-resonant energies. All the traversal times approach the classical time limit at very high incident energies.

6.1.3 Effect of the barrier width on the τ_{APT}

The dependence of τ_{APT} on the barrier width with $E < V_o$ is shown in Figure[6.7], for a barrier height of 1.0eV and for a barrier width in the range of 25\AA to 250\AA .

The τ_{APT} decreases as the incident energy of the particle increases and the τ_{APT} is inversely related to the transmission coefficient. The τ_{APT} is finite when the incident energy of the particle is equal to the barrier height V_o .

The dependence of τ_{APT} on barrier width, with incident energy of the particle more than the barrier height is shown in Figure[6.8], for a barrier height of 1.0eV and for a barrier width in the range from 25Å to 250Å. Small oscillations in the τ_{APT} can be seen as the width of the potential barrier increases.

The τ_{APT} decreases as the incident energy of the particle increases. It is to be noted that as the barrier thickness increases, small oscillations in the τ_{APT} can be observed. These oscillations are inversely proportional to the transmission coefficient. i.e. τ_{APT} valleys at resonant energies whereas the transmission coefficient peaks.

6.2 Double Barrier

The plot of the transmission coefficient and τ_{APT} is shown in Figure[6.10] for the structure shown in Figure[6.9]. Five quasi-bound energy states can be observed below the barrier height. The transmission coefficient is unity at these resonant energies levels. It is to be noted that τ_{APT} is minimum at the resonant energies. Thus the transmission coefficient is inversely related to τ_{APT} .

6.2.1 Comparison of τ_{APT} with Experimental Results

Structure 1: Barrier width = 50Å, Well width = 50Å, and Barrier height = 0.23 eV.

The plot of τ_{APT} and the transmission coefficient vs. the incident energy of the particle is shown in Figure[6.12]. The structure considered was a symmetrical rectangular double potential barrier with a barrier height of 0.23eV, barrier width of 50Å and a well width of 50Å as shown in Figure [6.11]. This same structure is chosen as it is well characterized experimentally in terms of the I - V characteristics and high frequency studies[47, 48]. It was reported by Sollner *et. al.*[47, 48] that the maximum frequency of operation of the resonant tunneling device is 1.2THz. It was also observed that there is one quasi-bound resonant energy state at 0.0791eV which is less than the barrier height. This value of 0.0791eV agrees with that obtained from our analytical solutions. At this resonant energy value, the τ_{APT} is a minimum and also the transmission coefficient attains unity. The estimated maximum frequency of operation, from analytical expression for τ_{APT} , is 0.8THz, i.e., frequency corresponding to the resonant energy, which is in good agreement with the experimental value of 1.2THz. This maximum frequency of operation was estimated taking into consideration only the τ_{APT} . The capacitance charging times at the depletion layers are not taken into consideration. Structure 2: Barrier width = 25Å, Well width = 45Å, and Barrier height = 1.0eV.

The plot of τ_{APT} and the transmission coefficient vs. the incident energy of the particle is shown in Figure[6.14]. The structure considered was a symmetrical rectangular double potential barrier with a barrier height of 1.0eV, barrier width of 25\AA and a well width of 45\AA as shown in Figure [6.13]. This structure was fabricated and experimentally studied for high frequency oscillations by Sollner *et.* al.[25, 47]. It was reported by Sollner *et. al.*, that the maximum frequency of operation of the above resonant tunneling device is 2.4THz. It was also reported that there are two quasi-bound resonant energy states, one at 0.154eV and the other at 0.581eV below the barrier height. These values agree well with the values obtained from other numerical solutions. The transmission coefficient is maximum and attains the value of unity at these resonant energy levels and τ_{APT} at these resonant energy levels is a minimum. The estimated maximum frequency of operation is 1.4THz which is in good agreement with the experimental results. The maximum frequency of operation was estimated by taking into consideration the τ_{APT} only.

6.2.2 Effect of barrier width on the APT time

A 3-dimensional surface plot of the τ_{APT} is shown in Figure[6.16], for a range of the barrier widths from 30Å to 100Å, well width of 30Å, and for a barrier height of 0.3eV, as shown in Figure[6.15]. The τ_{APT} approaches infinity when $E \rightarrow 0$. The τ_{APT} is inversely related to the transmission coefficient. The formation of troughs in the τ_{APT} at resonances indicate that at these resonant energy levels, the τ_{APT} is minimum. As the barrier thickness is increased, the formation of the resonant energy levels is more pronounced and τ_{APT} for a very thick barrier, at the resonance, is more than that for a thin barrier.

6.2.3 Effect of well width on the APT time

A 3-dimensional surface plot of the τ_{APT} is shown in Figure[6.18], for a range of well widths from 30Å to 110Å and a barrier width of 30Å, and for a barrier height of 1.0eV as shown in Figure[6.17]. A 3-dimensional surface plot of the τ_{APT} along with the transmission coefficient is shown in Figure[6.19] for the same structure shown in Figure[6.17]. More quasi-bound states with $E < V_o$ appear as the well width increases, as shown in Figure[6.18] and [6.19]. The formation of troughs in the τ_{APT} at resonances indicate that at these resonant energy levels, the τ_{APT} is minimum. τ_{APT} is minimum at resonant energies. When the width of the potential well is small, the number of resonant energies is small within the potential well. As the width of the potential well increases, the number of resonant energy levels increase and the energy spacing between any two adjacent resonant energy levels within the potential well, ΔE , decreases.



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Figure 6.1: The conduction band edge profile of a single rectangular potential barrier of width 200Å and height 0.3eV



Figure 6.2: Plot of the (a) Transmission Coefficient, and the (b) APT time, for a single rectangular potential barrier for $E < V_o$, with barrier width 200Å and barrier height 0.3eV



Figure 6.3: Plot of the (a) Transmission Coefficient, and the (b) APT time, for a single rectangular potential barrier for $E > V_o$, with barrier width 200Å and barrier height 0.3eV



Figure 6.4: Plot of the Traversal Times : (a) Dwell Time, (b) Phase-Delay Time, (c) Buttiker-Landauer Time, (d) APT time, and (e) Classical Time for $E < V_o$, with barrier width 200Å and barrier height 0.3eV.



Figure 6.5: Plot of the Traversal Times : (a) Dwell Time, (b) Phase-Delay Time, (c) Buttiker-Landauer Time, (d) APT time, and (e) Classical Time for $E > V_o$, with barrier width 200Å and barrier height 0.3eV.



Figure 6.6: Plot of the Traversal Times : (a) Dwell Time, (b) Phase-Delay Time, (c) Buttiker-Landauer Time, (d) APT time, (e) Classical Time, and the (f) Transmission Coefficient for $E > V_o$, with barrier width 200Å and barrier height 0.3eV.



Figure 6.7: 3-Dimensional surface plot of the APT time, for the case of $E < V_o$ with the barrier height 1.0eV and barrier width in the range $25\mathring{A}$ to $250\mathring{A}$.



Figure 6.8: 3-Dimensional surface plot of the APT time, for the case of $E > V_o$ with the barrier height 1.0eV and barrier width in the range $25\mathring{A}$ to $250\mathring{A}$.

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Figure 6.9: The conduction band edge profile of a symmetrical double rectangular potential barrier structure with a barrier height of 0.956eV, barrier width of 30Å and a well width of 100Å.



Figure 6.10: Plot of the (a) Transmission Coefficient and the (b) APT time for a symmetrical double rectangular potential barrier structure with a barrier height 0.956eV, barrier width 30\AA and a well width 100\AA , for $E < V_o$.



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Figure 6.11: The conduction band edge profile of a symmetrical double rectangular potential barrier structure with a barrier height 0.23eV, barrier width 50Å and a well width 50Å.

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Figure 6.12: Plot of the (a) Transmission Coefficient and the (b) APT time for a symmetrical double rectangular potential barrier structure with a barrier height 0.23eV, barrier width 50Å and a well width 50Å, for $E < V_o$.



Figure 6.13: The conduction band edge profile of a symmetrical double rectangular potential barrier structure with a barrier height 1.0eV, barrier width $25\mathring{A}$ and a well width $45\mathring{A}$.



Figure 6.14: Plot of the (a) Transmission Coefficient and the (b) APT time for $E < V_o$ for a symmetrical double rectangular potential barrier structure with a barrier height 1.0eV, barrier width $25\mathring{A}$ and a well width $45\mathring{A}$.



Figure 6.15: The conduction band edge profile of a symmetrical rectangular double potential barrier structure of barrier height 0.3eV, barrier width in the range from 30\AA to 100\AA and well width 30\AA , for $E < V_o$.



Figure 6.16: 3-Dimensional surface plot of the APT time for $E < V_o$. The barrier height is 0.3eV and the barrier width in the range from 30\AA to 100\AA and the well width is 30\AA .



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Figure 6.17: The conduction band edge profile of a symmetrical rectangular double potential barrier structure of barrier height 1.0eV, barrier width 30Å and the well width in the range from 30Å to 110Å.



Figure 6.18: 3-Dimensional surface plot of the APT time for $E < V_o$. The barrier height is 1.0eV and barrier width 30\AA and the well width in the range from 30\AA to 110\AA .

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Figure 6.19: 3-Dimensional surface plot of the (a) APT time and the (b) transmission coefficient for $E < V_o$. The barrier height is 1.0eV and barrier width is 30\AA and well width in the range from 30\AA to 110\AA .

Chapter 7

CONCLUSION

Starting from the analytical solution to the time-independent Schrödinger equation in one-dimension, and exploiting the analogy between the transmission line equation and the solution to the Schrödinger equation, an analytical expression for the Average Particle Traversal (APT) time, τ_{APT} , was derived in terms of the real part of the Quantum Mechanical Wave Impedance (QMWI). This approach was used to derive an analytical expression for the τ_{APT} through a single rectangular potential barrier under zero bias, and the results were compared with the dwell time, the phase-delay time, the Buttiker-Landauer time, the Collins-Barker numerical traversal time and the classical traversal time. The APT time is inversely proportional to the transmission coefficient. τ_{APT} approaches infinity as the incident energy tends to zero and as the energy goes to infinity, τ_{APT} tends to the classical time. The APT time is always more than the classical traversal time. The same approach was extended to obtain an analytical expression for the τ_{APT} through a symmetric double rectangular potential barrier structure under zero bias. The APT time is inversely proportional to the transmission coefficient and the τ_{APT} attains a minimum at resonant energies when the transmission coefficient is unity. The maximum frequency of oscillation of some of experimentally studied resonant tunneling structures were compared with those obtained using APT time. The agreement is good.

The capacitance charging time at the depletion regions were not taken into consideration. The

effective masses were assumed to be constant throughout the structure. The τ_{APT} in the free propagation regions, ahead and beyond the barriers, were not taken into consideration. The effect of the effective mass can be incorporated in this approach and an analytical expression for the τ_{APT} for a barrier structure with different outer edges can possibly be derived. An analytical expression can possibly be derived for the τ_{APT} through unsymmetrical double potential barriers. Coupled-quantum-wells effect can also be incorporated. As the pre-free-propagating region may play an important role, the traversal time through the pre-free-propagating region also should be considered, especially when comparison with experiments are made.

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Chapter 8

APPENDIX A

8.1 Complex Coefficients of Wave Function Solutions

The complex constants involved in the solutions to the Schrödinger Equation are given in this section. The suffix 1 and 2 indicate the real and imaginary parts of the constants, respectively.

$$A = \frac{e^{i2kd}}{i2k\alpha e^{\alpha d}} \left(\frac{\alpha + ik}{\alpha - ik}\right) \left[\left[(k^2 - \alpha^2) + (\alpha - ik)^2 e^{i2kd_1}\right] \sinh(\alpha d) + i2k\alpha \cosh(\alpha d)\right] - \left(\frac{\alpha + ik}{\alpha - ik}\right)$$
(8.1)

$$B = \frac{He^{ik2d}(\alpha + ik)}{i4k\alpha^2 e^{\alpha d}} [[(k^2 - \alpha^2) + e^{i2kd_1}(\alpha - ik)^2]\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)]$$
(8.2)

$$C = \frac{He^{i2kd}(\alpha - ik)}{i4k\alpha^2 e^{-\alpha d}} [[(k^2 - \alpha^2) + e^{i2kd_1}(\alpha + ik)^2]\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)]$$
(8.3)

$$D = \frac{He^{ikd}}{i2k\alpha} [(k^2 - \alpha^2)\sinh(\alpha d) + i2k\alpha\cosh(\alpha d)]$$
(8.4)

$$E = \frac{He^{ik(3d+2d_1)}}{i2k\alpha}(\alpha^2 + k^2)\sinh(\alpha d)$$
(8.5)

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$$F = \frac{He^{ik(2d+d_1)}(\alpha+ik)}{2\alpha e^{\alpha(2d+d_1)}}$$
(8.6)

$$G = \frac{He^{ik(2d+d_1)}(\alpha - ik)}{2\alpha e^{-\alpha(2d+d_1)}}$$
(8.7)

$$B_{1} = \alpha (k^{2} - \alpha^{2})(1 - e^{-2\alpha d}) \sin^{2}(kd_{1})$$

$$+ 2\alpha^{2}k(1 - e^{-2\alpha d}) \sin(kd_{1}) \cos(kd_{1})$$

$$+ k(k^{2} - \alpha^{2})(1 - e^{-2\alpha d}) \sin(kd_{1}) \cos(kd_{1})$$

$$+ \alpha k^{2}(1 - e^{-2\alpha d})(1 - 2\sin^{2}(kd_{1}))$$

$$- \alpha k^{2}(1 + e^{-2\alpha d})$$

(8.	8)
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$$B_{2} = k(k^{2} - \alpha^{2})(1 - e^{-2\alpha d}) \sin^{2}(kd_{1})$$

$$+ 2\alpha k^{2}(1 - e^{-2\alpha d}) \sin(kd_{1}) \cos(kd_{1})$$

$$-\alpha (k^{2} - \alpha^{2})(1 - e^{-2\alpha d}) \sin(kd_{1}) \cos(kd_{1})$$

$$-\alpha^{2} k(1 - e^{-2\alpha d})(1 - 2\sin^{2}(kd_{1}))$$

$$+\alpha^{2} k(1 + e^{-2\alpha d})$$

(8.9)

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$$C_{1} = \alpha(k^{2} - \alpha^{2})(e^{2\alpha d} - 1)\cos^{2}(kd_{1})$$

-2\alpha^{2}k(e^{2\alpha d} - 1)\sin(kd_{1})\cos(kd_{1})
+k(k^{2} - \alpha^{2})(e^{2\alpha d} - 1)\sin(kd_{1})\cos(kd_{1})
+\alpha k^{2}(e^{2\alpha d} - 1)(-1 + 2\cos^{2}(kd_{1}))
+\alpha k^{2}(e^{2\alpha d} + 1)

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(8.10)

$$C_{2} = \alpha (k^{2} - \alpha^{2})(e^{2\alpha d} - 1) \cos(kd_{1}) \sin(kd_{1})$$

$$+ 2\alpha k^{2}(e^{2\alpha d} - 1) \sin(kd_{1}) \cos(kd_{1})$$

$$- k(k^{2} - \alpha^{2})(e^{2\alpha d} - 1) \cos^{2}(kd_{1})$$

$$+ \alpha^{2} k(e^{2\alpha d} - 1)(-1 + 2\cos^{2}(kd_{1}))$$

$$+ \alpha^{2} k(e^{2\alpha d} + 1)$$

(8.11)

$$D_1 = \frac{2k\alpha\cos(kd)\cosh(\alpha d) + (k^2 - \alpha^2)\sin(kd)\sinh(\alpha d)}{2k\alpha}$$
(8.12)

$$D_2 = \frac{2k\alpha\cosh(\alpha d)\sin(kd) - (k^2 - \alpha^2)\cos(kd)\sinh(\alpha d)}{2k\alpha}$$
(8.13)

$$E_{1} = \frac{(\alpha^{2} + k^{2})\sin[k(3d + 2d_{1})]\sinh(\alpha d)}{2k\alpha}$$
(8.14)

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$$E_2 = \frac{-(\alpha^2 + k^2)\cos[k(3d + 2d_1)]\sinh(\alpha d)}{2k\alpha}$$
(8.15)

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$$F_1 = \frac{\alpha \cos[k(2d+d_1)] - k \sin[k(2d+d_1)]}{2\alpha e^{\alpha(2d+d_1)}}$$
(8.16)

$$F_2 = \frac{k \cos[k(2d+d_1)] + \alpha \sin[k(2d+d_1)]}{2\alpha e^{\alpha(2d+d_1)}}$$
(8.17)

$$G_1 = \frac{\alpha \cos[k(2d+d_1)] + k \sin[k(2d+d_1)]}{2\alpha e^{-\alpha(2d+d_1)}}$$
(8.18)

$$G_2 = \frac{\alpha \sin[k(2d+d_1)] - k \cos[k(2d+d_1)]}{2\alpha e^{-\alpha(2d+d_1)}}$$
(8.19)