IZMIR INSTITUTE OF TECHNOLOGY

# Tunneling Through a Potential Barrier

by

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*"I think I can safely say that nobody understands quantum mechanics..."*

Richard Phillips Feynman (May 11, 1918  February 15, 1988)

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# *Abstract*

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This is my undergraduate thesis. So far I have worked on tunneling and its classical, semi-classical and quantum description, then I looked some unsolved problems . I have learned about Hartman effect , tunneling time, semi-classical approximations ,path integral and a classical description of tunneling.

# Contents

# Chapter 1

# CLASSICAL DESCRIPTION AND UNCERTAINTY PRINCIPLE

## 1.1 CLASSICAL DESCRIPTION

Every day we encounter systems that are completely classical, i.e. systems that behave in accordance with the laws of classical physics. However,tunneling is a microscopic phenomenon where a particle can penetrate an in most cases pass through a potential barier,which is assumed to be higher than the kinetic energy of the particle.Therefore such motion is not allowed by the laws of classical dynamics. We begin our study of tunneling by investigating as to why tunneling is exclusively a quantum phenomena and does not have a classical counterpart. .[1] [2]

For people that have not heard of this before let me give a simple minded introduction. Imagine throwing a ball at a tree. Now, if the ball hits the tree then it bounces back and if you throw it fast and high enough it will clear the tree. Similarly, imagine a classical particle coming from the left towards a potential barrier. Suppose that the total energy (kinetic + potential) of the particle is less than the maximum height of the barrier. I am sure we all agree that the particle is going to bounce back from the barrier since it has insufficient energy to get over it. This is what classical mechanics would say and the question is what would quantum mechanics say for the same system? Surprisingly, according to quantum mechanics there is a very small but finite probability that the particle could be found to the right of the barrier! This phenomenon and various other generalizations is called as tunneling. Tunneling is rather important in many situations

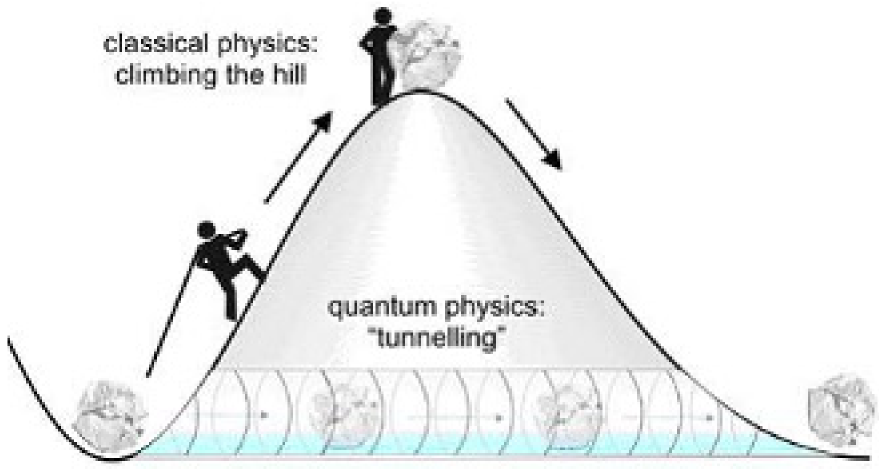



FIGURE 1.1

arising in fields ranging from Biology to modern computers. Hence, there are good reasons to try to understand tunneling and its effect on systems. .[3]

Let's try to understand this example by using the outside and inside barrier situations.

### 1.1.1 Outside Barrier

Particle with energy E moving the outside of barrier freely( $V = 0$) without any potensial,the total energy of the particle is ; $E = K + V$ and we can write that $K = \frac{p^2}{2m}$ or $K = \frac{1}{2}mv^2$

so $E = \frac{1}{2}mv^2 + V$ or $E = \frac{p^2}{2m} + V$ , and then we have found the velocity of the particle is $v = \sqrt{\frac{2}{m}(E - V)}$ , the momentum of the particle is $p = \sqrt{2m(E - V)}$

There are 2 regions (left outside where particle reflected and right outside where particle transmitted) and 2 boundary conditions ( $E > V$ and $V > E$) First we deal with the $E > V$ situation ;

Particle is easily scattering through the barier from left side to right side , so there is not any tunneling and we can describe the particle in both left and right side , inasmuch as the momentum of the particle is always found positive.

Outside the barrier, we can use the hamiltonian and lagrangian for describing the particle position and particle' behaviors.That's why the velocity of the particle is real outside the barrier $v = \sqrt{\frac{2}{m}(E - V)} > 0$ and there is not much words to say about it.

However , If the $V > E$ , particle can act as one way according to classical mechanics, it can be reflected after hit the barrier and there is not any possibility to pass other side of the barrier with lower energy than potential of the barrier.

### 1.1.2 Inside Barrier

Particle with energy E moving within a step potential with height $V > E$ is classically prohibited, since this would lead to an imaginary velocity $v = \sqrt{\frac{2}{m}(E-V)} < 0$ within the potential; however,one solution is that this prohibition is no longer necessary, if we extend Hamilton mechanics to complex space and allows particle to possess imaginary parts of position and momentum. We have seen in some papers that quantum tunneling is nothing but a classical motion emerged in complex space, which allows us to treat tunneling problems exactly by using classical Hamilton mechanics extended to complex space.[4]

So at the outset it seems as though tunneling is a purely quantum structure and "classically forbidden". That seems to be the end of the story. Is tunneling really an alien concept in classical mechanics? We can atleast ask, in the spirit of quantum-classical correspondence, as to what possible classical structure could give rise to this notion. It turns out that there is such a structure in classical mechanics contained in the complex time solutions to the classical equations of motion . But what does one "mean" by complex time? Isn't time always real? Well, I will let you think about it...but remember, we seem to be perfectly happy with the notion of a complex wavefunction in quantum mechanics! The principle of stationary action introduced by Lagrange, Hamilton, Jacobi and others states that a trajectory is a classical trajectory of the system if the first variations of the action functional vanishes. This leads to differential equations with time as the independent parameter. In general we can find perfectly valid classical solutions in the complex time domain! So there is nothing nonclassical about a complex time classical trajectory. We can take families of such classical tarjectories and get tunneling out of it!.[5] [6]

## 1.2 UNCERTAINTY PRINCIPLE

At the first sight the tunneling of a particle looks like a paradoxical problem, since if the height of the barrier is greater than the total energy of the particle,

$E = \frac{p^2}{2m} + V(x)$

then in the range b where $V(x) > E$ , the kinetic energy $\frac{p^2}{2m}$ is negative and p is imaginary, but this is not correct.

At the root of this paradox is our assumption that at each instant we know both the kinetic and the potential energy separately, or in other words we can assign values to the coordinate x and the momentum p simultaneously and this is in violation of the uncertainty principle. Here we want to know whether it is possible to determine the position of the particle when it is moving under the barrier or not. For this we observe that the particle can be at the point x where $E < V(x)$ but then according to the uncertainty principle its momentum is uncertain by an amount $\sqrt{\Delta p^2}$. Thus if we know the position of the particle to be x, then its total energy cannot be E. Since the transmission amplitude during tunneling is proportional to

$$\exp -\frac{1}{\hbar}\int_{x_0}^{x}\sqrt{2m(V(x)-E)}dx$$

where $x_0$ is the classical turning point, then the probability of finding the particle which is coming from the left to be on the right of the barrier, $x_0 + b$ is proportional to the square of this amplitude or to the factor

$$\exp -\frac{2}{\hbar}\int_{x_0}^{x_0+b}\sqrt{2m(V(x)-E)}dx$$

Now if we want a non-negligible probability then we must have

$$2\sqrt{2m(V_m - E)}b \approx \hbar$$

where $V_m$ is the maximum height of the potential. To find the position of the particle inside the barrier, we have to measure its coordinate with an accuracy $\Delta x < b$, therefore the uncertainty in momentum is

$$\Delta p^2 = \frac{\hbar^2}{4(\Delta x)^2}$$

by subtituting b from above equations , we find

$$\frac{\Delta p^2}{2m} = V_m - E$$

Thus the kinetic energy of the particle must be greater than the difference between the height of the barrier Vm and the total energy E [1].

A result similar to position-momentum uncertainity relation can be obtained from the time-energy uncertainty relation [7].

$$\Delta E \Delta t \approx \frac{\hbar}{2}$$

Again let us denote the energy of the incident particle by E. For a very short time At, the uncertainty in the energy is $\Delta E$, and for sufficiently small At, the energy of the particle E + $\Delta E$ is greater than the height of the barrier $V_m$. Tunneling takes place if in the time At the particle can traverse the barrier. For a rectangular barrier of width b this $\Delta t$ is given by

$$\Delta t = \frac{b}{\sqrt{(\frac{2}{m})(E+\Delta E - V_m)}}$$

and then we find $\Delta E$ to be the solution of the quadratic equation;

$$(\Delta E)^2 - \frac{(\hbar)^2}{2mb^2}\Delta E + (\frac{\hbar^2}{2mb^2})(V_m - E) = 0$$

and the condition for $\Delta E$ to be real is given by

$\frac{\hbar^2}{8mb^2} > V_m - E$ which is same as using position-momentum uncertainity relation.

★ We have used uncertainty principle for classical descripton, however uncertainty principle can be only used for the quantum descriptions.In my view , this approach is completely wrong regarding to classical description.

# Chapter 2

# SEMI-CLASSICAL APPROXIMATIONS

## 2.1 The WKB Approximation

The WKB (Wentzel, Kramers and Brillouin) method is the most widely used approximation for solving tunneling problems [8] , and while it is often applied to one-dimensional cases , it is possible to modify it in different ways to solve two or three-dimensional tunneling. In this part we discuss this approximate technique. However, We will not consider the another semi-classical approximation, i.e. the Miller-Good method [9].You can study yourself to this method.

The essential idea is as follows: Imagine a particle of energy E moving through a region where the potential V(x) is constant. If $E > V$ the wave function of this form

$\psi(x) = A\exp(\pm ikx)$ with $k = \dfrac{\sqrt{2m(E-V)}}{\hbar}$

* Now suppose that V(x) is not constant but varies rather slowly in comparison to $\lambda = \dfrac{2\Pi}{k}$,so that over a region containing many full wavelengths the potential is essential constant.Then it is reasonable to suppose that $\psi$ remains pratically sinusoidal, except that the wavelenght and the amplitude change slowly with x.This is the inspiration behind the WKB approximation.In effect , it identifies two different level of x-dependence: rapid oscillations , modulated by gradual variation in amplitude and wavelenght.

By the same token if $E < V$ ( and V is constant) then $\psi$ is exponential:

$\psi(x) = A\exp(\pm\kappa x)$ with $k = \dfrac{\sqrt{2m(E-V)}}{\hbar}$

And if V(x) is not constant , but varies slowly in comparison with $\frac{1}{\kappa}$, the solution remains pratically exponential, except that A and $\kappa$ are now slowly-varying functions of x.

### 2.1.1 Tunneling

Now Let's think about solution of tunneling by using WKB

I have assumed that $E > V$ so p(x) is real.But we can easily write down the corresponding result in the nonclassical region $(E < V)$ ;

Now we use the WKB solution which is calculated in Griffiths' Introduction to Quantum Mechanics book. [10]

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp(\pm\frac{1}{\hbar} \int |p(x)| dx)$$

To the left of the barrier $(x < 0)$ ;

$\psi(x) = A\exp(ikx) + B\exp(-ikx)$ where A is the incident amplitude, B is the reflected amplitude.

To the right of the barrier $(x > 0)$

$\psi(x) = F\exp(ikx)$ where F is the transmitted amplitude , and the transmission probability is $T = \dfrac{|F|^2}{|A|^2}$

now let's look inside the potential barrier where is tunneling region $(0 \leq x \leq a)$

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp(\frac{1}{\hbar} \int_0^x |p(x)| dx) + \frac{D}{\sqrt{|p(x)|}} \exp(-\frac{1}{\hbar} \int_0^x |p(x)| dx)$$

If the barrier is very high and/or wide ( which is to say, if the probability of tunneling is small), then the coefficient of the exponentially increasing term (C) must be small ( in fact it would be zero if the barrier were infinitely broad). The relativity amplitudes of the incident and transmitted waves are determined esentially by the total decrease of the exponential over the nonclassical region:

$$T = \frac{|F|^2}{|A|^2} \backsim \exp(-\frac{1}{\hbar} \int_0^x |p(x)| dx)$$

so that

$$T = \exp(-2\gamma) \text{ with } \gamma = \frac{1}{\hbar} \int_0^x |p(x)| dx$$

## 2.2 Path Integral

The path integral formulation of quantum mechanics is a description of quantum theory which generalizes the action principle of classical mechanics. It replaces the classical notion of a single, unique trajectory for a system with a sum, or functional integral, over an infinity of possible trajectories to compute a quantum amplitude.

The path integral formulation was developed in 1948 by Richard Feynman. Some preliminaries were worked out earlier, in the course of his doctoral thesis work with John Archibald Wheeler.

This formulation has proved crucial to the subsequent development of theoretical physics, because it is manifestly symmetric between time and space. Unlike previous methods, the path-integral allows a physicist to easily change coordinates between very different canonical descriptions of the same quantum system.

The path integral also relates quantum and stochastic processes, and this provided the basis for the grand synthesis of the 1970s which unified quantum field theory with the statistical field theory of a fluctuating field near a second-order phase transition. The Schrdinger equation is a diffusion equation with an imaginary diffusion constant, and the path integral is an analytic continuation of a method for summing up all possible random walks. For this reason path integrals were used in the study of Brownian motion and diffusion a while before they were introduced in quantum mechanics.

Recently path integrals have been expanded from Brownian paths to Lvy flights. The Lvy path integral formulation leads to fractional quantum mechanics and fractional Schrdinger equation.

### 2.2.1 Tunneling

We consider the path integral approach to one-dimensional tunneling.In this approach we formulate the tunneling problem with help of the Feynman propagator $D_f(x_f, x_i; T, 0)$ [11] [12], [13] , [14] . The square of the absolute value of this propagator is a measure of the probability of finding the particle which is initially at $x = x_i$ to be at $x =_f$ at the time T.

According to Feynman , we can determine this propagator by summing over the classical paths [15] ;

$D_f \sim \int [D(x) \exp[\frac{i}{\hbar} S(x)]$

For the problem of tunneling that we want to study, it is more convenient to replace $D_f(x_f, x_i; T, 0)$ by its energy Fourier transform,

$$D_f(x_f, x_i; E) = \int_0^\infty D(x) \exp[\frac{iET}{\hbar} D_f(x_f, x_i; T, 0)]dT$$

In the classical limit $\hbar \to 0$ , $\frac{iS}{\hbar}$ becomes large, and we find an approximate value for the integral using the method of stationary phase [16], [17].In this limit we get an expression which is similar to the WKB approximation,

$$D_f(x_f, x_i; T, 0) = f(x_f, x_i) \exp[\frac{i}{\hbar} S[x_{cl}] \ ,$$

here in this equation $f(x_f, x_i)$ is given by [14] ,

$$f(x_f, x_i = \frac{1}{[2\Pi k(x_f)k(x_i) \int_{x_i}^{x_f} \frac{dx}{(k(x))^3}]^{\frac{1}{2}}}$$

and $S[x_{cl}]$ is the classical action for a path joining the space time point $(x_f, T)$ to $(x_i, 0)$.This action is expressible as

$$S[x_{cl}] = \int_{x_i}^{x_f} k_{cl}(x)dx - E_{cl}T = \int_{x_i}^{x_f} \sqrt{2m[E_{cl} - V(x)]}dx - E_{cl}T$$

Here the constant $E_{cl}$ is the classical energy of this path and is related to T by the following relation

$$T = \int_{x_i}^{x_f} \sqrt{\frac{m}{2[E_{cl} - V(x)]}}dx$$

With the help of the stationary phase method, we can carry out the time integration in

$$D_f(x_f, x_i; E) \simeq \frac{m}{\sqrt{k(x_f)k(x_i)}} exp[i \int_{x_i}^{x_f} k_{cl}(x)dx$$

So far we have assumed that a real path exists for the motion of the particle , but we can generalize this method and apply it to the cases where tunneling occurs.

For a constant energy E, we can write $D_f(x_f, x_i; E)$ as a sum over these extended paths , $x_n$ ,which connects $x_i$ to $x_f$ ;

$$D_f(x_f, x_i; E) = \frac{m}{\sqrt{k(x_f)k(x_i)}} \sum_n K_n \ ,$$

where this $D_f$ is a semi-classical approximate form of the propagator, and the coefficients $K_n$ are determined by the following set of rules [14] :

(1) - In the classically allowed region we use the factor

$$\exp[i \int_{x_1}^{x_2} k(x)dx]$$

where $k(x) = \sqrt{k^2 - v(x)}$,

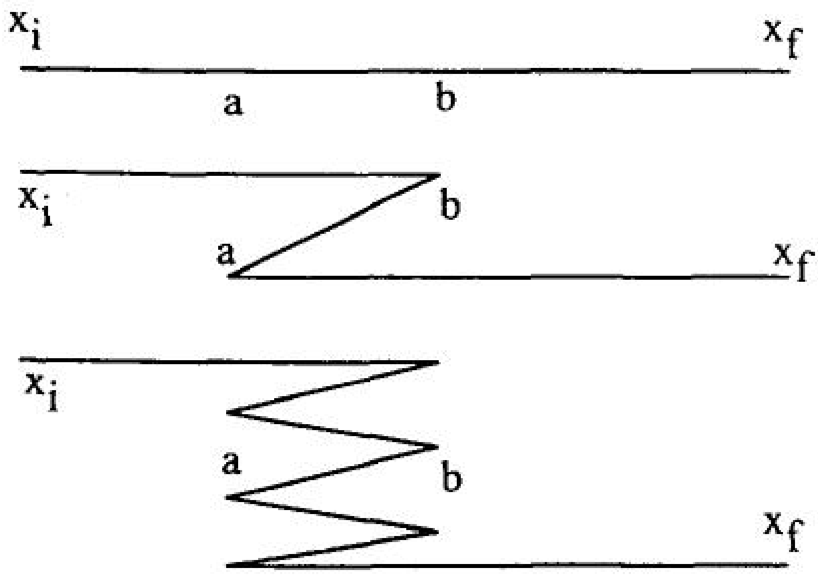



FIGURE 2.1: Possible extended classical paths connecting the initial point $x_i$ to the final point $x_f$, with a number of reflections inside the barrier.

whereas for the classically forbidden region, under the barrier the factor is

$\exp[-\int_{x_1}^{x_2} q(x)dx]$

where $q(x) = \sqrt{v(x) - k^2}$.

The way that we use these factors will be shown by studying a specific example below.

(2) - If the reflection from a classical turning point is from a part where the classical motion is allowed, we use a factor(-i). If the reflection is from the side where the classical motion is forbidden the factor that we use is (- $\frac{i}{2}$).

Let us consider the method of construction of $D_f(x_f, x_i; E)$ when there is a single barrier with turning points at a(E) and b(E), $b(E) > a(E)$ Fig.[2.1]

The trajectory of the particle starts at $x = x_i$ to the left of a(E) and ends at $x = x_f$ to the right of b(E).In the wave picture the simplest path consists of a wave emanating from $x_i$ , reaching the turning point $x = a(E)$ , and propagating under the barrier from a(E) to b(E), and finally moving from b(E) to $x_f$.For this case we can write the total amplitude as

$$D_f(x_f, x_i; E) = \frac{m}{\sqrt{k(x_f)k(x_i)}} \exp[i \int_{x_i}^{a} k(x)dx] * \{Z + (\frac{i}{2})^2 Z^3 + \ldots\} \exp[i \int_{b}^{x_f} k(x)dx]$$

where Z which is given by

$Z = \exp[-i \int_a^b q(x)dx]$

is the penetration factor in the WKB approximation. The infinite series in the curly bracket form a geometric series and thus can be summed to yield

$$\frac{Z}{1+\frac{1}{4}Z^2}$$

Then we find the coefficent of transmission to be equal to ;

$$|T(E)|^2 = |\frac{Z}{1+\frac{1}{4}Z^2}|^2 ,$$

where Z is a function of the energy E.

# Chapter 3

# QUANTUM DESCRIPTION

## 3.1 A Brief History of Quantum Tunneling

In 1896 Elster and Geitel found the exponential decay rate of radioactive substances experimentally three years after the discovery of natural radioactivity .[18]

In 1900 Rutherfod introduced the idea of half-lifeof these chemicals,i.e. the time that the number of radioactive nuclei reach one-half of their original number.[19]

In 1905 Schweidler showed the statistical nature of the decay.[20] This means that the probability of disintegration of a nucleus does not depend on the time of its formation and also the time that a particular nucleus decays can only be predicted statistically. This idea was verified empirically by Kohlrausch in 1906.[21] Later experiments showed that the decay width $\Gamma$ (which is related to the half-life $\tau$ by $\tau = \frac{ln2}{\Gamma}$ ) does not depend on external variables such as pressure, temperature or chemical environment.

The exponential law of decay can be written either in differential form as;

$\frac{dN(t)}{dt} = -\Gamma N(t)$ or as an integral form $N(t) = N_0 e^{(-\Gamma t)}$ ,

where $N_0$ is the original number of nuclei (at t=0), N(t) is their number at $t > 0$ , and $\Gamma$ is the decay probability per unit time.For the rate of decay one can use either $T = \frac{1}{\Gamma}$ or the half-life $\tau = T \ln(2)$

Instead of N(t) we can use $P(t) = \frac{N(t)}{N_0} = e^{(-\Gamma t)}$ which is usually referred to as the law of exponential decay.

By 1928, George Gamow had solved the theory of the alpha decay of a nucleus via tunnelling. Classically, the particle is confined to the nucleus because of the high energy requirement to escape the very strong potential. Under this system, it takes an enormous amount of energy to pull apart the nucleus. In quantum mechanics, however, there is a probability the particle can tunnel through the potential and escape. Gamow solved a model potential for the nucleus and derived a relationship between the half-life of the particle and the energy of the emission.[22] , [23] , [24]

Alpha decay via tunnelling was also solved concurrently by Ronald Gurney and Edward Condon. [25] , [26], [27] Shortly thereafter, both groups considered whether particles could also tunnel into the nucleus. After attending a seminar by Gamow, Max Born recognized the generality of quantum-mechanical tunnelling.[28] , [29] He realized that the tunnelling phenomenon was not restricted to nuclear physics, but was a general result of quantum mechanics that applies to many different systems.

1930's and 1940's there were many attempts to relate the dynamics of the electron current in a system of metal-semiconductor which was used in rectifying the current, to the tunneling of electrons in solids. But the models were not realistic enough and usually quantum theory was predicting a current in the opposite direction of the observed current. With the discovery of transistors in 1947, the tunneling of electrons received renewed attention. In 1950 the construction of semiconductors like Ge and Si had advanced to a point were it was possible to manufacture semiconductors of given characteristics.

In 1957 L. Esaki discovered tunnel diode and this discovery proved the electron tunneling in solids conclusively [30].Three years later i.e. in 1960, I. Giaever observed that if one or both of the metals are superconducting then the voltage-current curve provides interesting information regarding the state of superconductor (s). This experiment of Giaever was sufficiently accurate that it enabled one to measure the energy gap in superconductors. This gap appears when electrons form Cooper pairs, and the gap plays an essential role in the BCS theory of superconductivity [31].

The other major discovery was the theoretical work of B.D. Josephson in 1962 in connection with the tunneling between two superconductors separated by a thin layer of insulating oxide which serves as the barrier. Taking all of this as a single system, Josephson was able to predict the existence of a second current, i.e. the supercurrent in addition to the current foundby Giaever, and this he showed is due to the tunneling of electrons in pairs[32]. Only very recently the tunneling of an individual atom, e.g. hydrogen on a metal surface such as copper has been observed directly. A remarkable (non-classical) feature of the experiment is that the tunneling rate increases as the surface gets colder [33], [34] Today the theory of tunnelling is even applied to the early cosmology of the universe. Quantum tunnelling was later applied to other situations, such as the cold emission of electrons, and perhaps most importantly semiconductor and superconductor physics. Phenomena such as field emission, important to flash memory, are explained by quantum tunnelling. Tunnelling is a source of major current leakage in Very-large-scale integration (VLSI) electronics, and results in the substantial power drain and heating effects that plague high-speed and mobile technology. Another major application is in electron-tunnelling microscopes (see scanning tunnelling microscope) which can resolve objects that are too small to see using conventional microscopes. Electron tunnelling microscopes overcome the limiting effects of conventional microscopes (optical aberrations, wavelength limitations) by scanning the surface of an object with tunnelling electrons. Quantum tunnelling has been shown to be a mechanism used by enzymes to enhance reaction rates. It has been demonstrated that enzymes use tunnelling to transfer both electrons and nuclei such as hydrogen and deuterium. It has even been shown, in the enzyme glucose oxidase, that oxygen nuclei can tunnel under physiological conditions. [35]

## 3.2 Quantum Tunneling Through Barrier

Consider a particle of total energy E in the potential.In classical physics, if $E < V$ , the particle could never be found in the regions where $V(x) > E$, because that would imply that the kinetic energy $K = E - V$ was negative. Such intervals are referred to as the classically forbidden regions; intervals where $E > V(x)$ are the classically allowed regions. A particle in region II could never get out; it would be a bound state trapped by the potential, forever bouncing between points x2 and x3 . On the other hand, a particle in region I or III could never enter region II, but would bounce off the potential wall at points x1 and x4 , respectively. In quantum mechanics the physical state is governed by the Schrodinger equation, and generally there is no reason that the wavefunction must be exactly zero in regions where $E < V(x)$. This means that there is usually a finite probability to find a particle in the classically forbidden regions, and this fact gives rise to some remarkable phenomena which are inconceivable at the classical level. Nevertheless, the wave function does behave quite differently in the classically allowed and the classically forbidden regions, as one might expect, since classical behavior is an approximation to quantum mechanics, and should become exact in the h is greater than limit .This wholly non-classical phenomenon is called TUNNELING. Tunneling is a genuine quantum effect, a direct consequence of the matter wave structure of quantum mechanics. The two remarkable applications of tunneling are: (a) Resonant tunneling diodes, which are used as switching units in fast electronic circuits. (b) Scanning tunneling microscope (STM), based on the penetration of electrons near the surface of a solid sample through the barrier at the surface. These electrons form a "cloud" of probability outside the sample. Although the probability of detecting one of these electrons decays exponentially with distance (from the surface), one can induce and measure a current of these electrons and attain a magnification factor of 100 million large enough to permit resolution of a few hundredths the size of an atom. Gerd Binning and Heinrich Rohrer won the Noble Prize in Physics in 1986 for the invention of The STM.

Tunneling is a pure quantum mechanical phenomenon that a particle can cross a barrier with potential V, even if its total energy E is strictly less than V. Many phenomena related to tunneling are widely observed and applied in many areas of microscopic science and technology. Nevertheless, the understanding of this phenomenon to date does not seem complete yet.

### 3.2.1 Outside Barrier

A beam of particles coming from $x = -\infty$ meets a potential barrier described by $V(x) = V$ , where V is a positive constant, at x = 0.We have considered the incident beam of particles to have energy $0 < E < V$ and found the wavefunction for $x < 0$ and for $x > 0$, and described the transmission and reflection coefficients for this potential.

To begin with considering the time-independent Schrdinger equation for one particle, in one dimension.

This can be written in the forms $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + V(x) = E\Psi(x)$

To solve a problem , we divide the problem into two regions. We label $x < 0$ as Region I. In this region, the potential is zero and so the beam of particles is described by the free particle wavefunction. A particle coming from the left and moving to the right, which we label as the incident wavefunction, is described by:

$\psi_{inc}(x) = Ae^{[ikx]}$

When the beam encounters a potential barrier, some particles will be reflected back. So the total wavefunction in Region I is given by a sum of $incident + reflected$ wavefunctions. The reflected wavefunction, which moves to the left, is $\sim e^{[-ikx]}$.

We write the total wavefunction;

in Region I as:

$\psi = \psi_{inc}(x) + \psi_{ref}(x) = Ae^{[ikx]} + Be^{[-ikx]}$

in Region II as :

$\psi_{trans}(x) = Ce^{[\beta x]}$ ; $\beta^2 = \frac{2m}{\hbar^2}(V - E)$

So, to the left of the barrier, the wavefunction is oscillatory, while to the right it exponentially decays.

**Definition: Conditions the wavefunction must obey at a discontinuity**

The wavefunction must obey two conditions:

1. $\psi$ must be continuous

2. The first derivative $\frac{d\psi}{dx}$ must be continuous

After using this conditions , we find the relations between A , B and C .

$A + B = C$

$\frac{B}{A} = \dfrac{1 - i\dfrac{\beta}{k}}{1 + i\dfrac{\beta}{k}}$

$\dfrac{C}{A} = \dfrac{i2k}{ik - \beta}$

Now we calculate the probability current density for each wavefunction. This is given by:

$J = \frac{\hbar}{2mi}(\psi^* \frac{d\psi}{dx} - \psi \dfrac{d\psi^*}{dx})$

For , $\psi_{inc}(x) = Ae^{[ikx]}$ we find:

$J_{inc} = \frac{\hbar}{2mi}(i2kA^2) = \frac{\hbar}{m}(kA^2)$

A similar procedure shows that:

$J_{ref} = \frac{\hbar}{m}(kB^2)$

Now we calculate the current density for the transmitted current. The wavefunction for $x > 0$ is:

$J_{trans} = 0$

The reflection coefficient is found to be:

$R = \frac{J_{ref}}{J_{inc}} = \frac{B^2}{A^2} = 1$

$T = \frac{J_{trans}}{J_{inc}} = 0$

As expected, there is particle penetration into the barrier, but this tells us that no particles make it past the barrier there is 100 % reflection.

This quantum description is not different than classical description. Let's look the inside barrier.

### 3.2.2 Inside Barrier

Incident particles of energy E coming from the direction of $x = -\infty$ are incident on a square potential barrier V , where $E < V$ .

The potential is V for $0 < x < a$ and is 0 otherwise. Let's find the transmission coefficient.

We divide this problem into three regions:

Region I: $-\infty < x < 0$

Region II: $0 < x < a$

Region III: $a < x < \infty$

With the definitions:

$k^2 = \frac{2mE}{\hbar^2}$ , $\beta^2 = \frac{2m(V-E)}{\hbar^2}$

the wavefunctions for each of the three regions are:

$\phi_1(x) = Ae^{ikx} + Be^{-ikx}$

$\phi_2(x) = Ce^{\beta x} + De^{-\beta x}$

$\phi_3(x) = Ee^{ikx}$

Like above ;

**Definition: Conditions the wavefunction must obey at a discontinuity**

The wavefunction must obey two conditions:

1. $\phi$ must be continuous

2. The first derivative $\frac{d\phi}{dx}$ must be continuous

After using this conditions , we find the relations between A , B , C , D and E . However, We need only E and A for determining the transmission coefficient.

After doing some calculations like the outside barrier .We have found the transmission coefficient :

$T = (\frac{E}{A})^2 = \frac{1}{\frac{(k^2-\beta^2)^2}{4k^2\beta^2}\sinh(\beta a)^2+\frac{1}{2}}$

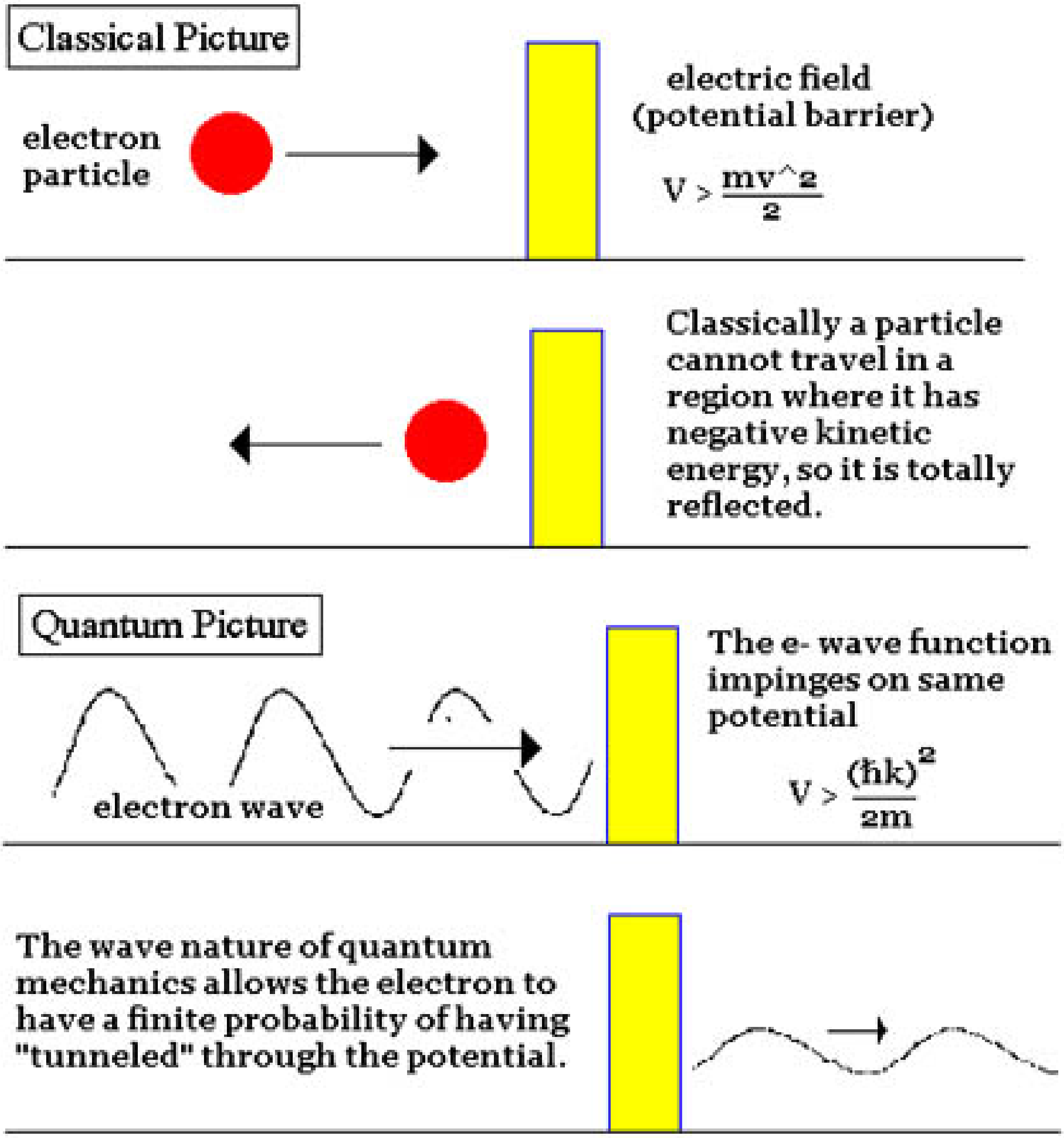
$T = \frac{1}{1+\frac{V^2\sinh^2(ka)}{4E(V-E)}}$

This differs from the predictions of classical physics. According to classical physics, a particle cannot make it past a barrier when $E < V$ . However according to this result there is a non-zero probability that the particle can make it past the barrier. This quantum effect is called **tunneling**. [7] , [36] , [10] , [37], [38] [39].

### Bohms Causal Theory

It is ironic that the same person who wrote the best account of the Copenhagen interpretation also created the best-known hidden variable theory. Bohms causal theory, which attributes a precise value to the position and the momentum of the particle, solves trivially, in a sense, the timing of events and durations. However, the durations or events timed in Bohms theory are, in general, hidden since we do not see the postulated trajectories.

For many the main problem with this theory though is that, according to the standard claim, it is impossible to determine if it is true or not,3 although the assumed equivalence of the predictions of the causal theory and the stan- dard approach have been recently questioned and debated for time correlations and double-slit experiments. In any case, the theory has had and has quite a number of devoted followers. Several authors have advocated the use of Bohms approach to in vestigate tunneling or arrival times.



Classical Picture
electron particle
electric field (potential barrier)
V > mv^2 / 2
Classically a particle cannot travel in a region where it has negative kinetic energy, so it is totally reflected.
Quantum Picture
electron wave
The e- wave function impinges on same potential
V > (ħk)^2 / 2m
The wave nature of quantum mechanics allows the electron to have a finite probability of having "tunneled" through the potential.


Figure 3.1

# Chapter 4

# UNSOLVED PROBLEMS

## 4.1 Tunneling Times

The tunneling time is an example of a duration type of quantity. Actually the word tunneling here is a red herring since the same conceptual problem arises without tunneling, even for free motion. The actual question is:

How long does a particle take to traverse a spatial region?

It is true, however, that tunneling enhances some of the puzzling aspects of the possible answers. There are hundreds of papers devoted to tunneling or traversal times. The modern stage of the tunneling-time conundrum started with a letter by Buttiker and Landauer in 1982 . They set a traversal time as the time characterizing the transition between sudden and adiabatic regimes in oscillating potential barriers. Very many different proposals appeared subsequently in the literature throughout the 1980s, with each author tending to defend their own time as the good one. The controversy has kept going all through the 1990s, moving however in the direction to a certain degree of consensus: that there is no single quantity that contains the whole and only truth about timing the particles traversal. The tunneling time is in fact one example of quantization of a classical quantity that involves products of noncommuting observables: a unique, classical question corresponds to different quantum versions. Comprehensive theories and experiments show explicitly several of these times.

### 4.1.1 Hartman Effect

The delay time for a quantum tunneling particle is independent of the thickness of the opaque barrier. This is called the Hartman effect and might result in particles traveling faster than light.

The Hartman effect is the tunnelling effect through a barrier where the tunnelling time tends to a constant for large barriers.[40] This was first described by Thomas Hartman in 1962.[41] This could, for instance, be the gap between two prisms. When the prisms are in contact, the light passes straight through, but when there is a gap, the light is refracted. There is a finite probability that the photon will tunnel across the gap rather than follow the refracted path. For large gaps between the prisms the tunnelling time approaches a constant and thus the photons appear to have crossed with a superluminal speed.[42] , [43] , [44]

However, an analysis by Herbert Winful from the University of Michigan suggests that the Hartman effect cannot actually be used to violate relativity by transmitting signals faster than c, because the tunnelling time ”should not be linked to a velocity since evanescent waves do not propagate”.[45] Winful means by this that the photons crossing the barrier are virtual photons only existing in the interaction and could not be propagated into the outside world.

Let’s look the Winful paper [1];

**New paradigm resolves old paradox of faster-than-light tunneling**

*Rethinking tunneling dynamics explains why tunneling time saturates with barrier length and why short delays do not imply superluminal group velocities.*

How long does it take a particle or wave packet to tunnel through a barrier? This question has occupied physicists since the early days of quantum mechanics, when it was suggested that the process is instantaneous. In tunneling, a particle lacking the energy to go over a classically impenetrable potential barrier can nevertheless end up on the other side, albeit with small probability. This process is the basis for devices such as the scanning tunneling microscope, which enables imaging with atomic-scale resolution. It is also at the origin of phenomena such as alpha decay, which sets off nuclear fission. Resolving the issue of tunneling time is thus of both fundamental and practical importance.

Several experiments to determine tunneling time have been carried out using single photons or classical electromagnetic pulses that can tunnel through forbidden regions in the form of evanescent waves. These measurements show that the peak of the much attenuated tunneling wave packet appears at the exit of a barrier sooner than the peak of a wave packet that traversed an equal distance in free space. Since the wave packet in free space travels with the speed of light c, the widely accepted conclusion from these

[1] 29 November 2007, SPIE Newsroom. DOI: 10.1117/2.1200711.0927

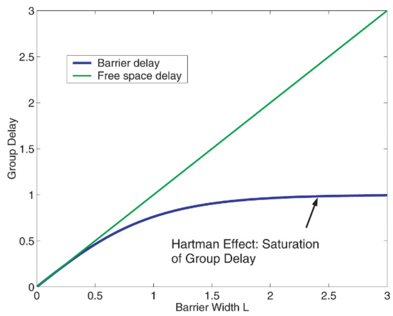



FIGURE 4.1: The Hartman effect, in which the tunneling time (group delay) of a wave packet saturates with barrier length.

experiments has been that tunneling wave packets travel with superluminal (faster-than-light) group velocities. An even more surprising result is that the tunneling time, as measured by the arrival of the peak, becomes independent of barrier length for thick enough barriers (see Figure 1). This phenomenon, predicted by Hartman in 1962 (and termed the Hartman effect), has been observed in several experiments and is at the crux of the tunneling time conundrum. How can the wave packet know the barrier length increased and thus speed up to cover the increased distance in the same time? Our work solves this mystery by introducing a new paradigm: the group delay in tunneling is the lifetime of stored energy escaping through both ends of the barrier. It is not the transit time from input to output, as has been assumed for decades.

A barrier is a filter (e.g., a multilayer dielectric mirror) that rejects a range of frequencies that lie within its stop band while transmitting frequencies outside this band. For a pulse to tunnel, its spectrum must be narrow enough to fit neatly within the stop band, as shown in Figure 2. A narrow spectrum means that the pulse is long in time and has a spatial extent greater than the barrier length. As a result, the barrier is essentially a lumped element with respect to the pulse envelope, and the interaction is quasi-static. When such a long pulse is incident on a barrier, a standing wave is formed in front of the barrier as a result of the interference between incident and reflected waves. Inside the barrier is an evanescent wave that is also a standing wave with an exponentially decaying amplitude. In a standing wave, the field at every spatial point oscillates up and down with the same phase, and the entire distributed structure acts as if it were a lumped element. In reality, because this evanescent standing wave is in contact with transmitting boundaries, the energy it stores can leak through the boundaries. This storage and release of energy leads to a time delay and thus a phase shift between output and input. For a long enough barrier, the amplitude transmission function is

$$T \sim \exp[(-kL) + i\phi(\Omega)]$$

The group delay is the derivative of the transmission phase shift with respect to frequency:

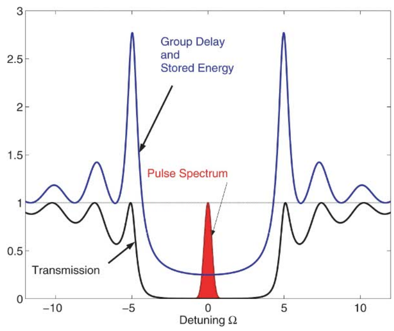



FIGURE 4.2: Black curve: Transmission of a barrier as a function of frequency detuning from the center (Bragg) frequency. The stop band is the region of low transmission (between 5 and 5). Blue curve: Normalized group delay, which is the same as the normalized stored energy. The normalized free-space delay and stored energy is 1. In the stop band, the barrier delay and stored energy are less than the free-space values.

$$\tau = \frac{\phi}{\Omega}$$

and it tells us the time at which the transmitted field attains a peak at the exit. The transmission and group delay are shown in Figure 2. Note that inside the stop band the group delay is less than that of a pulse in free space.

An interesting result is that the group delay is exactly equal to the stored energy in the barrier U divided by the incident power $P_{in}$ :

$$\tau_g = \frac{U}{P_{in}} = \frac{tanh(kL)}{\Omega_c}$$

where $\Omega_c$ is the width of the stop band. For a pulse whose center frequency is tuned to the Bragg frequency, the stored energy is proportional to tanh kL, a quantity that saturates with length. Since the group delay is proportional to stored energy, the Hartman effect or the saturation of the group delay with barrier length is thus explained by the saturation of stored energy. In the limit of a very long barrier, this delay saturates at the value $\tau_g = \frac{1}{\Omega_c}$ ,which is just the inverse of the filter bandwidth.

Since the group delay is proportional to the stored energy, we can now explain why the delay in the presence of a barrier is shorter than in its absence. Figure 3(a) shows the stored energy in a barrier-free region of length L when the peak of the input pulse is at $z = 0$. The group delay is the time it takes to move all that stored energy out of the region in the forward direction. When a barrier of the same length is introduced, the stored energy in the region is reduced below the free-space value as a result of destructive interference. The group delay is the time it takes for this energy to leave the barrier in both directions: it is a cavity lifetime. Since the stored energy in the barrier is less than that in free space, the delay will be shorter.

Because the delay is not a transit time, group velocity is not a valid concept, whereas group delay remains a useful quantity that tells us how long it takes for stored energy to

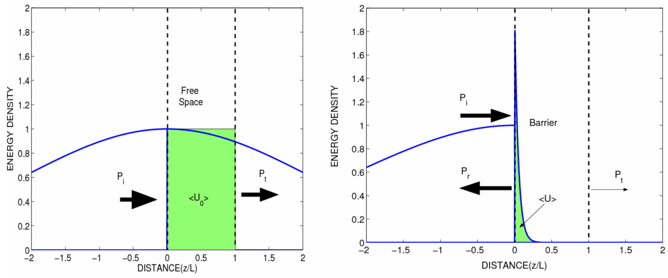



FIGURE 4.3: (a) Blue curve: Snapshot of incident pulse in free space at the instant its peak reaches $z = 0$. The green shaded area represents the energy stored in a region of length L for unity input power. (b) Blue curve: Snapshot of incident pulse and intensity distribution in the presence of barrier at the instant the peak reaches $z = 0$. The green shaded area representing stored energy in the barrier is much smaller than the free-space value.

be released out of both ends of the barrier, most of it leaving in the backward direction. Because the group delay is a cavity lifetime, it does not imply superluminal velocity. In all cases, the delay is much shorter than the pulse length. For this reason, a better measure of the duration of the tunneling event is just the length of the pulse. Finally, in the middle of the stop band the transmission is flat, and there is no dispersion in the group delay. This means that the phase is linear in frequency and there is a pure delay without distortion or reshaping.

Since tunneling is a phenomenon that is universal to all waves, whether matter, electromagnetic, water, or sound, a resolution of this problem has far-reaching implications. Our work has introduced a new paradigm that treats the group delay in tunneling as a lifetime rather than a transit time. This interpretation resolves the paradox of the Hartman effect and explains the anomalously short tunneling times observed in experiments without appealing to superluminal velocities. This opens the way to a deeper understanding of tunneling dynamics and to new methods to measure and control tunneling time.

### 4.1.2 Discussion

Understanding time in quantum mechanics is in fact intimately linked to un- derstanding quantum mechanics itself, in particular, the transition between the potentialities described by the formalism and actual events. However, we are far from a consensus on how, and even if, this transition takes place. Different solutions proposed for this theoretical lacuna amount to different answers for several of the mysteries related to time in quantum mechanics. We have paid particular attention to work done on tunneling times, and arrival times, two topics that have been controversial throughout the past two decades. Some results have been firmly established though, and much progress has been achieved in avoiding a number of stumbling blocks. For ex- ample, Paulis argument against the existence of a self-adjoint time operator in quantum mechanics is not a problem when realizing that observables are not necessarily linked to self-adjoint operators; similarly, difficulties pointed out by other authors, most prominently by Allcock, have been overcome; the multiplicity of quantum answers obtained for some unique classical questions (such as the traversal time) has been also well understood and formalized with a compact systematic theory. Of course different theoretical or experi- mental conditions may select one of them for a specific application. For the arrival time, in particular, distributions, which are optimal with respect to a number of classical constraints, have been identified.

All in all, we have reached a much better understanding of the phenomenol- ogy and underlying theoretical issues concerning time observables in quantum mechanics. Much remains to be done, and many issues are still contended, as the diverse character of the contributions to this volume will make clear. Nonetheless, we are convinced that the patient reader will have ample proof in the following chapters of the improvement in our understanding time in quantum mechanics that has taken place in the last decades. And we hope that the same reader will in turn contribute and improve on this work.

Chapter 5

# A NEW APPROACH

# Bibliography


[1] D.I.Blokhintsev. Quantum mechanics. *D.Reidel,Dordrecht Holland*, 16, 1964.

[2] Mohsen Razavy. *Quantum Theory of Tunneling*. World Scientific Publishing, 2003.

[3] M. V. Berry and K. E. Mount. *Rep. Prog. Phys.*, 35,(315), 1972.

[4] Joachim Ankerhold. *Quantum Tunneling in Complex Systems*. Springer-Verlag Berlin Heidelberg, 2007.

[5] V. P. Maslov and M. V. Fedoriuk. *Semiclassical Approximations in Quantum Mechanics*. Reidel, 1981.

[6] Arnaldo Donoso and Craig C. Martens. Quantum tunneling using entangled classical trajectories. *Phys. Rev. Lett.*, 87(22):223202, Nov 2001. doi: 10.1103/PhysRevLett.87.223202.

[7] Greiner W. *Quantum mechanics. An introduction*. Springer, 2001.

[8] N. Froman and P.O. Froman. Wkb approximation, contributions to the theory. *North-Holland Publishing Company, Amsterdam*, 1965.

[9] Jr. .C. Miller and Jr R.M. Good. Wkb -type approximation to the schrodinger equation. *Phys. Rev.*, 91(174), 1953.

[10] David J. Griffiths. *Introduction to Quantum Mechanics*. Benjamin Cummings, 2 edition, 2004.

[11] ] B.R. Holstein. Understanding alpha decay,. *Am. J. Phys.*, 64(1061), 1996.

[12] ] B.R. Holstein. Bound states, virtual states and nonexponential decay via path integrals. *Am. J. Phys.*, 51(897), 1983.

[13] B.R. Holstein and A.R. Swift. Barrier penetration via path integrals. *Am. J. Phys.*, 50(833), 1982.

[14] B.R. Holstein. , topics in advanced quantum mechanics. *(Addison-Wesley, Redwood, California*, (chp.5), 1992.

[15] ] R.P. Feynman and A.R. Hibbs. *Quantum Mechanics and Path Integrals.* (McGraw-Hill, New York, NY, 1965.

[16] R.B. Dingle. *Asymptotic Expansions: Their Derivation and Interpretation.* ( Academic Press , New York, NY,Chap. VI, 1973.

[17] L.S. Schulman. *Techniques and Applications of Path Integrations.* ( JohnWiley Sons, New York NY, 1981.

[18] J.Elster and H.Geitel. Bequerel rays. *Wied Ann.*, 66(735), 1889.

[19] E. Rutherford. Radioactive substance emitted from thorium compounds. *Phil. Mag.*, 49(1), 1900.

[20] E.R. von Schweidler. Premier congres de radiologie. *Liege*, 1905.

[21] K.W.F. Kohlrausch. Variation in radioactive transformation. *Akad.Wiss.Wien Sitz Ber.*, 115(637), 1906.

[22] G.Gamow. Quantum theory of atomic nucleus. *Z.f.Phys.*, 51(204), 1928.

[23] G.Gamow. Quantum theory of nucler disintegration. *Nature*, 122(805), 1928.

[24] G.Gamow. Consittution of atomic nuclei and radioactivity. *Oxford University Press , London*, 1931.

[25] R.W.Gurney and E.U. Condon. Wave mechanics and radioactive disintegration. *Nature*, 122(439), 1928.

[26] R.W.Gurney and E.U. Condon. Quantum theory and radioactive disintegration. *Phys. Rev.*, 33(127), 1929.

[27] R.W.Gurney and E.U. Condon. Nuclear levels and artificial disintegration. *Nature*, 123(565), 1929.

[28] H. Geiger and J.M.Nuttall. Ranges of a particles from uranium. *Phil.Mag.*, 23(439), 1912.

[29] M. Born. Theory of nuclear disintegration. *Z. f. Phys.*, 58(306), 1929.

[30] L.Esaki. Long journey into tunneling. *Proc. of the IEEE*, 62(825), 1974.

[31] I.Giaever. Electron tunneling and superconductivity. *Science*, 183(1253), 1974.

[32] B.D.Josephson. The discovery of tunneling supercurrent. *Science*, 184(527), 1974.

[33] L.J.Lauhon and W.Ho. Direct observation of the quantum tunneling of single hydrogen atoms with a scanning tunneling microscope. *Phys.Rev.Lett*, 85(4566), 2000.

[34] A. Yazdani. Watching an atom tunnel. *Nature*, 409(471), 2001.

[35] Andrew W Munro Nigel S Scrutton P. Leslie Dutton and Michael J Sutcliffe. Introduction. quantum catalysis in enzymes: beyond the transition state theory paradigm. *hilos Trans R Soc Lond B Biol Sci.*, 361(1472), 2006.

[36] Lifshitz. Landau. *Quantum mechanics: non-relativistic theory*, volume 3. Pergamon, 3 edition, 1991.

[37] David McMahon. *Quantum Mechanics Demystified*. McGraw-Hill Professional, 1 edition, 2005.

[38] J. Greensite. *Lecture Notes on Quantum Mechanics*. Physics and Astronomy Department ,San Francisco State University, 2003.

[39] M. Shifman. Quantum tunneling, 2002. URL http://www.citebase.org/abstract?id=oai:arXiv.org:quant-ph/0204156.

[40] J.C. Martinez and E. Polatdemir. Origin of the hartman effect. *Physics Letters A*, 351(31-36), 206.

[41] T. E. Hartman. Tunneling of a wave packet. *J. Appl. Phys.*, 33(3427), 1967.

[42] Herbert G. Winful. Comment on macroscopic violation of special relativity by nimtz and stahlhofen. *Arxiv*, 2007.

[43] A. Stahlhofen G. Nimtz. Evanescent modes and tunnelling instantaneously act a distance. *IP Conf. Proc*, Volume 977:pp. 310–315, March 6, 2008.

[44] Nimtz A. Haibel U. Walter G. Zero time space: How quantum tunneling broke the light speed. *John Wiley & Sons*, 2008.

[45] Herbert G. Winful. Delay time and the hartman effect in quantum tunneling. *Phys. Rev. Lett.*, 91(260401), December 2003.