

# **ENTROPIC TUNNELING TIME AND ITS APPLICATIONS**

**A Thesis Submitted to  
the Graduate School of Engineering and Sciences of  
İzmir Institute of Technology  
in Partial Fulfillment of the Requirements for the Degree of**

**MASTER OF SCIENCE**

**in Physics**

**by  
Tuğrul GÜNER**

**December 2014  
İZMİR**

We approve the thesis of **Tuğrul GÜNER**

**Examining Committee Members:**

---

**Prof. Dr. Durmuş Ali DEMİR**  
Department of Physics, İzmir Institute of Technology

---

**Assoc. Prof. Dr. Haldun SEVİNÇLİ**  
Department of Materials Science and Engineering, İzmir Institute of Technology

---

**Assoc. Prof. Dr. Özgür ÇAKIR**  
Department of Physics, İzmir Institute of Technology

**15 December 2014**

---

**Prof. Dr. Durmuş Ali DEMİR**  
Supervisor, Department of Physics  
İzmir Institute of Technology

---

**Prof. Dr. Nejat BULUT**  
Head of the Department of  
Physics

---

**Prof. Dr. Bilge KARAÇALI**  
Dean of the Graduate School of  
Engineering and Sciences

# **ACKNOWLEDGMENTS**

I would like to thank to my supervisor Prof.Dr. Durmuş Ali DEMİR for his endless efforts and support in this thesis. I am very grateful to benefit from his experience, and deep knowledge. It is a great honour for me to work with him. Besides, I want to thank Ozan SARGIN for his help, corrections, support, and my family, my friends, and Özge ÇAYLIOĞLU for their support, and motivation.

# ABSTRACT

## ENTROPIC TUNNELING TIME AND ITS APPLICATIONS

Quantum tunneling is one of the most interesting consequences of quantum behaviour. However, even though it is known and understood well, due to non-existence of a time operator in quantum mechanics, estimating what time it takes for a particle to cross a barrier remains an open question. There are some attempts like phase time, dwell time, Larmor clock, Buttiker-Landauer, and Feynman Path Integral approaches. These definitions do not agree with each other and with experiment.

In this thesis work, tunneling time problem is studied in a rather new context. Knowing time necessitates momentum, we deal with momentum state vectors and define entropy accordingly. This entropy, which gives a temperature, defines a thermal energy in the tunneling region. With this thermal energy and uncertainty principle, resulting time deviation of the particle from the classically instantaneous is stated as our tunneling time, entropic tunneling time. Moreover, we compare this tunneling time with recent experiments in detail, and find that, it is in very good agreement with the data. Then, we apply this entropic tunneling time to  $\alpha$  - decay, STM and creation of universe from nothing to predict natural time scale of these processes.

# ÖZET

## ENTROPİK TÜNELLEME ZAMANI VE UYGULAMALARI

Kuantum tünelleme, kuantum mekaniğinin en ilginç sonuçlarından biridir. Ama iyi bilinmesine ve anlaşılmasına rağmen, kuantum mekaniğinde zaman operatörü yazılmayışından ötürü, bir parçacığın bariyeri ne kadar zamanda katedeceği açık bir soru olarak durmaktadır. Bu sorunu çözmek için faz zamanı, dwell zamanı, Larmor saati, Buttiker-Landauer, ve Feynman Yol İntegrasyonu yaklaşımı gibi bazı girişimler mevcut olsada, henüz daha bir fikir birliğine varılamamıştır.

Bu tezde, tünelleme zamanı problemi oldukça yeni bir bağlamda çalışıldı. Zamanı anlamak momentumu gerekli kılar, ve dolayısıyla, entropiyi tanımlamak için momentum durum vektörleri kullanıldı. Bu entropi, ki ayrıca bir sıcaklık ifade eder, tünelleme bölgesi için termal enerji tanımlar. Bu termal enerji ve belirsizlik ilkesi neticesinde, parçacık için sonuçlanan ve klasik olarak anlık ifade edilen zamandan sapmayı temsil eden zaman tanımı bizim tünelleme zamanımız, entropik tünelleme zamanı, olarak belirlendi. Dahası, bu modeli deney ile detaylıca karşılaştırdık ve deney sonuçlarıyla oldukça iyi bir şekilde uyduğunu bulduk. Bunun üzerine, entropik tünelleme zamanını  $\alpha$ -bozunumu'na, STM'e ve evrenin tünellemesi'ne, bu süreçlerin doğal zaman skalasını belirleyebilmek için uyguladık.

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# CHAPTER 1

## INTRODUCTION

Quantum tunneling (for general information you can check (Griffiths, 2005), or for more detailed information (Razavy, 2003)) is a pure quantum mechanical phenomenon enabled by the uncertainty principle which can be explained simply as a penetration of subatomic particles into classically forbidden region. Ordinarily, if a subatomic particle interacts with a barrier that exceeds its energy, we would expect it to be reflected by the barrier. However, as we mentioned above, contrary to our senses, quantum mechanics implies non-vanishing probability for any particle to cross this type of barriers. This interesting result of quantum mechanics' physical relevance was first established by Gamow during his work on the  $\alpha$ -decay (Gamow, 1928a,b, 1931). Max Born is the one who generalizes and formulates this effect. Then technological applications such as tunnel diode of Esaki (Esaki, 1976) and STM (Binning and Rohrer, 1993) followed. Today, quantum tunneling is known to enable various physical (Razavy, 2003), chemical (McMahon, 2003), biological (Lambert et al., 2013), and complex systems (Ankerhold, 2007) phenomena.

With the increasing attention to quantum tunneling and its technological applications, having still no consensus (why there is no consensus on this problem will be explained in Section.1.2 in detail) on the answer of the question, what time it takes for the particle to cross the barrier, is an important ongoing problem. In this work, we develop a novel formulation for tunneling time in order to solve this problem (Demir, 2014), and in addition to this, we apply this tunneling time formula to some well-known cases as numerical applications (Demir and Guner, 2014). In general, we divide this thesis into three main chapters, and one can follow these chapters according to given information below.

In the first chapter, we give brief information about quantum tunneling. We summarise two main approaches that are used for analytical calculations of the tunneling. These two approaches, which are Rectangular Potential Barrier as a constant potential case and WKB Approximation as a slowly varying potential case respectively, are the subsections of the first chapter. Next, we give a quick review and critics of some existing well known approaches such as Phase Time (Wigner, 1955; Hauge and Støvneng, 1989), Dwell Time, Larmor Clock (Baz', 1967a,b; Büttiker, 1983), Buttiker-Landauer Approach (Büttiker and Landauer, 1982, 1985) in one subsection and Feynman Path Integral Approach (Sokolovski and Baskin, 1987) in another subsection alone. We separate the last one from the others because it fits the experimental data better than any other tunneling time approaches as we will see in Chapter 2

explicitly.

Second chapter consists of the formulation of our approach in detail. However, in addition to development of the tunneling time formula theoretically in one section by following (Demir, 2014), we analyse the latest experiment about tunneling time in detail in the remaining section. This experiment compares several important and common approaches which have already been investigated briefly in section.1.2, with the tunneling time data that are taken by the velocity map imaging spectrometer (VMIS) and the colt-target recoil-ion momentum spectrometer (COLTRIMS) (these techniques will be explained in Section.2.2, but for more detail see the experiment section of (Landsman et al., 2013)). Thanks to this experiment, we are able to state that our formulation of tunneling time is consistent with, and is in good agreement with the experiment.

In third chapter, we apply this approach to some well known cases that are using tunneling such as  $\alpha$ -decay, *STM*, and *creation of universe from nothing* by following (Demir and Guner, 2014).

In last chapter, we will conclude our work, and you can find further details in Appendix section.

## **1.1. Review of the Quantum Tunneling**

### **1.1.1. Rectangular Potential Barrier**

Rectangular potential barrier is the simplest case, and therefore, commonly studied while teaching quantum tunneling. According to the time-independent Schroedinger equation, exact analytical solution exists when we deal with this type of constant potential case. This is important because for any potential function  $V(x)$ , solving this Schroedinger equation exactly is not easy and for most of the cases, impossible. However, approximation like WKB which we will see it the following subsection in detail, will be used but only for the specific cases. For the rectangular potential barrier as one can see in Fig.1.1, we have

$$V(x) = \begin{cases} V_0, & 0 \leq x \leq L \\ 0, & \text{elsewhere} \end{cases}$$

Separating all three regions and solving as a stationary case, we have:

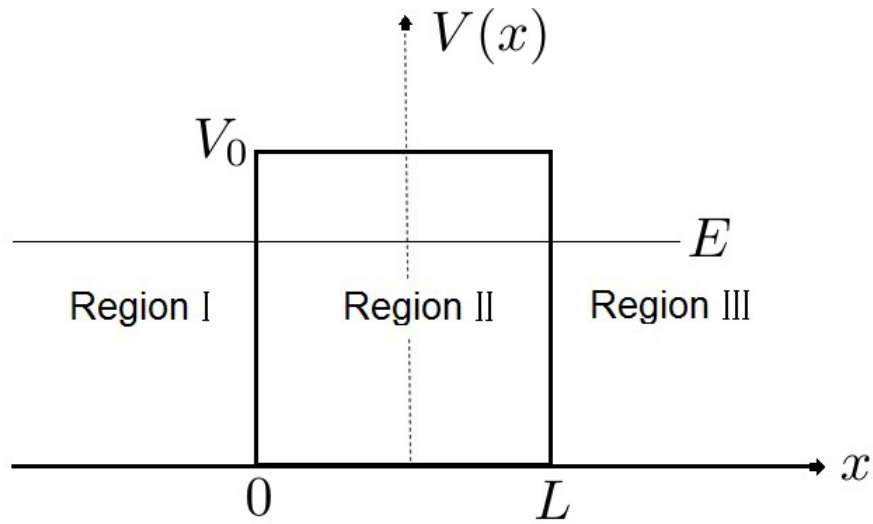


Figure 1.1. Simple Illustration of the Rectangular Potential Barrier

**Region I:**

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_I(x)}{dx^2} = E\psi_I(x) \quad (1.1)$$

where  $E$  is energy of the particle. Then resulting differential equation is:

$$\frac{d^2\psi_I(x)}{dx^2} + k^2\psi_I(x) = 0 \quad (1.2)$$

where  $k = \frac{2mE}{\hbar^2}$  with  $m$  is mass of the particle. Solution is then:

$$\psi_I = Ae^{ikx} + Re^{-ikx} \quad (1.3)$$

**Region II:**

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}(x)}{dx^2} + V_0\psi_{II}(x) = E\psi_{II}(x) \quad (1.4)$$

Differential form becomes:

$$\frac{d^2\psi_{II}(x)}{dx^2} - \kappa^2\psi_{II}(x) = 0 \quad (1.5)$$

where  $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$ . Solution is then:

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x} \quad (1.6)$$

### Region III:

This region has exactly same solution with Eq.(1.1) because  $V(x) = 0$  here. Therefore, we expect a solution  $\psi_{III}(x) = Fe^{ikx} + Ge^{-ikx}$  but we have to be aware that, there is no reflected particle in region III because if particle crosses the barrier, moves forward, cannot be reflected by any other potential barrier according to Fig.1.1. This simplifies the result as:

$$\psi_{III}(x) = Te^{ikx} \quad (1.7)$$

### Transmission and Reflection Coefficients

We've constructed our wavefunction and investigated its analytical behaviour.

$$\psi(x) = \begin{cases} \psi_I = Ae^{ikx} + Re^{-ikx}, & x \leq 0 \\ \psi_{II} = Ce^{\kappa x} + De^{-\kappa x}, & 0 \leq x \leq L \\ \psi_{III} = Te^{ikx}, & x \geq L \end{cases}$$

Now, it is important to find transmission ( $t = \frac{|T|^2}{|A|^2}$ ) and reflection ( $r = \frac{|R|^2}{|A|^2}$ ) coefficients because, first, these lead to information about the probabilities that represent particle's possible status, and second, we will see in Section.1.2 that some of the known tunneling time approaches need especially this transmission coefficient to calculate tunneling time. To do

so, we should use continuity conditions at the boundaries. First condition is:

$$\psi_I(0) = \psi_{II}(0) \quad (1.8)$$

Second condition is:

$$\dot{\psi}_I(0) = \dot{\psi}_{II}(0) \quad (1.9)$$

Third condition is:

$$\psi_{II}(L) = \psi_{III}(L) \quad (1.10)$$

And last condition is:

$$\dot{\psi}_{II}(L) = \dot{\psi}_{III}(L) \quad (1.11)$$

All of these Eqs.(1.8 - 1.11) lead to following equalities:

$$A + R = C + D \quad (1.12)$$

$$A - R = \frac{\kappa}{ik}(C - D) \quad (1.13)$$

$$Ce^{\kappa L} + De^{-\kappa L} = Te^{ikL} \quad (1.14)$$

$$Ce^{\kappa L} - De^{-\kappa L} = \frac{ik}{\kappa}Te^{ikL} \quad (1.15)$$

Using Eqs.(1.14) and (1.15), we express two coefficients  $C$  and  $D$  in terms of  $T$ :

$$C = \frac{T}{2}e^{(ik-\kappa)L} \left(1 + \frac{ik}{\kappa}\right) \quad (1.16)$$

$$D = \frac{T}{2} e^{(ik+\kappa)L} \left(1 - \frac{ik}{\kappa}\right) \quad (1.17)$$

If we put these  $C$  and  $D$  in Eqs.(1.12) and (1.13), we get:

$$\frac{T}{A} = \frac{4e^{-ikL}}{4 \cosh \kappa L + 2i\left(\frac{\kappa^2 - k^2}{\kappa k}\right) \sinh \kappa L} \quad (1.18)$$

Then, transmission coefficient is,

$$t = \frac{|T|^2}{|A|^2} = \frac{4}{4 \cosh^2 \kappa L + \left(\frac{\kappa^2 - k^2}{\kappa k}\right)^2 \sinh^2 \kappa L} \quad (1.19)$$

Particle must be either transmitted or reflected, therefore,  $t + r = 1$  must be satisfied and this simplifies the calculation of reflection coefficient, which is:

$$r = \frac{|R|^2}{|A|^2} = 1 - t = \frac{4\left(\frac{\kappa^2 + k^2}{\kappa k}\right)^2 \sinh^2 \kappa L}{4 \cosh^2 \kappa L + \left(\frac{\kappa^2 - k^2}{\kappa k}\right)^2 \sinh^2 \kappa L} \quad (1.20)$$

### 1.1.2. WKB Approximation

The WKB (Wentzel (Wentzel, 1926), Kramers (Kramers, 1926) and Brillouin (Brillouin, 1926)) method is an approximation to time-independent schrodinger equation while dealing with a potential function  $V(x)$  depending on  $x$ , as you see in Fig.1.2. In this case, analytical solution of this

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (1.21)$$

time-independent Schroedinger equation as we mentioned early, is not easy. Here, assumption of this WKB approximation is simple; potential function  $V(x)$  slowly varies with respect to the position  $x$ . According to this, we propose a solution similar to the constant potential case as you see in Eqs.(1.3) and (1.7). Therefore, expected solution is of the form

$$\psi(x) = A e^{\frac{i}{\hbar}\phi(x)} \quad (1.22)$$

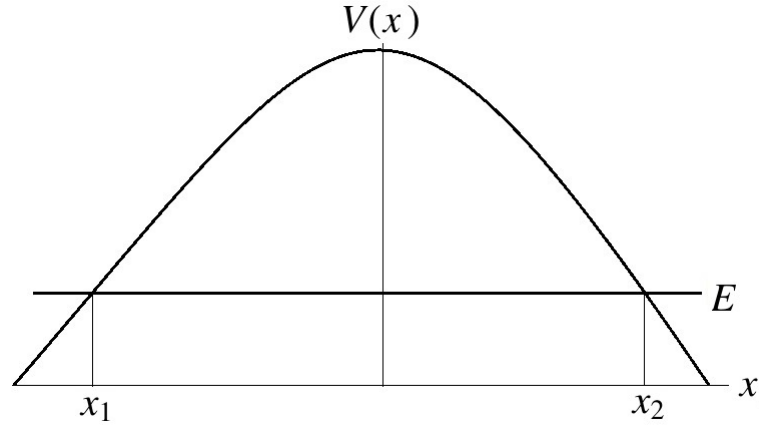


Figure 1.2. Simple Illustration of the Potential Barrier for the WKB Method

Now, putting Eq.(1.22) into (1.21) leads to the following equation for  $\phi(x)$ ,

$$-i\hbar \frac{d^2\phi(x)}{dx^2} + \left( \frac{d\phi(x)}{dx} \right)^2 + 2m(V(x) - E) = 0 \quad (1.23)$$

Notice that, if we set  $\phi(x) = \pm\hbar kx$ , or  $\phi(x) = \pm i\hbar\kappa x$ , then we would immediately get the solutions of the rectangular potential barrier for related regions, but with these  $\phi(x)$ , first term of the Eq.(1.23) vanishes. On the other hand, since Eq.(1.23) is a non-linear equation, we have to start making approximations to solve this equation. Therefore, based on this negligible property of this first term and its proportionality to  $\hbar$  (where  $\hbar \rightarrow 0$  in the classical limit), we treat this  $\hbar$  as an indication of smallness<sup>1</sup> and we are able to expand the function  $\phi(x)$  in the power series in terms of it,

$$\phi(x) = \phi_0(x) + \hbar\phi_I(x) + \frac{\hbar^2}{2}\phi_{II}(x) + \dots \quad (1.24)$$

---

<sup>1</sup>Details can be found in [http://www.pha.jhu.edu/courses/171\\_303/WKB\\_notes\\_brandsen.pdf](http://www.pha.jhu.edu/courses/171_303/WKB_notes_brandsen.pdf)

From now on, all we have to do is placing the above expansion into the Eq.(1.23) and by equating every coefficient of power of  $\hbar$  term by term to zero, we obtain

$$\left(\frac{d\phi_0(x)}{dx}\right)^2 + 2m(V(x) - E) = 0 \quad (1.25)$$

$$-\frac{i}{2} \frac{d^2\phi_0(x)}{dx^2} + \frac{d\phi_0(x)}{dx} \frac{d\phi_I(x)}{dx} = 0 \quad (1.26)$$

$$-i \frac{d^2\phi_I(x)}{dx^2} + \frac{d\phi_0(x)}{dx} \frac{d\phi_{II}(x)}{dx} + \left(\frac{d\phi_I(x)}{dx}\right)^2 = 0 \quad (1.27)$$

We see explicitly that,  $\phi_0(x)$ ,  $\phi_I(x)$  and  $\phi_{II}(x)$  will be solved sequentially because each higher order term depends on the previous terms. However, we have to notice that, we keep the  $\phi_{II}(x)$  as the highest term because WKB method only considers  $\phi_0(x)$  and  $\phi_I(x)$  terms and this highest term enables us to show that why this and remaining higher order terms vanish. Our assumption of slowly varying potential plays its crucial role at this point. For the  $E < V(x)$  case, Eq.(1.25) solved as

$$\phi_0(x) = \pm i \int^x q(x) dx \quad (1.28)$$

where  $q(x) = \sqrt{2m(V(x) - E)}$ . Now, we are able to solve the Eq.(1.26), and the solution is:

$$\phi_I(x) = \frac{i}{2} \log q(x) \quad (1.29)$$

As a final step, solution of the Eq.(1.27) is:

$$\phi_{II}(x) = i \frac{m}{2q(x)^3} \frac{dV(x)}{dx} - i \frac{m^2}{4} \int^x \frac{1}{q(x)^5} \left(\frac{dV(x)}{dx}\right)^2 dx \quad (1.30)$$

Here comes the main assumption, and approximation of the WKB method. We have already told that potential must be slowly varying with respect to  $x$ , and since  $\phi_{II}(x) \propto \frac{dV(x)}{dx}$ , this



means that third term in the Eq.(1.24) is negligible

$$\left| \frac{\hbar^2}{2} \phi_{II}(x) \right| \ll 1 \quad (1.31)$$

and this leads to a constraint that must be satisfied to ensure that WKB is applicable:

$$\left| \frac{\hbar^2 m \frac{dV(x)}{dx}}{4q(x)^3} \right| \ll 1 \quad (1.32)$$

What we have left is, since  $\phi_{II}$  and the following terms negligible, by taking the non-negligible first two terms in Eq.(1.24) and putting it into the Eq.(1.22), we obtain the wavefunction solution of the WKB method,

$$\psi(x) = \frac{A}{\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int^x q(x) dx} \quad (1.33)$$

of course, general solution is a linear combination, but keeping exponentially decaying term only is enough for now.

So far, we have determined the wavefunction of the particle inside the tunneling region according to the WKB method. Now, we need to find what is the transmission coefficient related to this method. However, we know that, at the turning points  $x_1$  and  $x_2$ ,  $q(x_1) = q(x_2) = 0$  and this diverges the wavefunction in Eq.(1.33). Therefore, connection formula is necessary to move forward. This connection formula involves Airy functions, and contains lengthy calculations while finding the transmission coefficient. We leave this content to Appendix A, and writing down the exact result of the transmission coefficient here,

$$T_{trans} = \frac{1}{\cosh^2 \Phi} \quad (1.34)$$

where

$$\Phi = \frac{1}{\hbar} \int_{x_1}^{x_2} q(x) dx \quad (1.35)$$

is Hamilton's characteristic function (also known as Gamow factor) in units of  $\hbar$  within the tunneling region.

## 1.2. Review of the Tunneling Time Problem

Tunneling is a genuine quantum phenomenon as we already mentioned. Solving Schroedinger equation, in WKB approximation if not exactly, gives wavefunction inside and outside the tunneling region. This, however, gives no information about tunneling time. The question of *tunneling time*, and therefore defining an average *speed* for a particle that represents the barrier crossing was first pointed out by Condon (Condon and Morse, 1931). Then, MacColl attempted to solve this problem just a year later (MacColl, 1932). Afterwards, this problem almost did not take attention up to fifties. Problem of defining a tunneling time is challenging and this is not surprising because in quantum theory time is not an operator whose expectation value can be evaluated by using the wave-function. From fifties, to date, it is also for this particular reason that various tunneling time definitions which we have already mentioned above have been introduced: Büttiker-Landauer, Larmor approach, phase time, and dwell time. However, contrary to their *raison d'être*, all these time definitions utilize a sort of time operator because they all involve derivatives with respect to energy  $E$  or potential  $V(x)$  (Yamada, 2004). Compared to them, the Feynman path integral (FPI) approach is particularly interesting because it involves times taken by individual classical trajectories yet tunneling time is still controversial (details can be found in Section.1.2.2). Now, we will investigate some of the main tunneling time approaches (there are many reviews about these time approaches that contain both theoretical and experimental point of views, and hence, one can find more technical details in these reviews (Olkhovsky and Recami, 1992; Landauer and Martin, 1994; Privitera et al., 2004; Winful, 2006; Maji et al., 2007), and in thesis (Eser, 2011)).

### 1.2.1. Phase Time, Dwell Time, Larmor Clock and Buttiker-Landauer Approaches

Phase time approach is about tracking the position of a peak of very narrow wavepacket around a determined wave number  $k_0$ . Mostly, stationary phase is considered, and therefore, notation of simple rectangular potential barrier in Section.1.1.1 is valid here. Under right circumstances and neglecting the dispersion effects (Olkhovsky and Recami, 1992; Olkhovsky et al., 2001), one can take this peak of the wave-packet as a reference point.

We have to note that, this peak of the wavepacket is consisting of the Fourier components of the form

$$\psi(x, t; k) = |T|e^{i(kx - \frac{Et}{\hbar} + \alpha(k))} \quad (1.36)$$

which dominates the surrounding phase variation around  $k_0$ , and hence, prohibits the destructive interference. Here  $E$  is energy of the particle,  $t$  is time and  $\alpha(k)$  comes from the  $T \rightarrow |T|e^{i\alpha(k)}$  as phase shifting term to represent contribution of transmission.

We are able to find position of the peak, where the phase is maximum, and hence, stationary as we told earlier. This will be achieved simply;

$$\frac{d}{dk}\psi(x, t; k) = \frac{d}{dk}\left(|T|e^{i(kx - \frac{Et}{\hbar} + \alpha(k))}\right) = 0 \quad (1.37)$$

Result of this derivation is,

$$x - \frac{dE}{dk} \frac{t}{\hbar} + \frac{d\alpha(k)}{dk} = 0 \quad (1.38)$$

and position  $x$  that satisfies above equation is the position of the peak wave-packet which we call it as  $x = x_D(t)$ . Then,

$$x_D(t) = \frac{dE}{dk} \frac{t}{\hbar} - \frac{d\alpha(k)}{dk} \quad (1.39)$$

but to understand what the equation above means, we also have to evaluate the case without the barrier. In this case, there aren't any transmission or reflection coefficients, and we must consider just a free particle that is moving as a wave-packet of the form

$$\psi(x, t; k) = Ce^{i(kx - \frac{Et}{\hbar})} \quad (1.40)$$

where  $C$  is the amplitude. Applying same procedure which is about finding the location of the peak of the wave-packet, we have

$$\frac{d}{dk}\psi(x, t; k) = \frac{d}{dk}\left(Ce^{i(kx - \frac{Et}{\hbar})}\right) = 0 \quad (1.41)$$

then resulting peak position  $x = x_F$  for this free particle case is

$$x_F = \frac{dE}{dk} t \quad (1.42)$$

This  $x_F$  is nothing but the first term in the Eq.(1.39), and rearranging  $x_D$  gives

$$x_D = x_F - \frac{d\alpha(k)}{dk} \quad (1.43)$$

By looking at the equation above, we immediately conclude that, the term

$$\frac{d\alpha(k)}{dk} = \delta x \quad (1.44)$$

represents the spatial delay caused by the barrier, phase shift of the particle due to the transmission. In addition to this spatial delay, one will also find a temporal delay by using equation of motion,

$$\delta\tau = \frac{\delta x}{v_G} \quad (1.45)$$

where  $v_G$  is the group velocity, and if we rewrite the Eq.(1.42) as

$$x_F = v_G t \quad (1.46)$$

then the group velocity is nothing but the

$$v_G = \frac{1}{\hbar} \frac{dE}{dk} \quad (1.47)$$

using both (1.44) and (1.47), temporal delay in Eq.(1.45) becomes

$$\delta\tau = \frac{\frac{d\alpha(k)}{dk}}{\frac{1}{\hbar} \frac{dE}{dk}} = \hbar \frac{d\alpha(k)}{dE} \quad (1.48)$$

We have found temporal delay explicitly. Now, we are able to write down the tunneling time as *phase time* which is nothing but the sum of the time that it takes a particle to move a distance without any barrier and the contribution of the barrier as  $\delta\tau$ ,

$$\tau_t = \frac{x_2 - x_1}{v_G} + \delta\tau \quad (1.49)$$

where  $x_2$  and  $x_1$  here represents two distant points external to the barrier region, but barrier region be somewhere in between these two points. One important note is that, if we call  $x_1$  a point in region I of Fig.(1.1), then  $x_1 \ll 0$  and  $x_2$  a point in region III, then  $x_2 \gg L$ , because this time is meaningful only when this narrow wave-packet moves completely out of the tunneling region. On the other hand, explicitly, *phase time* (1.49) is

$$\tau_t = \frac{x_2 - x_1}{v_G} + \hbar \frac{d\alpha(k)}{dE} \quad (1.50)$$

but in general, for simplicity, they use (1.45) to take into  $v_G$  parenthesis, and therefore

$$\tau_t = \frac{1}{v_G} \left( x_2 - x_1 + \frac{d\alpha(k)}{dk} \right) \quad (1.51)$$

this is transmission delay of the phase time approach. In the same way, one finds the reflection time by again adding phase term to reflection amplitude which is  $R \rightarrow |R|e^{i\beta(k)}$  where  $\beta(k)$  represents the phase term here. This time wavefunction is of the form

$$\psi(x, t; k)_r = |R|e^{i(-kx - \frac{Et}{\hbar} + \beta(k))} \quad (1.52)$$

and location of the peak of the wave-packet is

$$\frac{d}{dk} \psi(x, t; k)_r = \frac{d}{dk} \left( |R|e^{i(-kx - \frac{Et}{\hbar} + \beta(k))} \right) \quad (1.53)$$

from here, we get

$$-x - \frac{dE}{dk} \frac{t}{\hbar} + \frac{d\beta(k)}{dk} = 0 \quad (1.54)$$

therefore, solution for the position of the peak  $x = x_{RD}$  of the reflected wave-packet is

$$x_{RD} = -\frac{dE}{dk} \frac{t}{\hbar} + \frac{d\beta(k)}{dk} \quad (1.55)$$

this time, the term representing the group velocity  $v_G$  of the without barrier case  $-\frac{dE}{dk} \frac{1}{\hbar}$  is with a minus sign because reflected wave-packet moves in opposite direction. Here,  $\frac{d\beta(k)}{dk} = \delta x$  term is now representing the spatial delay and leads to a

$$\delta\tau = \frac{\delta x}{v_G} = \frac{1}{v_G} \frac{d\beta(k)}{dk} \quad (1.56)$$

temporal delay. Then, one finds the reflection delay as

$$\tau_r = \frac{1}{v_G} (-x_1 - x_1 + \delta\tau) \quad (1.57)$$

if we compare this Eq.(1.57) with the transmission delay in Eq.(1.51), we immediately see that, here instead of  $x_2$ , there exists a  $-x_1$ , and this is simply because of starting from the point  $x_1$ , wave-packet travels and comes back to  $x_1$  again with  $-v_G$ , therefore  $\frac{x_2}{v_G} \rightarrow \frac{x_1}{-v_G}$ . Writing the reflection delay explicitly,

$$\tau_r = \frac{1}{v_G} \left( -2x_1 + \frac{d\beta(k)}{dk} \right) \quad (1.58)$$

So far, we've found both the transmission and reflection delay for this phase time approach. However, there is some serious criticism about this approach. Mainly, we know that incoming peak of the wave-packet consists of several different energetic components. Therefore, some of these components of the Fourier may be reflected while peak of this wave-packet get transmitted. One can argue about physical validity of this approach due to whether the resulting wave-packet represents incoming one or not (Landauer and Martin, 1994). Also, again similar reasoning, some of these Fourier components may be higher than the potential  $V_0$  of the barrier, and hence, delay becomes unconnected to tunneling or even if there exists no components exceeding the potential  $V_0$ , there will be some components very close to it, and this will cause these components to be transmitted more effectively. As a result, emerging packet will have a higher velocity which implies that, tunneling is an electron accelerator (Hauge and Støvneng, 1989; Landauer and Martin, 1994).

Another well-known approach, dwell time, is first introduced by Smith (Smith, 1960), and it is an average time spent by a particle during its motion in the specific bounded region. It is defined as

$$\tau^D = \frac{1}{v_{in}} \int_{x_1}^{x_2} |\psi(x)|^2 dx \quad (1.59)$$

where  $v_{in}$  is the incoming flux. This Eq.(1.59) tells us that, dwell time is the average of probability of finding the particle in the region of interest over the flux that represents the same region but without any interaction, which is then simply the free wave-packet group velocity  $v_{in} = v_G$  for this particular region.

Calculating dwell time is straightforward. For the case of simple rectangular potential barrier in Section.1.1.1, we know that in tunneling region  $0 < x < L$ , wavefunction is

$$\psi(x) = Ce^{\kappa x} + De^{-\kappa x} \quad (1.60)$$

where  $C$  is (1.16),  $D$  is (1.17) and  $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$ . We continue by calculating the probability density of the tunneling region using (1.60) with the turning points  $x_1 = 0$ , and  $x_2 = L$

$$|\psi(x)|^2 = |C|^2 e^{2\kappa x} + |D|^2 e^{-2\kappa x} + C^*D + CD^* \quad (1.61)$$

one will simply calculate these coefficients, and result is

$$\left. \begin{aligned} |C|^2 &= \frac{|T|^2}{4} e^{-2\kappa L} \frac{(k^2 + \kappa^2)}{\kappa^2} \\ |D|^2 &= \frac{|T|^2}{4} e^{2\kappa L} \frac{(k^2 + \kappa^2)}{\kappa^2} \\ C^*D &= \frac{|T|^2}{4} \left( 1 - 2\frac{ik}{\kappa} - \frac{k^2}{\kappa^2} \right) \\ CD^* &= \frac{|T|^2}{4} \left( 1 + 2\frac{ik}{\kappa} - \frac{k^2}{\kappa^2} \right) \end{aligned} \right\} \quad (1.62)$$

now, integrating the probability density in Eq.(1.61)

$$\int_0^L |\psi(x)|^2 dx = \frac{|C|^2}{2\kappa} (e^{2\kappa L} - 1) - \frac{|D|^2}{2\kappa} (e^{-2\kappa L} - 1) + (C^*D + CD^*)L \quad (1.63)$$

and putting the coefficients in (1.62), we get

$$\int_0^L |\psi(x)|^2 dx = \frac{|T|^2}{8\kappa} (e^{2\kappa L} - 1) e^{-2\kappa L} \frac{(k^2 + \kappa^2)}{\kappa^2} - \frac{|T|^2}{8\kappa} (e^{-2\kappa L} - 1) e^{2\kappa L} \frac{(k^2 + \kappa^2)}{\kappa^2} + \frac{|T|^2}{4} \left( 2 - 2 \frac{k^2}{\kappa^2} \right) L \quad (1.64)$$

if we simplify this result,

$$\int_0^L |\psi(x)|^2 dx = \frac{|T|^2}{4\kappa^3} \left( (k^2 + \kappa^2) \sinh(2\kappa L) + 2L \frac{(\kappa^2 - k^2)}{\kappa^2} \right) \quad (1.65)$$

where  $|T|^2$  is the transmission coefficient in Eq.(1.19). Solution is then

$$\int_0^L |\psi(x)|^2 dx = \frac{4\kappa^2 k^2}{4(4\kappa^2 k^2 \cosh^2 \kappa L + (\kappa^2 - k^2)^2 \sinh^2 \kappa L)} \left( \frac{(k^2 + \kappa^2)}{\kappa^3} \sinh(2\kappa L) + 2L \frac{(\kappa^2 - k^2)}{\kappa^2} \right) \quad (1.66)$$

So, dwell time  $\tau^D = \frac{1}{v_{in}} \int_0^L |\psi(x)|^2 dx$  is found by dividing (1.66) to  $v_{in} = v_G = \frac{\hbar k}{m}$ , also dividing and multiplying by  $\kappa$

$$\tau^D = \frac{mk}{\hbar\kappa} \left( \frac{(\kappa^2 + k^2) \sinh 2\kappa L + 2\kappa L(\kappa^2 - k^2)}{4\kappa^2 k^2 \cosh^2 2\kappa L + (\kappa^2 - k^2)^2 \sinh^2 2\kappa L} \right) \quad (1.67)$$

this is the *dwell time* for the tunneling region.

Main criticism about this approach is that as we have already mentioned above, this time in Eq.(1.67) measures how much time the particle spends inside the barrier region. Therefore, one cannot make a specific conclusion about which this time corresponds to: *reflection time* or *transmission time* (Büttiker and Landauer, 1982; Leavens and Aers, 1989).

Now, we will investigate the Büttiker - Landauer approach. This approach is known as one type of clock approaches in literature. Simply, idea is summarised as: there is a time modulated barrier, and particle interacts with this barrier by absorbing or emitting quanta. Hence, by analysing this external effect of modulating barrier to tunneling particle, one will get the information of tunneling time. This is possible because of the existing dependency of tunneling time to modulation frequency. Here, there are two cases, in low frequency



modulation, particle sees a static barrier because its crossing time is lower than the period, and hence, it sees only a part of the modulation cycle. The other case, higher frequency modulation, this time particle sees several modulation cycles because, unlike the previous case, crossing time is now higher than the period, and as a result, particle interacts with the time-averaged barrier.

We begin with defining the potential function

$$V(t) = V_0 + V_L \cos wt \quad (1.68)$$

here,  $V_0$  represents the static potential, and  $V_L$  represents the amplitude of this modulation of the barrier. Then, Hamiltonian becomes

$$H = \frac{p^2}{2m} + V_0 + V_L \cos wt \quad (1.69)$$

we know the solution of energy eigenfunctions  $\phi_E(x) = \psi_{II} = Ce^{\kappa x} + De^{-\kappa x}$  which have Hamiltonian  $H = \frac{p^2}{2m} + V_0$  already from the Section.1.1.1. Therefore, we need to add the time evolution part by using

$$i\hbar \frac{\partial}{\partial t} \phi_t(t) = \hat{H} \phi_t(t) \quad (1.70)$$

which is

$$i\hbar \frac{\partial}{\partial t} \phi_t(t) = (E + V_L \cos wt) \phi_t(t) \quad (1.71)$$

therefore, solution is nothing but the

$$\phi_t(t) = e^{-\frac{iE}{\hbar}t} e^{-\frac{iV_L}{\hbar\omega} \sin wt} \quad (1.72)$$

as a result, wave-function is found as

$$\psi(x, t) = \phi_E(x) e^{-\frac{iE}{\hbar}t} e^{-\frac{iV_L}{\hbar\omega} \sin wt} \quad (1.73)$$

we have to express  $\psi(x, t)$  so that, it contains the related absorbed and emitted quanta  $E \pm n\hbar\omega$  caused by the time modulated barrier. Therefore, we use the identity

$$e^{\frac{x}{2}\left(\frac{c^2-1}{c}\right)} = \sum_{n=-\infty}^{n=\infty} J_n(x)c^n \quad (1.74)$$

for the last term  $e^{-\frac{iV_L}{\hbar\omega} \sin \omega t}$  in Eq.(1.73) where  $J_n(x)$  is the Bessel function of first kind. After expanding  $\sin \omega t = \frac{e^{i\omega t} - e^{-i\omega t}}{2i}$ , then we immediately get this term by  $x \rightarrow \frac{V_L}{\hbar\omega}$ , and  $c \rightarrow e^{-i\omega t}$ . What we get is

$$e^{-\frac{iV_L}{\hbar\omega} \sin \omega t} = e^{-\frac{iV_L}{\hbar\omega} \left(\frac{e^{i\omega t} - e^{-i\omega t}}{2i}\right)} = \sum_{n=-\infty}^{n=\infty} J_n\left(\frac{V_L}{\hbar\omega}\right) e^{-in\omega t} \quad (1.75)$$

and resulting wavefunction is

$$\psi(x, t) = \phi_E(x) e^{-\frac{iE}{\hbar}t} \sum_{n=-\infty}^{n=\infty} J_n\left(\frac{V_L}{\hbar\omega}\right) e^{-in\omega t} \quad (1.76)$$

now, we will understand by looking at (1.76) that, particle can absorb or emit quanta as  $\pm n\hbar\omega$  due to this interaction with the time modulated barrier. However, to simplify this expansion, we take care of only the neighbourhood absorbed or emitted quanta energies, which are  $E \pm \hbar\omega$ . This assumption leads us to conclude that, there are three wave-functions with the energies  $E$ ,  $E + \hbar\omega$ , and  $E - \hbar\omega$ . Here, wave-function with energy  $E$  represents the case that particle is under static potential effect only. On the other hand, since the amplitude of the modulation  $V_L$  is small, we will expand the  $\left(\frac{V_L}{\hbar\omega}\right)$  term while getting these three wave-functions. According to the fact that  $\frac{V_L}{\hbar\omega} \ll 1$ , then

$$J_n\left(\frac{V_L}{\hbar\omega}\right) \sim \left(\frac{V_L}{\hbar\omega}\right)^n \frac{1}{\Gamma(n+1)} \quad (1.77)$$

one gets

$$J_n\left(\frac{V_L}{\hbar\omega}\right) \propto \left(\frac{V_L}{\hbar\omega}\right)^n \quad (1.78)$$

Last step is about determining the  $\phi_E(x)$  term in the wave-function (1.76). This term is simply calculated in same way that we did in the Section.1.1.1 while dealing with the simple rectangular potential barrier case. However, here, there are three wave-functions and we label related parameters using the same notation in Section.1.1.1 ( $k, \kappa, T$ ) with the energy  $E$  as  $k_{\pm}, \kappa_{\pm}$ , and  $T_{\pm}$  that  $(k_+, \kappa_+, T_+)$  corresponds to  $E + \hbar\omega$ ,  $(k_-, \kappa_-, T_-)$  corresponds to  $E - \hbar\omega$  energies.

One further assumption is, we consider  $\hbar\omega \ll E$  and  $\hbar\omega \ll V_0 - E$  since  $V_L \cos \omega t$  is a small perturbation. Therefore,

$$k_{\pm} = \frac{\sqrt{2m(E \pm \hbar\omega)}}{\hbar} = \frac{\sqrt{2mE(1 \pm \frac{\hbar\omega}{E})}}{\hbar} \quad (1.79)$$

which will be written as

$$k_{\pm} = \frac{\sqrt{2mE}}{\hbar} \sqrt{1 \pm \frac{\hbar\omega}{E}} \approx \frac{\sqrt{2mE}}{\hbar} (1 \pm \frac{\hbar\omega}{2E}) \quad (1.80)$$

result is then

$$k_{\pm} \approx k(1 \pm \frac{\hbar\omega}{2E}) \quad (1.81)$$

where  $E = \frac{\hbar^2 k^2}{2m}$ . Making the same calculations for the  $\kappa_{\pm}$

$$\kappa_{\pm} = \frac{\sqrt{2m(V_0 - (E \pm \hbar\omega))}}{\hbar} = \frac{\sqrt{2m(V_0 - E)(1 \mp \frac{\hbar\omega}{V_0 - E})}}{\hbar} \quad (1.82)$$

with using same approach again, we get

$$\kappa_{\pm} \approx \kappa(1 \mp \frac{\hbar\omega}{2(V_0 - E)}) \quad (1.83)$$

where  $V_0 - E = \frac{\hbar^2 \kappa^2}{2m}$ .

Solving for the related transmission amplitudes which is multiplied with the related trans-

mitted wave-functions, then we immediately get

$$T_{\pm} = T \frac{V_L}{2\hbar w} (e^{\pm\tau w} - 1) \quad (1.84)$$

from here, we calculate the relative intensity by

$$|T_{\pm}|^2 = |T|^2 \left( \frac{V_L}{2\hbar w} \right)^2 (e^{\pm w(\frac{mL}{\hbar\kappa})} - 1)^2 \quad (1.85)$$

where  $|T|^2$  is the transmission coefficient in Eq.(1.19). Büttiker-Landauer defined this crossing time for the simple rectangular potential barrier as you see above,  $\tau_T^{BL} = \frac{mL}{\hbar\kappa}$  where  $L$  is the barrier width  $x_2 - x_1$ . This time they found measures the duration of interaction between particle and time modulated barrier.

For the opaque barriers (when  $\kappa L$  is large),  $T_+$  grows exponentially, but  $T_-$  decays in same speed. These authors then define the tunneling time for this case as the difference between  $|T_+|^2$  and  $|T_-|^2$ ,

$$\tanh w\tau = \frac{|T_+|^2 - |T_-|^2}{|T_+|^2 + |T_-|^2} \quad (1.86)$$

and one will determine tunneling time  $\tau$  by measuring the  $|T_+|^2$  and  $|T_-|^2$ .

Last approach that we will investigate in this subsection is the Larmor clock. Again this is the same type of approach belongs to the clock type approaches like Büttiker-Landauer approach. However, in this case, applying the method of Baz' which was proposed in the paper (Baz', 1967a,b) to calculate collision times based on the Larmor precession, Rybachenko (Rybachenko, 1967) computed the tunneling time. It considers a charged particle which is tunneling through a barrier under the effect of a weak magnetic field  $\vec{B} = B_0\hat{z}$  in  $\hat{z}$  direction. Here, spin-1/2 particles are polarized in  $\hat{x}$  direction, which you see in Fig.1.3<sup>2</sup>. As a result, while particle is crossing the barrier, due to the existence of this infinitesimal magnetic field, its spin axis will rotate, and hence, this rotation will provide the necessary information for

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<sup>2</sup>This image is taken from the (Olkhovsky and Recami, 1992)

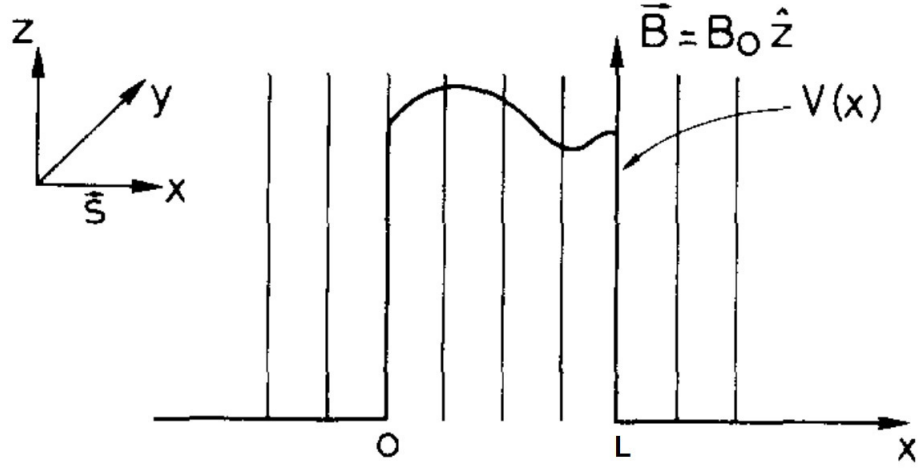


Figure 1.3. Set-up of the Larmor clock approach

the tunneling time. we get

$$\tau_{Tra} = \frac{\theta_{Tra}}{w} \quad (1.87)$$

for average time corresponding to transmission

$$\tau_{Ref} = \frac{\theta_{Ref}}{w} \quad (1.88)$$

for average time corresponding to reflection. Here  $w = -\frac{eB_0}{2mc}$  is the Larmor frequency,  $\theta_{Tra}$  corresponds to angular rotation by transmitted particles, and  $\theta_{Ref}$  corresponds to angular rotation by reflected particles. With this additional action of the magnetic field, Hamiltonian becomes in the region  $0 \leq x \leq L$  with turning points  $x_1 = 0$ , and  $x_2 = L$

$$\hat{H}_L = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) - \mu \vec{B} \hat{\sigma} \quad (1.89)$$

then, the solution of the time-independent Schroedinger equation

$$\hat{H}_L \psi(x, s) = E \psi(x, s) \quad (1.90)$$

where  $\psi(x, s)$  contains the spin wave-function. Wave-function solution for this region inside the barrier is changed due to the energy shift  $-\mu\vec{B}\hat{\sigma}$ , but here, our main concern is about understanding what happens to transmission and reflection coefficients. By switching on the magnetic field, one changes both coefficients of the wave-function inside the barrier region, and also change both transmission  $T$  and reflection  $R$  coefficients. According to Rybachenko (Rybachenko, 1967), this change will be written as:

$$\hat{T} = \hat{I}T + \mu\vec{B}\hat{\sigma}\frac{\delta T}{\delta E} \quad (1.91)$$

$$\hat{R} = \hat{I}R + \mu\vec{B}\hat{\sigma}\frac{\delta R}{\delta E} \quad (1.92)$$

where  $\hat{I}$  is identity matrix. Here,  $\frac{\delta}{\delta E} = \frac{d}{dE} - \left(\frac{\partial}{\partial E}\right)$ .

If we apply these transmission and reflection operators in (1.91) and (1.92) respectively, we will get the shifted spin wave-function according to the spin wave-function of the incident particle. Then, by using this shift, one finds the rotation angles as

$$\theta_{Tra} = 2\mu B_0 \text{Im} \left( \frac{\delta \ln |T|}{\delta E} \right) \quad (1.93)$$

$$\theta_{Ref} = 2\mu B_0 \text{Im} \left( \frac{\delta \ln |R|}{\delta E} \right) \quad (1.94)$$

Using these angular rotations in the times we give in Eqs.(1.87) and (1.88), we immediately get

$$\tau_{Tra} = \hbar \text{Im} \left( \frac{\delta \ln |T|}{\delta E} \right) \quad (1.95)$$

$$\tau_{Ref} = \hbar \text{Im} \left( \frac{\delta \ln |R|}{\delta E} \right) \quad (1.96)$$

These are the corresponding Larmor clock for both transmission  $\tau_{Tra}$  and reflection  $\tau_{Ref}$  times.

Before ending this subsection, we should give brief criticism about these clock type of approaches. As you notice that, one will introduce many degrees of freedom as a clock. We learned time modulated barrier, and spin degree of freedom achieve this, but there is no limit

here. Which one of the clock approaches leads to a better tunneling time, or which one is true, is an unknown question among these approaches.

As we have pointed earlier in the introduction, obviously there is no consensus on the tunneling time. This is because, there are several approaches existing in the literature, and all of them have some serious disadvantages as we already mentioned while criticising the related approaches above.

## 1.2.2. Feynman Path Integral Approach

Feynman Path Integral approach is proposed by Sokolovski and Baskin in 1987, and it is conceptually based on the Feynman Path Integration which makes this approach distinctive according to the other approaches we have investigated above. Here, classical trajectories are considered over all paths in the region  $\Omega$ , and due to this classicality, this approach is also known as *semi-classical approach*. This certain region  $\Omega$  includes all possible paths between  $x_1$  and  $x_2$  with time  $t_2 - t_1$  under the influence of the potential  $V(x)$ . Note that,  $t_1$  is the time when particle is in  $x_1$ , and  $t_2$  is the time when this moving particle is detected at the  $x_2$ . Therefore, any particle that is following a classical path  $\mathbf{x}(t)$  in this region  $\Omega$  will be represented by a time expression that gives the time spent by a particle as you see in Fig.1.4<sup>3</sup>, which is

$$\tau_{\Omega}^{cl} = \int_{t_1}^{t_2} \Theta(x(t)) dt \quad (1.97)$$

where  $\Theta_{\Omega}(x(t))$  is a functional depending on the related path of the particle, and it obeys

$$\Theta_{\Omega}(x(t)) = \begin{cases} 1, & x(t) \in \Omega \\ 0, & \text{otherwise} \end{cases}$$

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<sup>3</sup>This image is taken from the (Sokolovski and Baskin, 1987)

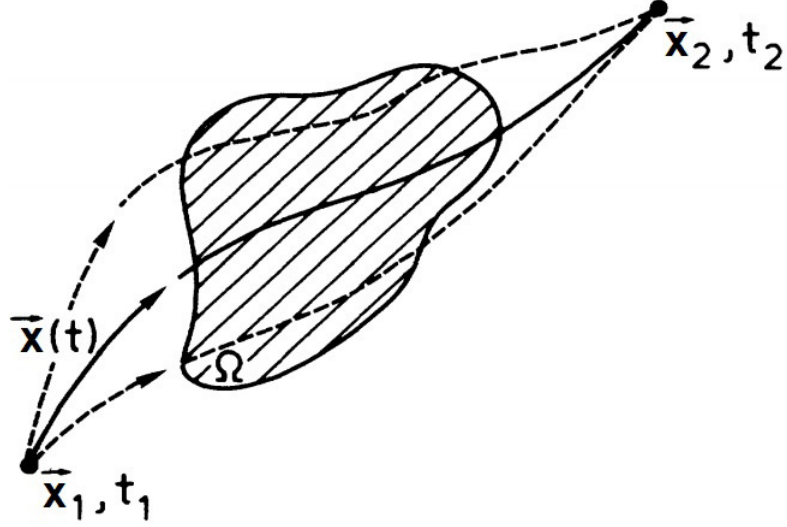


Figure 1.4. Simple illustration of the domain  $\Omega$  that contains the classical trajectories of Feynman Path Integral approach

this condition above leads to a more general form for the definition of time. In one-dimensional case, Eq.(1.97) will be written as

$$\tau_{\Omega}^{cl} = \int_{t_1}^{t_2} dt \int_{\Omega} \delta(x - x(t)) dx \quad (1.98)$$

and thanks to this delta function  $\delta(x - x(t))$  property, we are able to ensure that only paths that are belonging to this  $\Omega$  region are chosen. From here, by taking the mean value for the functional  $\tau_{\Omega}^{cl}[x(\cdot)]$ , which also means taking the time average of those paths, we get

$$\tau_{\Omega} = \langle \tau_{\Omega}^{cl}[x(\cdot)] \rangle \quad (1.99)$$

Here, for any functional  $G[x(\cdot)]$ , mean value is taken as

$$\langle G[x(\cdot)] \rangle = \frac{\int Dx(\cdot) G[x(\cdot)] e^{\frac{i}{\hbar} S[x(\cdot)]}}{\int Dx(\cdot) e^{\frac{i}{\hbar} S[x(\cdot)]}} \quad (1.100)$$



where  $S[x(\cdot)]$  is the action, and explicitly

$$S[x(\cdot)] = \int_{t_1}^{t_2} L dt = \int_{t_1}^{t_2} \left( \frac{1}{2} m \dot{x}(\cdot)^2 - V(x(\cdot), t) \right) dt \quad (1.101)$$

to calculate Eq.(1.99), Sokolovski and Baskin have used the time functional form in Eq.(1.98), and then putting it into the mean value definition in Eq.(1.100), they have got

$$\tau_{\Omega} = \langle \tau_{\Omega}^{cl}[x(\cdot)] \rangle = i\hbar \int_{t_1}^{t_2} dt \int_{\Omega} \frac{\delta \ln \langle x_2, t_2 | x_1, t_1 \rangle}{\delta V(x)} \quad (1.102)$$

where  $\langle x_2, t_2 | x_1, t_1 \rangle$  is the propagator which takes particle from  $x_1$  to  $x_2$  with the time interval  $t_2 - t_1$ . Also  $\frac{\delta}{\delta V}$  is a functional derivative, and it is defined for any function  $G[f(x)]$  as

$$\frac{\delta G[V(x)]}{\delta V(y)} = \lim_{\epsilon \rightarrow 0} \frac{G[V(x) + \epsilon \delta(x - y)] - G[V(x)]}{\epsilon} \quad (1.103)$$

However, this equation above (1.102) is a generalized way of calculating the time using Feynman Path Integral formulation. From here, using the same calculations, now, we have to find an expression for the tunneling time. It is necessary to distinguish reflection and transmission amplitudes for this case, and this will be done by considering particle that is starting its motion far from the left of the barrier, and it is detected after a long time in the right of the barrier. We follow Sokolovski and Baskin, and then set

$$\left. \begin{array}{l} x_1 \rightarrow -\infty \\ \tau \rightarrow \infty \\ \frac{|x_1|}{\tau} = v \\ x_2 > a \end{array} \right\} \quad (1.104)$$

which satisfies the conditions we have mentioned above. With the help of these conditions, authors found

$${}^T \tau_{\Omega} = i\hbar \int_{x_1}^{x_2} \frac{\delta \ln (T e^{i\alpha})}{\delta V(x)} \quad (1.105)$$

is the transmission time and

$${}^R\tau_{\Omega} = i\hbar \int_{x_1}^{x_2} \frac{\delta \ln (Re^{i\beta})}{\delta V(x)} \quad (1.106)$$

is the reflection time where  $T$  is the transmission amplitude,  $R$  is the reflection amplitude,  $\alpha$  and  $\beta$  are the phase shifts for the transmission and reflection respectively.

As you notice by looking at these transmission and reflection times that, corresponding times are complex. Not only these but also the generalized time  $\tau_{\Omega}$  in Eq.(1.102) is complex in general. This complexity of resulting times make sense and they are expected because, we know that for the tunneling process, momentum is imaginary, and therefore, particle has both imaginary velocity and time while following the classical path. Since this approach is a time average of these classical paths inside the region  $\Omega$ , having complex time is not a surprising result. Here, main criticism about this approach is based on these facts; complex time and also, the other important criticisms are, this resulting time is a average time of the all paths inside the region  $\Omega$  (Fertig, 1990; Martin, 1996), and there will be important consequences of the interference of these paths (Fertig, 1993; Sokolovski and Connor, 1991, 1993; Mugnai and Ranfagni, 1992) which cannot be controlled.

# CHAPTER 2

## ENTROPIC TUNNELING TIME

### 2.1. Derivation of the Entropic Tunneling Time

First, we have to answer the question of how time reveals itself. In other words, what is the key ingredient of expressing time? In classical realm, the time elapsed while a particle moves from one point to another cannot be determined without knowing its momentum at each point in between. Therefore, holding the information of momentum is the answer (in this section, the content that we are covering is available in (Demir, 2014)). This is because momentum is the generator of translations and, with strict energy conservation, it becomes  $\sqrt{2m(E - V(x))}$  for a material point moving along  $x$  axis with mass  $m$ , potential energy  $V(x)$  and total energy  $E$ . The tunneling region, bounded by the turning points  $x_1$  and  $x_2 > x_1$  at which  $V(x_1) = E = V(x_2)$  and between which  $E < V(x)$ , has the particle diffusing with imaginary momentum. This necessitates time to turn into pure imaginary direction  $dt \rightarrow id\tau$  where  $d\tau = (m/q(x)) dx$  (see Zeh (2007) for time arrow) with

$$q(x) = \sqrt{2m(V(x) - E)} \quad (2.1)$$

being the momentum modulus in tunneling region. The crucial point is that tunneling, being instantaneous in real time, violates causality. Tunneling time, however, must be real and finite (Landauer, 1989) as was discussed in (Low and Mende, 1991; Demir, 1998; Grossmann, 2000) by kinematic approaches (spatial discretum causes Zeno effect (Demir and Sargin, 2014)).

In search for a phenomenological approach that can evade problems with tunneling process, we develop a novel formulation building upon the three observations below:

1. For a proper formulation of tunneling time, we consider only those states having definite momentum, and among them we specialize to that state which diffuses the particle from  $x_1$  to  $x_2$  straight. (Constant potentials and smooth potentials admitting WKB approximation accommodate such states.)
2. Imaginary time takes propagators in quantum mechanics into partition functions in equilibrium statistical mechanics (Feynman and Hibbs, 1965), and thus, we resort to

statistical methods in defining the tunneling time. (Probabilistic interpretation enables statistical methods for individual quantum states.)

3. While the energy  $E$  of the particle is fixed everywhere, the thermal energy is not, and it facilitates thus formulation of a real tunneling time representative of the entropy production in tunneling region.

These elements give rise to a consistent framework in which tunneling time can be formulated in verity and its application to most recent attoclock measurements exhibits remarkable agreement with experimental data.

The wave-function describing diffusion from  $x_1$  to  $x$  where  $x_1 < x < x_2$

$$\psi(x) \propto \frac{1}{\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_1}^x q(x') dx'} \quad (2.2)$$

is an approximate solution of the Schroedinger equation in WKB approximation as we already analysed in Section.1.1.2. This wave-function is an approximate eigenfunction of the momentum operator with approximate eigenvalue  $iq(x)$ . Its deviation from exact momentum eigenfunction, proportional to  $dV(x)/dx$ , is small in the WKB regime (see Section.1.1.2). In effect, particles tunnel with a nearly definite momentum under smooth potentials.

The imaginary time, when interpreted as inverse temperature, is known to convert quantum mechanical propagators into statistical mechanical partition functions (Feynman and Hibbs, 1965). This fact can be interpreted to indicate that, statistical methods can provide correct framework for addressing tunneling time problem. In statistical approach, entropy is the core observable and it is proportional to  $-p \log p$  for an event with probability  $p$ . This Boltzmann definition takes on different forms depending on the system under consideration. It is taken, for instance,  $(p - p^r)/(r - 1)$  for non-extensive statistical systems (Tsallis, 1988),  $-\log p$  for applications in medical data analysis (Pincus et al., 1991), and  $(1/(r - 1)) \log p^r$  for entanglement in quantum systems (Renyi, 1961). For quantum tunneling, following (Demir, 2014), we take it in the form

$$S(p) = k_B p \log(1 - \log p) \quad (2.3)$$

where  $k_B$  is the Boltzmann constant. Just as the Boltzmann entropy, this novel entropy vanishes at the points of impossibility ( $p = 0$ ) and certainty ( $p = 1$ ). Its loglog form, which exhibits double exponential Gompertz distribution (Gompertz, 1825) even for uniform  $p$ , can have requisite distributional structure to account for the diffusive tunneling dynamics

stemming from the evanescent wave in (2.2).

In (2.3),  $p$  is the probability that the tunneling particle diffuses till  $x_2$  after entering the barrier region at  $x_1$ . It is necessarily proportional to  $\psi^\dagger(x_2)\psi(x_2)$ . Moreover, irrespective of whether the particle tunnels to reach  $x = x_2$  or is reflected to reappear at  $x = x_1$ , at the beginning of scattering, it must be situated at  $x = x_1$  with certainty. This condition is fulfilled by taking

$$p = \frac{\psi^\dagger(x_2)\psi(x_2)}{\psi^\dagger(x_1)\psi(x_1)} = e^{-2\Phi} \quad (2.4)$$

where

$$\Phi = \frac{1}{\hbar} \int_{x_1}^{x_2} q(x) dx \quad (2.5)$$

is Hamilton's characteristic function in units of  $\hbar$  within the tunneling region. It follows from (2.2). The use of (2.4) in (2.3) returns the entropy produced during diffusion from  $x_1$  to  $x_2$ . Thermodynamically, energy rate of change of entropy gives reciprocal temperature, and for the tunneling entropy in (2.3) it reads

$$\frac{1}{T} = \frac{\partial S}{\partial E} = -2 \frac{k_B}{\hbar} \tau \exp(-2\Phi) \left( \frac{1}{1+2\Phi} + \log \frac{1}{1+2\Phi} \right) \quad (2.6)$$

where

$$\tau = \int_{x_1}^{x_2} \frac{m dx}{q(x)} \quad (2.7)$$

is the modulus of the classical tunneling time (which is pure imaginary as mentioned above equation (2.1)). It is not surprising that the temperature  $T$  is proportional to the reciprocal  $\tau$  (Feynman and Hibbs, 1965).

The energy  $E$  of the particle is strictly constant throughout its motion inside and outside the tunneling region. It is known with certainty. Then, in view of energy-time uncertainty, only an infinite time lapse can be associated with  $E$ . In contrast to  $E$ , however, the thermal energy  $k_B T$  varies as in (2.6) and physically a finite time interval can well be associated with it. The finite time interval must be nothing but the time elapsed between the disappearance of the particle at  $x_1$  and its reappearance at  $x_2$ . In other words, the time

interval has every reason to qualify as the tunneling time  $\Delta t$  provided that tunneling process is properly completed. Again, following (Demir, 2014), this requirement is assured by the uncertainty product

$$\left(T_{trans} \times 2\pi k_B T\right) \times \left(\Delta t\right) = \frac{\hbar}{2} \quad (2.8)$$

where the factor of  $2\pi$  converts  $k_B T$  into Matsubara frequency (Matsubara, 1955) of the particle. In this equation,  $T_{trans}$  (1.34) is transmission coefficient from  $x_1$  to  $x_2$ . It must be present in (2.8) because in case it vanishes ( $T_{trans} \rightarrow 0$ ) the tunneling time must tend to infinity ( $\Delta t \rightarrow \infty$ ) in complete consistency with the nonoccurrence of tunneling. In the WKB regime (details of this transmission coefficient corresponding to WKB approach can be found in Appendix (A))

$$T_{trans} = \frac{1}{\cosh^2 \Phi} \quad (2.9)$$

so that the tunneling time in (2.8) takes the form

$$\Delta t = -\frac{\tau}{2\pi} \cosh^2 \Phi \exp(-2\Phi) \left( \frac{1}{1+2\Phi} + \log \frac{1}{1+2\Phi} \right) \quad (2.10)$$

which is proportional to the classical time  $\tau$ . In the classical limit, where  $\Phi \rightarrow \infty$ , one gets  $\Delta t \rightarrow \infty$ . This infinite limit affirms that the entropic tunneling time is a genuine real time (Low and Mende, 1991), not the norm of an imaginary time like  $\tau$ .

## 2.2. Test of the Entropic Tunneling Time by Experiment

We now study if the entropic tunneling time (2.10) agrees with experimental data. The electric fields of high-intensity lasers reshape Coulomb potential in atoms to generate a potential barrier through (see Fig.2.1) which electrons can tunnel to continuum (Keldysh, 1965). At the peak value  $\mathcal{E}$  of the electric field, an atomic electron possesses the potential energy

$$V(\xi) = -\frac{Z}{\xi} - \mathcal{E}\xi \quad (2.11)$$

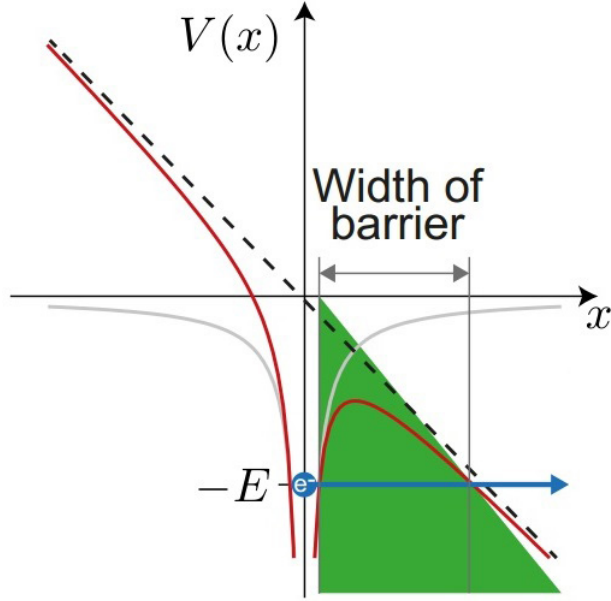


Figure 2.1. Illustration of the potential barrier that is reshaped by the high-intensity laser.

in atomic units (see Appendix B.1 for the detailed calculations of atomic units representation). The Coulomb potential, proportional to the atomic number  $Z$ , turns to linear Stark form at large  $\xi$  ( $\xi = \frac{x}{a_0}$  where  $a_0$  is the Bohr radius). The electron energy  $E_I$  remains unchanged up to second order in  $\mathcal{E}\xi$  by symmetry. Advancements in ultrafast science, where strong laser fields are used to ionize atoms, are able to observe the tunneling phenomenon and measure the tunneling time (Steinberg et al., 1993; Uiberacker et al., 2007; Eckle et al., 2008; Haessler et al., 2010; Smirnova et al., 2009). In spite of various factors affecting the experiments (Lein, 2012; Torlina et al., 2014; Shafir et al., 2012; Sabbar et al., 2014), improving on previous single-particle tunneling time measurements (Eckle et al., 2008), Landsman and her collaborators have recently performed a refined measurement of the tunneling time of electrons in He atom (Landsman et al., 2013). We base our phenomenological analysis below on the data from this recent experiment.

In the experimental set-up, laser intensity  $3.5152 \times 10^{16} \text{ W/cm}^2 \mathcal{E}^2$  is varied from  $0.730 \times 10^{14} \text{ W/cm}^2$  to  $7.50 \times 10^{14} \text{ W/cm}^2$  by varying the peak electric field  $\mathcal{E}$  from 0.046 to 0.146 in atomic units (curiously, experiment reports results at  $\mathcal{E} = 0.04$ , too)(for the details see Appendix B.3). The electron energy  $E_I = -0.8941 \text{ a.u.}$  is the first ionization energy of He. Momentum distribution of continuum electrons are obtained by cold-target recoil-ion momentum spectrometer (COLTRIMS) and velocity map imaging spectrometer (VMIS) (see the experiment section of (Landsman et al., 2013) for details). The VMIS is

used particularly at low laser intensities. Quantum tunneling is ensured to be the dominant ionization mechanism by keeping Keldysh parameter small. The experimental results are given in Fig. 3 of (Landsman et al., 2013). Depicted in Fig. 3 (a) are different tunneling times that we have already investigated in Section.1.2 contrasted with experiment's own results. Given in Fig. 3 (b) and (d) are tunneling times as functions of the peak electric field  $\mathcal{E}$  and barrier width (approximated as  $E_I/\mathcal{E}$  a.u. in the experiment). The experiment concludes that among all widely-used tunneling time definitions only the FPI time comes closest to its data points (see Fig. 3 (b) and (d)).

For testing our model, we pick up the potential energy (2.11) and use parameters of the experiment in the formulae leading to  $\Delta t$  in (2.10). By increasing  $\mathcal{E}$  from 0.05 a.u. to 0.09 a.u., one finds turning points as:  $\xi_L$  ( $\xi_L = \frac{\hat{E}_I + \sqrt{\hat{E}_I^2 - 4\mathcal{E}Z}}{2\mathcal{E}}$ ) increases from 2.616 a.u. to 3.387 a.u.,  $\xi_R$  ( $\xi_R = \frac{\hat{E}_I - \sqrt{\hat{E}_I^2 - 4\mathcal{E}Z}}{2\mathcal{E}}$ ) decreases from 15.290 a.u. to 6.561 a.u. (see Appendix B.2 for detailed calculations of these turning points), and correspondingly, modulus of the classical imaginary time  $\tau$  decreases from 693.045 as to 396.845 as. At these extremes, the entropic tunneling time  $\Delta t$  decreases from 73.066 as to 12.365 as. Numerically, thus, it takes attosecond times for particle to wend the laser-induced nano-width He barrier. This theoretical prediction affirms the attoclock experiments studying tunneling time (Steinberg et al., 1993). Basically, attosecond tunneling times must be the characteristic time scale in nano-width eV-barriers.

We plot in Figs.(2.2) and (2.3) the entropic tunneling time (2.10) as a function of the peak electric field  $\mathcal{E}$  and experiment's barrier width  $E_I/\mathcal{E}$  (which is not the true barrier width  $\xi_R - \xi_L$ ). The minimum entropic tunneling time  $(\Delta t)_{min}$ , shown by filled triangles in Figs. 2.2 and 2.3, is superimposed on Fig. 3 (b) and (d) of (Landsman et al., 2013)<sup>1</sup>. The figure ensures that the minimum of the entropic tunneling time is indeed the shortest time among all theoretical predictions and experimental data (see Fig. 3 (a) of (Landsman et al., 2013)). The FPI time (Sokolovski and Baskin, 1987; Fertig, 1990; Martin, 1996; Sokolovski et al., 1994), the theoretical prediction coming closest to the experimental data, overlies data in the left panel and crosses over data in the right panel. The entropic time, although what is plotted in Figs. 2.2 and 2.3 is only its minimum, performs even better than the FPI time as indicated especially by the right panel. Overall, what is interesting is that, in both panels of Figs. 2.2 and 2.3, the minimum entropic time  $\Delta t$  stays congruent to the experimental data by closely following it from a distance. Barring various factors affecting the experiment (Lein, 2012; Torlina et al., 2014; Shafir et al., 2012; Sabbar et al., 2014; Keldysh, 1965; Landsman

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<sup>1</sup>digitized by using <http://arohatgi.info/WebPlotDigitizer/>



et al., 2013)), actual value of the entropic time has every reason to agree with the experiment. The entropic tunneling time  $\Delta t$  is depicted by filled triangles. It is seen to stay congruent

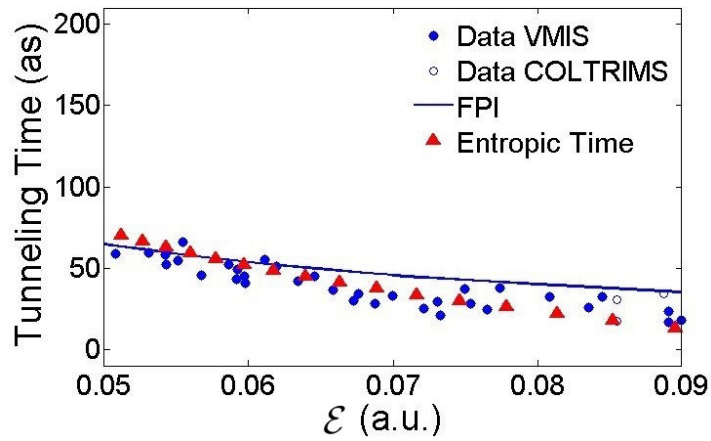


Figure 2.2. Tunneling times as functions of peak electric field  $\mathcal{E}$ .

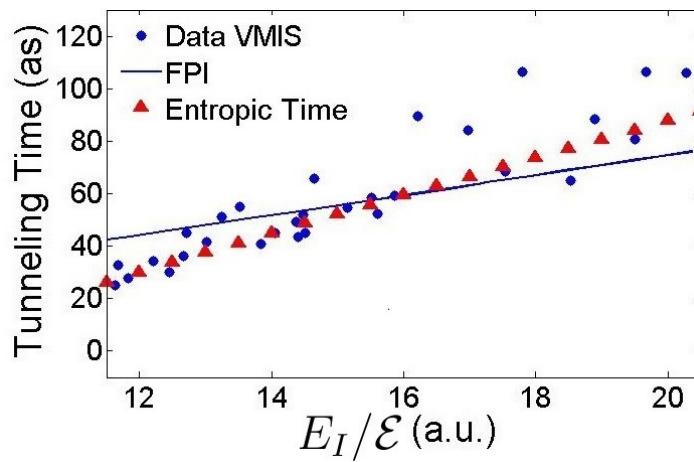


Figure 2.3. Tunneling times as functions of experimental barrier width  $E_I/\mathcal{E}$ .

to the experimental data throughout. The right panel specifically shows how the minimum entropic time adheres to the experimental data while the FPI time diverges away from data

at the asymptotics <sup>2</sup>.

In summary, in the present study, we have founded a new tunneling time formula and verified it with most recent experimental data. The formula works. It has far-reaching consequences in basic sciences and technological applications because knowing the lower bound means knowing the highest speed with which the reaction under concern proceeds.

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<sup>2</sup>Data of the experiment

# CHAPTER 3

## APPLICATIONS OF THE ENTROPIC TUNNELING TIME

### 3.1. $\alpha$ - decay

$\alpha$  - decay is a type of radioactive decay and a well known process. In addition, stability of nucleus has a strict line, and this provides an important information about when  $\alpha$ -decay becomes a dominant process for the unstable nuclei. As you see in the Fig.3.1<sup>1</sup>, if

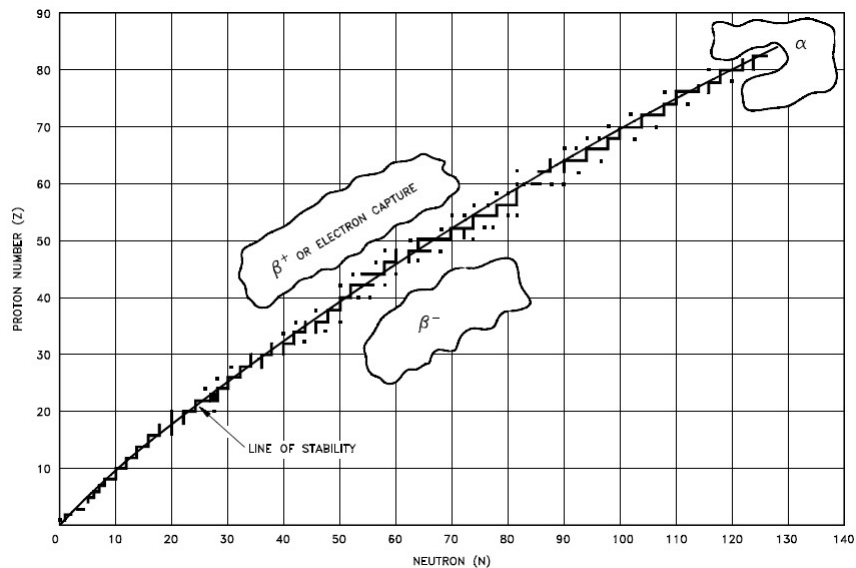


Figure 3.1. Stability curve of the radioactivity

the mass exceeds 83 or neutron number is higher than 126, nucleus starts to emit  $\alpha$  particles to become more stable.

How this  $\alpha$  escapes from the nucleus was a challenging problem. But it was understood that,

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<sup>1</sup>this image is taken from the [http://knowledgepublications.com/doi/doi\\_nuclear\\_physics\\_detail.htm](http://knowledgepublications.com/doi/doi_nuclear_physics_detail.htm)



Now, we are starting to analyse the solution <sup>3</sup> with first considering the potential energy function which is of the form

$$V(x) = \begin{cases} \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 x}, & x \geq R \\ -B, & x < R \end{cases}$$

where  $B$  is the nuclear binding energy, and  $R$  is radius of the Parent nucleus. We set  $l = 0$  for the centrifugal potential  $\frac{l(l+1)\hbar^2}{2mx^2}$  for simplicity. By looking at this potential above, we immediately find the turning point which  $E = V(x_2)$ , and hence

$$x_2 = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 E} \quad (3.2)$$

To calculate tunneling time (2.10)(Demir, 2014; Demir and Guner, 2014) for the  $\alpha$ -decay of any radioactive element like Uranium, we have to find Gamow factor  $\Phi$  of Eq.(1.35). Gamow factor is written for this case with  $x_1 = R$  as

$$\Phi = \frac{1}{\hbar} \int_R^{x_2} \sqrt{2m_\alpha \left( \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 x} - E \right)} dx \quad (3.3)$$

where  $m_\alpha$  is the mass of the  $\alpha$  particle, and if we set

$$\frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 x} = \frac{E x_2}{x} \quad (3.4)$$

we can simplify the term inside of the square root. Therefore, Eq.(3.3) becomes

$$\Phi = \frac{1}{\hbar} \int_R^{x_2} \sqrt{2m_\alpha E \left( \frac{x_2}{x} - 1 \right)} dx \quad (3.5)$$

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<sup>3</sup>further details can be found in <https://fenix.tecnico.ulisboa.pt/downloadFile/3779576931836/Ex8Serie1/>

simplified  $\Phi$  becomes

$$\Phi = \frac{\sqrt{2m_\alpha E}}{\hbar} \int_R^{x_2} \sqrt{\frac{x_2}{x} - 1} dx \quad (3.6)$$

this integral is solved easily when we set

$$x \equiv x_2 \sin^2 u \quad (3.7)$$

which leads to  $dx = 2x_2 \cos u \sin u du$ , and then

$$\Phi = \frac{\sqrt{2m_\alpha E}}{\hbar} \int \left( \sqrt{\frac{x_2}{x_2 \sin^2 u} - 1} \right) 2x_2 \cos u \sin u du \quad (3.8)$$

using the  $\cos^2 u = 1 - \sin^2 u$  for the term in square root, then integration reduces to

$$\Phi = \frac{\sqrt{2m_\alpha E}}{\hbar} 2x_2 \int \cos^2 u du \quad (3.9)$$

resulting integral is simply  $\int \cos^2 u du = \frac{1}{2}(u + \sin u \cos u)$ , and using (3.7), we get for  $u$  as

$$u \equiv \arcsin \sqrt{\frac{x}{x_2}} \quad (3.10)$$

then, analytical solution for the Gamow factor  $\Phi$  becomes

$$\Phi = \frac{\sqrt{2m_\alpha E}}{\hbar} 2x_2 \frac{1}{2} \left[ \arcsin \sqrt{\frac{x}{x_2}} \Big|_R^{x_2} + \sin \left( \arcsin \sqrt{\frac{x}{x_2}} \right) \cos \left( \arcsin \sqrt{\frac{x}{x_2}} \right) \Big|_R^{x_2} \right] \quad (3.11)$$

and applying integral limits, we get the total result

$$\phi = \frac{\sqrt{2m_\alpha E}}{\hbar} x_2 \left[ \frac{\pi}{2} - \arcsin \sqrt{\frac{R}{x_2}} - \sqrt{\frac{R}{x_2}} \cos \left( \arcsin \sqrt{\frac{R}{x_2}} \right) \right] \quad (3.12)$$

In addition to this calculation of  $\Phi$ , we have to also calculate  $\tau$  in (2.7) to be able to get the numerical value of our tunneling time (2.10). We write  $\tau$  for the  $\alpha$ -decay as

$$\tau = \int_R^{x_2} \frac{m_\alpha}{q(x)} dx = m_\alpha \int_R^{x_2} \frac{1}{\sqrt{2m_\alpha \left( \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 x} - E \right)}} dx \quad (3.13)$$

following the same calculation of  $\Phi$  above, what we get is

$$\tau = \frac{m_\alpha}{\sqrt{2m_\alpha E}} \int_R^{x_2} \frac{1}{\sqrt{\frac{x_2}{x} - 1}} dx \quad (3.14)$$

with the help of Mathematica (Wolfram Research, 2010), we get the result for this integral as

$$\tau = \frac{m_\alpha}{\sqrt{2m_\alpha E}} \left[ -x \sqrt{\frac{x_2}{x} - 1} \Big|_R^{x_2} - \frac{x_2}{2} \arctan \left( \frac{(2x - x_2) \sqrt{\frac{x_2}{x} - 1}}{2(x - x_2)} \right) \Big|_R^{x_2} \right] \quad (3.15)$$

applying integral limits

$$\tau = \frac{m_\alpha}{\sqrt{2m_\alpha E}} \left[ \frac{x_2}{4\pi} + R \sqrt{\frac{x_2}{R} - 1} + \frac{x_2}{2} \arctan \left( \frac{(2R - x_2) \sqrt{\frac{x_2}{R} - 1}}{2(R - x_2)} \right) \right] \quad (3.16)$$

gives us the analytical expression of  $\tau$ . Before applying our tunneling time approach to this  $\alpha$ -decay via Gamow factor  $\Phi$ , and  $\tau$ , we have to mention that,  $E$  must be determined by using the binding energy formula. This formula is necessary because this type of nuclear processes involve change in the binding energy, and one will calculate the energy of the  $\alpha$  particle by considering it as absorbing the released energy that determines its kinetic energy. Therefore, released energy, and hence, kinetic energy of the  $\alpha$  particle is

$$E = (m_{parent} - m_{daughter} - m_\alpha) c^2 \quad (3.17)$$

where  $m_{parent}$  is the atomic mass of the parent nucleus, and  $m_{daughter}$  is the atomic mass of resulting daughter nucleus. Knowing the energy of  $\alpha$  particle is not enough, and also, we

have to determine radius of the related nucleus by using an empirical formula <sup>4</sup>

$$\text{Approximated radius of the nucleus: } R \approx 1.07 \times 10^{-15} \text{m} \times A^{\frac{1}{3}} \quad (3.18)$$

where  $A$  is the atomic mass number. Putting numerical values of these parameters  $x_2$ ,  $R$ , and  $E$  into the expressions of  $\tau$ , and  $\Phi$ , we obtain the tunneling times (2.10) for  $\alpha$ -decays of different isotopes of nucleus Uranium (U), Thorium (Th), Polonium (Po), Protactinium (Pa), and Bismuth(Bi) as you see in Table 3.1 and in Fig.(3.3) <sup>5</sup>.

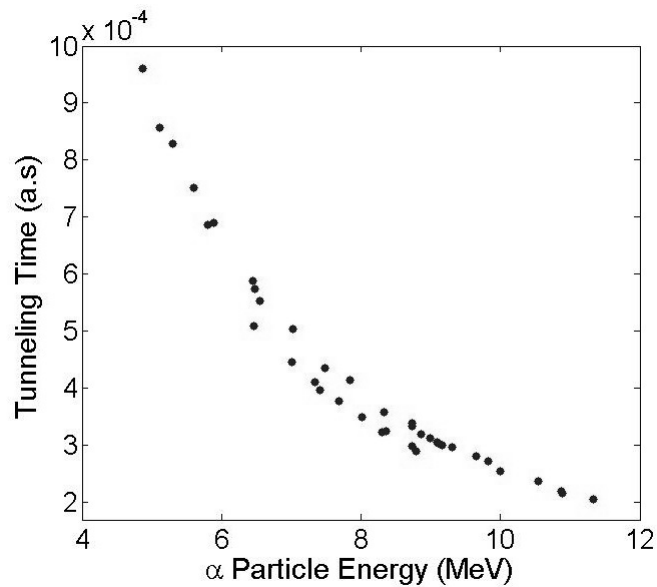


Figure 3.3. Plot of the  $\alpha$ -decay tunneling times

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<sup>4</sup>details can be found in <http://physics.bu.edu/py106/notes/RadioactiveDecay.html>

<sup>5</sup>Mass of the  $\alpha$ -particle is taken as  $m_\alpha = 4.001506\text{u}$ .



Table 3.1. Calculated tunneling times for  $\alpha$ -decay processes of different elements. Here extra term  $t_c = \frac{x_2 - R}{c}$  represents the time it takes for a photon to travel this barrier region.  $fm$  is femtometer,  $as$  is attosecond, and  $u$  is atomic mass unit.

Parent Nucleus	$m_{parent}(u)$	$R(fm)$	$m_{daughter}(u)$	$E(MeV)$	$\Delta t(as)$	$t_c(as)$
$^{218}_{92}U$	218.023540	6.439800	214.011500	9.826900	0.000273	0.000066
$^{220}_{92}U$	220.024720	6.459400	216.011062	11.336000	0.000206	0.000055
$^{222}_{92}U$	222.026090	6.478900	218.013284	10.541000	0.000238	0.000060
$^{224}_{92}U$	224.027605	6.498300	220.015748	9.656100	0.000281	0.000068
$^{226}_{92}U$	226.029339	6.517600	222.018468	8.736300	0.000339	0.000077
$^{228}_{92}U$	228.031374	6.536800	224.021467	7.837000	0.000414	0.000088
$^{230}_{92}U$	230.033940	6.555800	226.024903	7.025400	0.000504	0.000101
$^{232}_{92}U$	232.037156	6.574800	228.028741	6.445200	0.000588	0.000112
$^{234}_{92}U$	234.040952	6.593600	230.033139	5.883600	0.000690	0.000125
$^{236}_{92}U$	236.045568	6.612300	232.038055	5.603700	0.000752	0.000132
$^{238}_{92}U$	238.050788	6.631000	234.043601	5.299600	0.000828	0.000141
$^{240}_{92}U$	240.056592	6.649500	236.049870	4.865800	0.000960	0.000155
$^{210}_{90}Th$	210.015075	6.360000	206.003827	9.088000	0.000306	0.000072
$^{212}_{90}Th$	212.012980	6.380100	208.001840	8.987300	0.000313	0.000073
$^{214}_{90}Th$	214.011500	6.400100	210.000495	8.861300	0.000321	0.000074
$^{216}_{90}Th$	216.011062	6.420000	211.999794	9.106700	0.000304	0.000071
$^{218}_{90}Th$	218.013284	6.439800	214.000108	10.887000	0.000216	0.000056
$^{220}_{90}Th$	220.015748	6.459400	216.003533	9.990100	0.000255	0.000063
$^{222}_{90}Th$	222.018468	6.478900	218.007140	9.162700	0.000300	0.000071
$^{224}_{90}Th$	224.021467	6.498300	220.011028	8.333300	0.000358	0.000080
$^{226}_{90}Th$	226.024903	6.517600	222.015375	7.483500	0.000436	0.000091
$^{228}_{90}Th$	228.028741	6.536800	224.020212	6.551500	0.000554	0.000107
$^{230}_{90}Th$	230.033134	6.555800	226.025410	5.800500	0.000687	0.000124
$^{232}_{90}Th$	232.038055	6.574800	228.0310703	5.110800	0.000857	0.000143
$^{190}_{84}Po$	189.995101	6.151300	185.984239	8.727900	0.000300	0.000070
$^{192}_{84}Po$	191.991335	6.172800	187.980874	8.353800	0.000325	0.000074
$^{194}_{84}Po$	193.988186	6.194200	189.978082	8.020800	0.000350	0.000077
$^{196}_{84}Po$	195.985535	6.215400	191.975785	7.690600	0.000378	0.000082
$^{198}_{84}Po$	197.983389	6.236500	193.974012	7.342600	0.000411	0.000086
$^{200}_{84}Po$	199.981799	6.257400	195.972774	7.014200	0.000447	0.000091
$^{214}_{91}Pa$	214.020920	6.400100	210.00944	9.304400	0.000298	0.000070
$^{220}_{91}Pa$	220.02188	6.459400	216.008720	10.872000	0.000220	0.000057
$^{224}_{91}Pa$	224.025626	6.498300	220.014763	8.728900	0.000334	0.000076
$^{230}_{91}Pa$	230.034541	6.555800	226.026098	6.471300	0.000575	0.000110
$^{186}_{83}Bi$	185.996600	6.107800	181.985670	8.791400	0.000291	0.000068
$^{188}_{83}Bi$	187.99227	6.129700	183.981870	8.296900	0.000324	0.000073
$^{192}_{83}Bi$	191.98546	6.172800	187.976010	7.410700	0.000398	0.000084
$^{196}_{83}Bi$	195.980667	6.215400	191.972230	6.465700	0.000509	0.000100

### 3.2. STM

STM (Scanning Tunneling Microscope) is an important instrument that was developed by Binnig and Rohrer in 1981 and they earned the Nobel Prize in Physics in 1986 for this invention. This instrument images surfaces at the atomic level by using quantum tunneling. One can use STM with two different ways: *constant current* and *constant height*. First one provides better resolution since tip arranges itself to make current fixed, and latter one is faster but only appropriate for the atomically flat surfaces since the vertical position of the tip remain unchanged. One can visualize this set up as in Fig.3.4<sup>6</sup>. As you see in

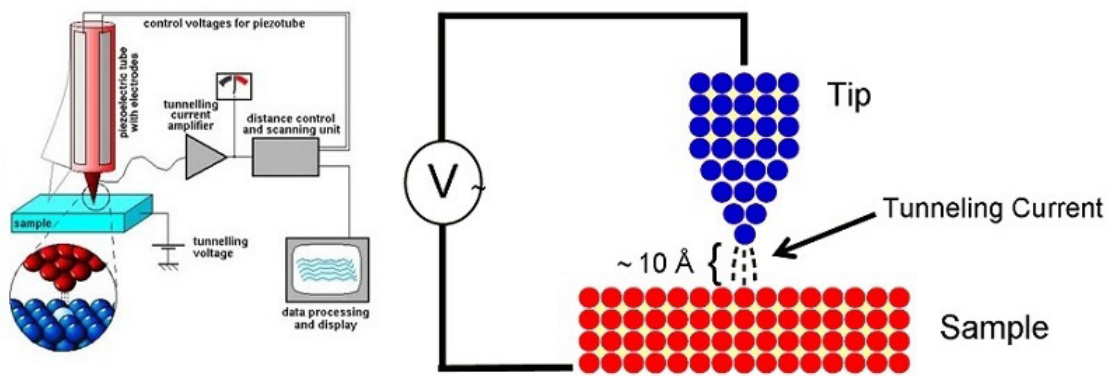


Figure 3.4. Illustration of the STM set-up and tip-sample interaction

this figure, a conducting tip brought very close to the conducting sample. Conductivity is necessary because these free electrons form the tunneling current when bias voltage is applied because this bias voltage make electrons to start tunneling between this gap of tip and sample. This gap which also means a barrier width  $x_2 - x_1$  is typically  $\leq 10\text{\AA}$  for the best resolution because as you see in Eq.(1.19) that, transmission coefficient ( $t \approx e^{-2\kappa L}$ ) decays exponentially as barrier width  $L (x_2 - x_1)$  increases, and therefore, is very sensitive to change in any distance of tip from the sample.

To apply our tunneling time approach in Eq.(2.10) (Demir, 2014; Demir and Guner, 2014) to

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<sup>6</sup>These images are taken from the (left)[http://www.iap.tuwien.ac.at/www/surface/STM\\_Gallery/stm\\_schematic.html](http://www.iap.tuwien.ac.at/www/surface/STM_Gallery/stm_schematic.html), and (right)<http://www.personal.psu.edu/ewh10/ResearchBackground.htm>

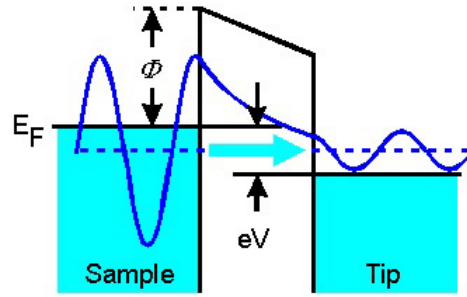


Figure 3.5. Simple illustration of the tunneling process in STM

STM, we have to understand how we deal with this system first. Most of the studies consider potential function as constant, and hence, we treat this system as an approximately a rectangular potential barrier (details and other approaches can be found in (Pitarke et al., 1989) and (Olesen et al., 1996)). This simple approach is illustrated in Fig.3.5<sup>7</sup>. According to this approach, we use  $\kappa$  in Section.1.1.1,

$$\kappa = \frac{\sqrt{2m(\phi - E)}}{\hbar} \quad (3.19)$$

where  $\phi$  is the work-function here,  $E$  is electron's energy, and  $m$  is the mass of electron.  $\phi$  is work-function because it represents the height that is corresponding to the interval between  $E_F$  (fermi-energy level) and top of the barrier. This work-function is approximately taken as average

$$\phi = \frac{1}{2}(\phi_S + \phi_T) \quad (3.20)$$

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<sup>7</sup>This picture is taken from the <http://www2.fkf.mpg.de/ga/research/stmtutor/stmtheo.html>

where  $\phi_S$  is the work-function of the sample, and  $\phi_T$  is the work function of the tip. Therefore,  $\Phi$  in Eq.(1.35) found as

$$\Phi = \frac{\sqrt{2m(\phi - E)}}{\hbar} \int_{x_1}^{x_2} dx \quad (3.21)$$

and if we set turning points as  $x_1 = 0$ , and  $x_2 = L$ , result becomes

$$\Phi = \frac{\sqrt{2m(\phi - E)}}{\hbar} L \quad (3.22)$$

from here, we approximately treat the system as <sup>8</sup>

$$\Phi \approx \frac{\sqrt{2m\phi}}{\hbar} L \quad (3.23)$$

since applied bias voltage is small compared to the work-function  $eV \ll \phi$ . In other words, if we look at the  $\kappa$  term in (3.19), we see that there is energy of the particle  $E$  in terms of  $eV$  due to applied voltage  $V$ , and if we keep bias voltage very small, then  $\phi - E$  term becomes dominated by the work-function  $\phi$  which leads to a  $\Phi$  solution as we seen in (3.23) or we simply consider that electrons are having energies oscillating around the fermi-energy level  $E_F$  that allows us to take  $E = E_F = 0$  approximately.

In addition to  $\Phi$ , we also need to calculate  $\tau$  (2.7) in this case appropriate for STM where  $x_1 = 0$ , and  $x_2 = L$ , which is

$$\tau = \int_0^L \frac{m dx}{q(x)} \quad (3.24)$$

and where  $q(x) = \sqrt{2m(\phi - E)} \approx \sqrt{2m\phi}$ , then  $\tau$  becomes

$$\tau \approx \frac{m}{\sqrt{2m\phi}} L \quad (3.25)$$

---

<sup>8</sup><http://www2.fkf.mpg.de/ga/research/stmtutor/stmtheo.html>

We apply our tunneling time formula in (2.10) to STM using these  $\Phi$  (3.23), and  $\tau$  (3.25). To obtain numerical data, we consider different samples, and three different tip-sample distances  $L(1\text{\AA}, 5\text{\AA}, \text{ and } 8\text{\AA})$  as you see in Table 3.2 and Fig.(3.6-3.8), and we take Tungsten (W) as tip material which has a work-function as  $\phi_T = 4.55\text{eV}$ . We should note that the time it takes for photon to travel these widths are  $t_c = 0.3333\text{as}$  for  $1\text{\AA}$ ,  $t_c = 1.667\text{as}$  for  $5\text{\AA}$ , and  $t_c = 2.667\text{as}$  for  $8\text{\AA}$  respectively.

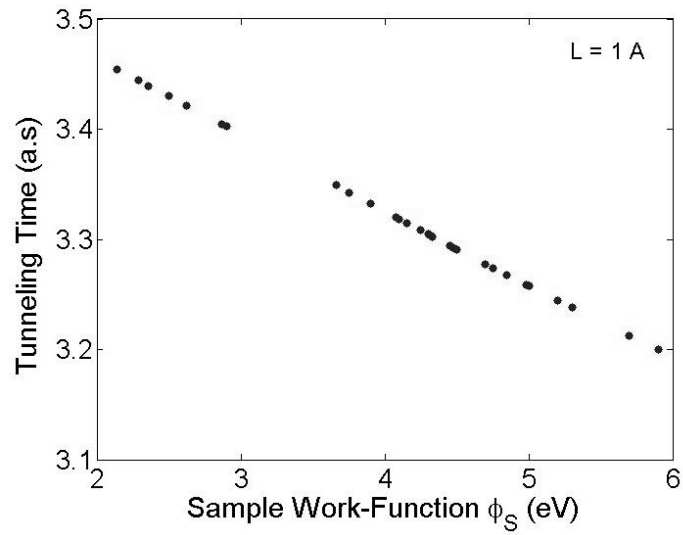


Figure 3.6. Plot of the STM tunneling times for  $1\text{\AA}$

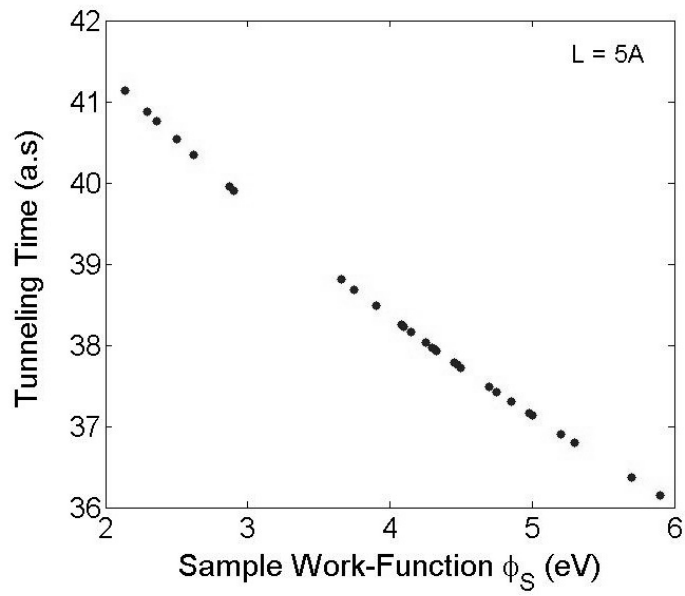


Figure 3.7. Plot of the STM tunneling times for  $5 \text{ \AA}$

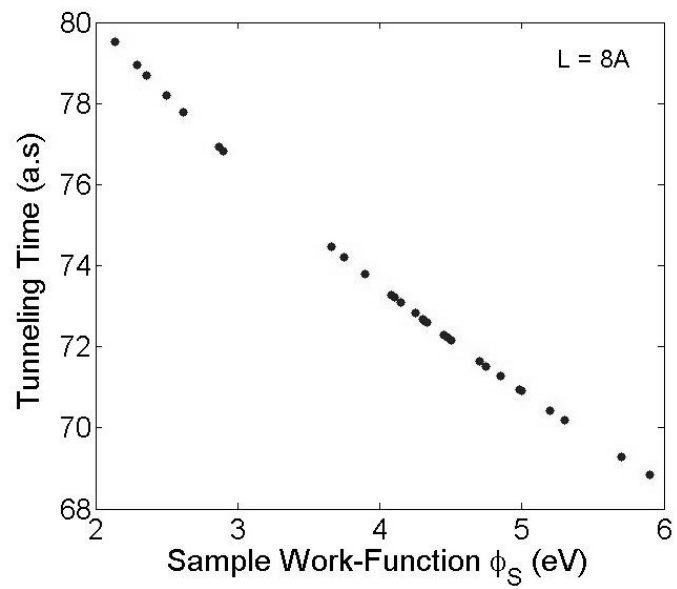


Figure 3.8. Plot of the STM tunneling times for  $8 \text{ \AA}$

Table 3.2. Calculated tunneling times for different samples in STM.

Sample	$\phi_S$ (eV)	Width (Å)	$\Delta t$ (as)	Sample	$\phi_S$ (eV)	Width (Å)	$\Delta t$ (as)
Ag	4.30	1	3.3046	Al	4.15	1	3.3149
Ag	4.30	5	37.9723	Al	4.15	5	38.1620
Ag	4.30	8	72.6869	Al	4.15	8	73.0915
As	3.75	1	3.3426	Au	5.3	1	3.2379
As	3.75	5	38.6866	Au	5.3	5	36.7961
As	3.75	8	74.2140	Au	5.3	8	70.1892
B	4.45	1	3.2944	Ba	2.62	1	3.4217
B	4.45	5	37.7864	Ba	2.62	5	40.3404
B	4.45	8	72.2906	Ba	2.62	8	77.7812
Be	4.98	1	3.2588	Bi	4.31	1	3.3039
Be	4.98	5	37.1569	Bi	4.31	5	37.9598
Be	4.98	8	70.9530	Bi	4.31	8	72.6602
C	5	1	3.2575	Ca	2.87	1	3.4043
C	5	5	37.1339	Ca	2.87	5	39.9501
C	5	8	70.9044	Ca	2.87	8	76.9354
Cd	4.08	1	3.3197	Li	2.9	1	3.4022
Cd	4.08	5	38.2518	Li	2.9	5	39.9043
Cd	4.08	8	73.2833	Li	2.9	8	76.8362
Ti	4.33	1	3.3026	Cr	4.5	1	3.2910
Ti	4.33	5	37.9349	Cr	4.5	5	37.7252
Ti	4.33	8	72.6069	Cr	4.5	8	72.1603
Cs	2.14	1	3.4543	Cu	4.7	1	3.2775
Cs	2.14	5	41.1347	Cu	4.7	5	37.4842
Cs	2.14	8	79.5104	Cu	4.7	8	71.6479
Eu	2.5	1	3.4300	Fe	4.75	1	3.2741
Eu	2.5	5	40.5332	Fe	4.75	5	37.4249
Eu	2.5	8	78.2000	Fe	4.75	8	71.5219
Ga	4.32	1	3.3032	Hg	4.475	1	3.2927
Ga	4.32	5	37.9473	Hg	4.475	5	37.7557
Ga	4.32	8	72.6335	Hg	4.475	8	72.2253
K	2.29	1	3.4443	Se	5.9	1	3.1997
K	2.29	5	40.8798	Se	5.9	5	36.1550
K	2.29	8	78.9542	Se	5.9	8	68.8368
Mg	3.66	1	3.3489	Mn	4.1	1	3.3184
Mg	3.66	5	38.8086	Mn	4.1	5	38.2260
Mg	3.66	8	74.4757	Mn	4.1	8	73.2283
Na	2.36	1	3.4395	Ni	5.20	1	3.2444
Na	2.36	5	40.7629	Ni	5.20	5	36.9073
Na	2.36	8	78.6997	Ni	5.20	8	70.4246
Pb	4.25	1	3.3080	Pt	5.70	1	3.2122
Pb	4.25	5	38.0351	Pt	5.70	5	36.3638
Pb	4.25	8	72.8208	Pt	5.70	8	69.2766
Si	4.85	1	3.2674	Zn	3.90	1	3.3322
Si	4.85	5	37.3075	Zn	3.90	5	38.4865
Si	4.85	8	71.2724	Zn	3.90	8	73.7854

### 3.3. Creation of Universe from Nothing

Understanding origin of the universe, and also, trying to provide a satisfactory explanation for the "Universe from nothing" are still ongoing studies in physics. In this section, we want to apply our tunneling time formula (2.10) (Demir, 2014; Demir and Guner, 2014) to the universe that emerges by tunneling at the beginning. This idea of tunneling universe is a point of view towards understanding origin of the universe, and explaining the "Universe from nothing". To do so, first (details can be found in (Stenger, 2006)), we have to understand how this tunneling occurs, and we need to get the Hamiltonian representing this initial stage of the universe to find corresponding potential. Following Atkatz (Atkatz, 1994), one can write action for FRW universe as

$$S \equiv \int dt L = \frac{3\pi c^4}{4G_N} \int dt \left[ -\frac{1}{c^2} \left( \frac{\partial a}{\partial t} \right)^2 a + a \left( 1 - \frac{a^2}{a_0^2} \right) \right] \quad (3.26)$$

where  $a$  is scale factor that represents the radius,  $a_0 = \sqrt{\frac{3c^2}{\Lambda}}$ ,  $c$  is speed of light,  $\Lambda$  is cosmological constant, and  $G_N$  is Newton's gravitational constant. Therefore, Lagrangian is

$$L = \frac{3\pi c^4}{4G_N} \left[ -\frac{1}{c^2} \left( \frac{\partial a}{\partial t} \right)^2 a + a \left( 1 - \frac{a^2}{a_0^2} \right) \right] \quad (3.27)$$

and note that,  $k = 1$  which means we have considered FRW universe as closed, and depending on the variable  $a$ . From here, using our classical mechanics knowledge, we get canonical momentum via Lagrangian above.

$$p_c = \frac{\partial L}{\partial \dot{a}} = \frac{3\pi c^4}{4G_N} \left( -\frac{2a}{c^2} \frac{\partial a}{\partial t} \right) \quad (3.28)$$

where  $\dot{a} = \frac{\partial a}{\partial t}$ . Then, one gets the Hamiltonian using the canonical momentum  $p_c$  we have found above

$$H = p_c \dot{a} - L = p_c \dot{a} - \frac{3\pi c^4}{4G_N} \left[ -\frac{1}{c^2} \dot{a}^2 a + a \left( 1 - \frac{a^2}{a_0^2} \right) \right] \quad (3.29)$$



and by looking at the Eq.(3.28), if we represent  $\dot{a}$  in terms of canonical momentum  $p_c$

$$\dot{a} = \frac{c^2 p_c}{-\left(\frac{3\pi c^4}{4G_N}\right) 2a} \quad (3.30)$$

if we put (3.30), in Hamiltonian form (3.29), what we get is

$$H = \frac{c^2 p_c^2}{-\left(\frac{3\pi c^4 a}{2G_N}\right)} - \frac{3\pi c^4}{4G_N} \left[ -\frac{ac^4 p_c^2}{\left(-\frac{3\pi c^4 a}{2G_N}\right)^2} + a \left(1 - \frac{a^2}{a_0^2}\right) \right] \quad (3.31)$$

combining all terms leads to a

$$H = -\frac{c^2 p_c^2 G_N}{3\pi c^4 a} - \frac{3\pi c^4}{4G_N} a \left(1 - \frac{a^2}{a_0^2}\right) \quad (3.32)$$

and then

$$H = -\frac{G_N}{3\pi c^4} \left[ \frac{c^2 p_c^2}{a} + 4 \left(\frac{3\pi c^4}{4G_N}\right)^2 a \left(1 - \frac{a^2}{a_0^2}\right) \right] \quad (3.33)$$

from here, one will express term that contains  $p_c$  in terms of  $\dot{a}$  using the (3.30), and as a result, one gets

$$H = -\frac{3\pi c^4}{4G_N} \left[ \frac{1}{c^2} a \left(\frac{da}{dt}\right)^2 + a \left(1 - \frac{a^2}{a_0^2}\right) \right] \quad (3.34)$$

according to this Hamiltonian, if we set  $H = 0$ , we immediately get

$$\frac{1}{c^2} \left(\frac{da}{dt}\right)^2 + \left(1 - \frac{a^2}{a_0^2}\right) = 0 \quad (3.35)$$

which is one of the Friedmann equations with  $k = 1$ . On the other hand, if we use canonical quantization by

$$p_c = -i\hbar \frac{\partial}{\partial a} \quad (3.36)$$

then Hamiltonian (3.33) becomes

$$H = -\frac{G_N}{3\pi c^4} \left[ -\frac{c^2 \hbar^2}{a} \frac{\partial^2}{\partial a^2} + 4 \left( \frac{3\pi c^4}{4G_N} \right)^2 a \left( 1 - \frac{a^2}{a_0^2} \right) \right] \quad (3.37)$$

and multiplying and dividing this Hamiltonian by  $2m$ , and taking into  $\frac{1}{a}$  and  $c^2$  parenthesis,

$$H = -\frac{2mG_N c^2}{3\pi c^4 a} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial a^2} + \frac{4}{2mc^2} \left( \frac{3\pi c^4}{4G_N} \right)^2 a^2 \left( 1 - \frac{a^2}{a_0^2} \right) \right] \quad (3.38)$$

when we set  $H\psi = E_n\psi = 0$ ,

$$-\frac{2mG_N c^2}{3\pi c^4 a} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial a^2} + \frac{4}{2mc^2} \left( \frac{3\pi c^4}{4G_N} \right)^2 a^2 \left( 1 - \frac{a^2}{a_0^2} \right) \right] \psi = 0 \quad (3.39)$$

this Hamiltonian that is having zero eigenvalue for the energy which represents empty space without any energy at the beginning of the universe, is Wheeler-DeWitt equation, and wave-function  $\psi$  here is the wave-function of the universe (Hartle and Hawking, 1983).

We can write inside the bracket of Hamiltonian (3.39) in terms of potential and kinetic energy terms.

$$H = -\frac{2mG_N c^2}{3\pi c^4 a} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial a^2} + V(a) \right] \psi = 0 \quad (3.40)$$

Therefore,

$$V(a) = \frac{4}{2mc^2} \left( \frac{3\pi c^4}{4G_N} \right)^2 a^2 \left( 1 - \frac{a^2}{a_0^2} \right) \quad (3.41)$$

is the potential function that we are looking for. We illustrate this potential as Fig.(3.9)<sup>9</sup> now, to calculate tunneling time for universe, first, we have to calculate  $\Phi$  in (2.5) again, re-writing it in terms of  $a$ , taking turning points as  $x_1 = 0$ ,  $x_2 = a_0$ , and setting  $E = 0$  because of the

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<sup>9</sup>This image is taken from the Atkatz (Atkatz, 1994)

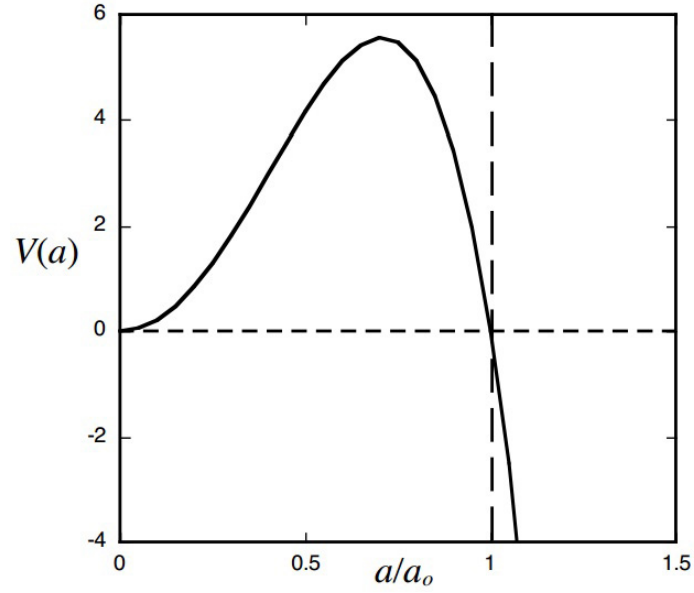


Figure 3.9. Illustration of the potential  $V(a)$

Wheeler-DeWitt condition, what we get is

$$\Phi = \frac{1}{\hbar} \int_0^{a_0} \sqrt{2mV(a)} da = \frac{1}{\hbar} \int_0^{a_0} \sqrt{2m \frac{4}{2mc^2} \left( \frac{3\pi c^4}{4G_N} \right)^2 a^2 \left( 1 - \frac{a^2}{a_0^2} \right)} da \quad (3.42)$$

this leads to

$$\Phi = \frac{1}{\hbar} \frac{2}{c} \left( \frac{3\pi c^4}{4G_N} \right) \int_0^{a_0} \sqrt{a^2 \left( 1 - \frac{a^2}{a_0^2} \right)} da \quad (3.43)$$

this integral is taken simply by arranging it as

$$\Phi = \frac{1}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \int_0^{a_0} \frac{a}{a_0} \sqrt{a^2 - a_0^2} da \quad (3.44)$$

and then setting  $a_0^2 - a^2 \equiv u$  gives,

$$\Phi = \frac{1}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \left( -\frac{1}{3a_0} (a_0^2 - a^2)^{\frac{3}{2}} \Big|_0^{a_0} \right) \quad (3.45)$$

then solution is

$$\Phi = \frac{1}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \frac{a_0^2}{3} \quad (3.46)$$

but we already set  $a_0^2 = \frac{3}{\Lambda}$  due to empty space, and

$$\Phi = \frac{1}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \frac{1}{\Lambda} \quad (3.47)$$

Since there exists ambiguity on the numerical value of  $\Lambda$ , the precise value of which is unknown, we have to leave our tunneling time formula (2.10) as a function of  $\Lambda$ .

To apply our tunneling time formula (2.10), also, we have to evaluate  $\tau$  in (2.7), which results as

$$\tau = m \frac{2G_N}{3\pi c^3} \int_0^{a_0} \frac{da}{\sqrt{a^2(1 - \frac{a^2}{a_0^2})}} \quad (3.48)$$

and this ntegral is obviously a divergent one. To move on, first, we need to put this integral into non-dimensional form by making  $\frac{a}{a_0} = \eta$  which

$$\int_0^{a_0} \frac{da}{\sqrt{a^2(1 - \frac{a^2}{a_0^2})}} = \int_0^1 \frac{d\eta}{\sqrt{\eta^2(1 - \eta^2)}} \quad (3.49)$$

and second, we call this divergent integral

$$\int_0^1 \frac{d\eta}{\sqrt{\eta^2(1 - \eta^2)}} = C_0 \quad (3.50)$$

and this  $C_0$  is estimated by the Mathematica (Wolfram Research, 2010) approximately as

$$C_0 = 9.59068 \quad (\text{with the error estimation } 0.40208) \quad (3.51)$$

when we express mass  $m$  in terms of planck mass

$$m = \frac{3\pi}{2} \left( \frac{\hbar c}{G_N} \right)^{\frac{1}{2}} \quad (3.52)$$

we get for the  $\tau$  as

$$\tau = \frac{3\pi}{2} \left( \frac{\hbar c}{G_N} \right)^{\frac{1}{2}} \frac{2G_N}{3\pi c^3} C_0 \quad (3.53)$$

which simplifies to

$$\tau = \left( \frac{\hbar G_N}{c^5} \right)^{\frac{1}{2}} C_0 \quad (3.54)$$

if we put (3.47), and (3.54) into our tunneling time formula in (2.10), we get analytical

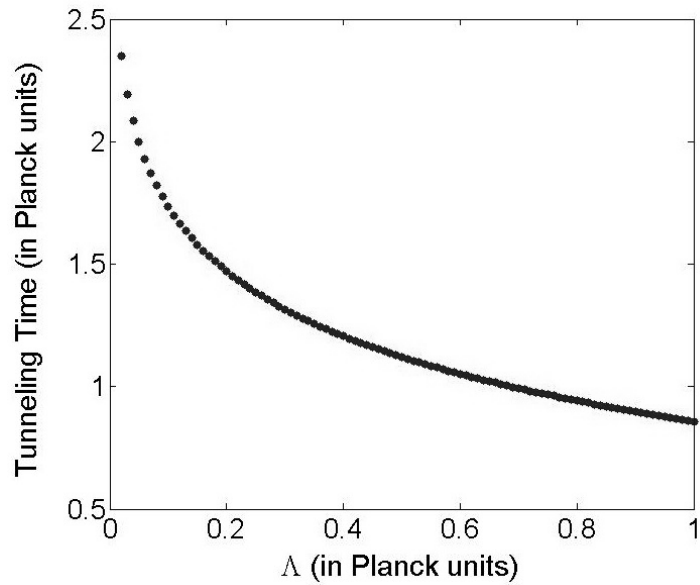


Figure 3.10. Plot of the tunneling time of the universe with respect to cosmological constant  $\Lambda$  in Planck units

expression as a function of  $\Lambda$ ,

$$\Delta t = -\frac{\left(\frac{\hbar G_N}{c^5}\right)^{\frac{1}{2}}}{2\pi} C_0 \cosh^2 \left( \frac{1}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \frac{1}{\Lambda} \right) \exp \left( \frac{-2}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \frac{1}{\Lambda} \right) \times \left( \frac{1}{1 + \left( \frac{2}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \frac{1}{\Lambda} \right)} + \log \frac{1}{1 + \left( \frac{2}{\hbar} \left( \frac{3\pi c^3}{2G_N} \right) \frac{1}{\Lambda} \right)} \right) \quad (3.55)$$

however, in cosmological scale, we have to use planck units where  $\hbar = G_N = c = 1$ , and as a result

$$\Delta t = -\frac{C_0}{2\pi} \cosh^2 \left( \frac{3\pi}{2\Lambda} \right) \exp \left( \frac{-3\pi}{\Lambda} \right) \left( \frac{1}{1 + \left( \frac{3\pi}{\Lambda} \right)} + \log \frac{1}{1 + \left( \frac{3\pi}{\Lambda} \right)} \right) \quad (3.56)$$

where  $\Lambda$  is dimensionless here. This tunneling time is the expression of how long it takes for the universe to tunnel from its origin to the critical radius  $a_0$ . If we find  $\Lambda$  precisely, then this tunneling time formula will give us the Planck order of this time. You find in Fig.3.10 tunneling times of the universe as a function of cosmological constant  $\Lambda$  in Planck units.

## CHAPTER 4

### CONCLUSION

In this thesis work, we proposed a new formulation for tunneling time. Unlike the well-known approaches as we already mentioned in Section.1.2, this entropic tunneling time approach contains statistical methods due to deterministic behaviour of the time, and also due to correlation between propagator and partition function that exists when time flows in imaginary direction. In addition to statistical nature, quantum mechanical contribution as uncertainty principle played a fundamental role while constructing the entropic tunneling time. Then, after deriving the tunneling time formula, we analysed the latest tunneling time experiment (Landsman et al., 2013) in detail, and compared our tunneling time expression with its data. As a result of this comparison, we found that, our theoretical predictions fit well to the data. As the next step, we apply this tunneling time formula to  $\alpha$ -decay, STM, and creation of universe from nothing, and our results indicate femtosecond-attosecond times at characteristic sizes. Consequently, the entropic tunneling time formalism, with direct applications given here, can serve as a useful tool to define time costs of various biological, chemical, physical and technological processes.

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# APPENDIX A

## TRANSMISSION COEFFICIENT IN WKB APPROACH

According to Section.1.1.2, we have found that wavefunction is of the form (1.33). However, we have mentioned that, solution is a linear combination which we didn't consider the whole solution in that section. Now, to calculate transmission coefficient appropriately<sup>1</sup>, we have to write down solution for the wavefunction  $\psi(x)$  for all regions. By looking at Fig.1.2, we separate solution for every region. Therefore, similar to the simple rectangular potential barrier case in Section.(1.1.1), we write

$$\psi(x) = \begin{cases} \frac{A}{\sqrt{p(x)}} e^{\frac{i}{\hbar} \int_{x_1}^x p(x) dx} + \frac{R}{\sqrt{p(x)}} e^{-\frac{i}{\hbar} \int_{x_1}^x p(x) dx}, & x \leq x_1 \\ \frac{C}{\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_1,2}^x q(x) dx} + \frac{D}{\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_1,2}^x q(x) dx}, & x_1 \leq x \leq x_2 \\ \frac{T}{\sqrt{p(x)}} e^{\frac{i}{\hbar} \int_{x_2}^x p(x) dx}, & x \geq x_2 \end{cases} \quad (\text{A.1})$$

where  $p(x) = \sqrt{2m(E - V(x))}$ . One immediately notices that, both  $p(x)$  and  $q(x)$  diverge at the turning points. Therefore, boundary conditions containing these points become problematic, and without using the boundary conditions, finding transmission and reflection coefficients are not possible. Solution is, we have to analyse neighbourhood of these turning points with approximating the change of the the potential as linear.

We have two cases here, around  $x_1$  which  $V'(x_1) = \frac{\partial V(x_1)}{\partial x} > 0$ , and around  $x_2$  which  $V'(x_2) = \frac{\partial V(x_2)}{\partial x} < 0$ . For the case of  $V'(x_1) > 0$ , we write potential as

$$V(x) \approx V(x_1) + V'(x_1)(x - x_1) \quad (\text{A.2})$$

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<sup>1</sup>Further details of this calculation of the transmission coefficient can be found in, Marcus A. M. de Aguiar, "The WKB Approximation"(lecture, IFGW - UNICAMP, November 12, 2013). <http://sites.ifi.unicamp.br/aguiar/files/2014/10/wkb1.pdf>

and we know that  $V(x_1) = E$  since  $x_1$  is turning point, therefore

$$V(x) \approx E + V'(x_1)(x - x_1) \quad (\text{A.3})$$

if we put (A.3) into the time-independent Schroedinger equation,

$$\left( \frac{\hat{p}^2}{2m} + E + V'(x_1)(x - x_1) \right) \psi(x) = E\psi(x) \quad (\text{A.4})$$

which is then

$$\left( \frac{\hat{p}^2}{2m} + V'(x_1)x \right) \psi(x) = V'(x_1)x_1\psi(x) \quad (\text{A.5})$$

and we have to solve this equation. Since  $\hat{p}^2$  term contains second order differentiation, first, we turn this position representation to the momentum representation  $\psi(x) \rightarrow \psi(p)$  to make it easier, and after finding the solution in terms of momentum wave-function, we use Fourier transformation to get wave-function in position representation. So, according to the momentum representation which  $\hat{x} = i\hbar\frac{\partial}{\partial p}$ ,  $\hat{p} = p$ , (A.5) becomes

$$\frac{p^2}{2m}\psi(p) + i\hbar V'(x_1)\frac{\partial\psi(p)}{\partial p} = V'(x_1)x_1\psi(p) \quad (\text{A.6})$$

and rearranging this equation

$$\frac{\psi'(p)}{\psi(p)} = i\left( \frac{p^2 - 2mV'(x_1)x_1}{2m\hbar V'(x_1)} \right) \quad (\text{A.7})$$

where  $\psi'(p) = \frac{\partial\psi(p)}{\partial p}$ . And, solution of this first order differential equation is simply,

$$\psi(p) = C e^{\frac{ip}{6m\hbar V'(x_1)}(p^2 - 6mx_1 V'(x_1))} \quad (\text{A.8})$$

we find momentum wavefunction, and therefore, position wavefunction is

$$\psi(x) = \frac{C}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ip}{6m\hbar V'(x_1)}(p^2 - 6mx_1 V'(x_1))} e^{\frac{ipx}{\hbar}} dp \quad (\text{A.9})$$

from here, since cosine term is symmetric, and sinus term is antisymmetric between  $-\infty$  and  $\infty$  according to the point zero, we write the exponential function above only depending on the cosine term with limits from 0 to  $\infty$ . Therefore, if we set  $\frac{2C}{\sqrt{2\pi\hbar}} \rightarrow C'$ , then

$$\psi(x) = C' \int_0^{\infty} \cos\left(\frac{p^3}{6m\hbar V'(x_1)} + \frac{p(x - x_1)}{\hbar}\right) dp \quad (\text{A.10})$$

to see what this integral leads to, we should define variables

$$j = p \left( \frac{1}{2m\hbar V'(x_1)} \right)^{\frac{1}{3}} \quad (\text{A.11})$$

and

$$z = (x_1 - x) \left( \frac{2mV'(x_1)}{\hbar^2} \right)^{\frac{1}{3}} \quad (\text{A.12})$$

then, (A.10) becomes

$$\psi(x) = C'' \int_0^{\infty} \cos\left(\frac{j^3}{3} - jz\right) dj \quad (\text{A.13})$$

where  $C' \rightarrow C''$  due to emerging constants while  $dp \rightarrow (2m\hbar V'(x_1))^{1/3} dj$ . Notice that, Eq.(A.13) is nothing but the

$$\psi(x) = D \frac{1}{\pi} \int_0^{\infty} \cos\left(\frac{j^3}{3} - jz\right) dj \equiv D Ai(-z) \quad (\text{A.14})$$

where  $Ai(-z)$  is the airy function. Since  $z = 0$  at the turning points  $x_1 = x$ , we are not able to benefit from this result. Therefore, assuming  $\hbar^2/mV'(x_1) \ll 1$ , it makes  $z$  to become very large when move away from the turning points. By doing this, on find approximate wavefunctions  $\psi(x)$  representing the WKB approximation. Since  $z$  becomes very large, integral



in Eq.(A.13) starts to oscillate very rapidly. Hence, we need to find stationary behaviour of  $\frac{\partial}{\partial j}(\frac{j^3}{3} - jz) = 0$  that is hiding inside this cosine function which makes some constant contribution to the integral. Following this assumption, and using the integral representation of the airy function, we get

$$Ai(-z) = \begin{cases} \sqrt{\frac{\pi}{\sqrt{z}}} \cos(\frac{2z^{3/2}}{3} - \pi/4), & x < x_1, \text{ hence } z > 0 \\ \sqrt{\frac{\pi}{4\sqrt{-z}}} e^{-\frac{2}{3}(-z)^{3/2}}, & x > x_1, \text{ hence } z < 0 \end{cases} \quad (\text{A.15})$$

now, we have to arrange them in terms of  $q(x)$  and  $p(x)$  to make these to become most appropriate form for the WKB approach. We achieve this by

$$\int_{x_1}^x q(x') dx' = \int_{x_1}^x \sqrt{2m(V(x) - E)} dx' \quad (\text{A.16})$$

using (A.3)

$$\int_{x_1}^x q(x') dx' \approx \int_{x_1}^x \sqrt{2mV'(x_1)(x - x_1)} dx' \quad (\text{A.17})$$

this integration then results as

$$\int_{x_1}^x q(x') dx' \approx \frac{2}{3}(x - x_1)^{3/2} \sqrt{2mV'(x_1)} = \hbar \frac{2}{3}(-z)^{3/2} \quad (\text{A.18})$$

with the same way,

$$\int_{x_{1,2}}^x p(x') dx' \approx -\frac{2}{3}(x_1 - x)^{3/2} \sqrt{2mV'(x_1)} = -\hbar \frac{2}{3}z^{3/2} \quad (\text{A.19})$$

using these and

$$z^{1/2} = \frac{p(x)}{(2m\hbar V'(x_1))^{1/3}} \quad (\text{A.20})$$

$$(-z)^{1/2} = \frac{q(x)}{(2m\hbar V'(x_1))^{1/3}} \quad (\text{A.21})$$

then, what we get for this case of  $V'(x_1) > 0$  is

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' + \pi/4\right), & x < x_1 \\ \frac{1}{2\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_1}^x q(x') dx'}, & x > x_1 \end{cases} \quad (\text{A.22})$$

Now, for the case of  $V'(x_2) < 0$ , again following the same steps that we have already done above, we immediately get

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_2}^x p(x') dx' - \pi/4\right), & x > x_2 \\ \frac{1}{2\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_2}^x q(x') dx'}, & x < x_2 \end{cases} \quad (\text{A.23})$$

However, these  $\psi(x)$  solutions around the turning points  $x_1$  and  $x_2$  in terms of the approximated Airy function  $Ai(-z)$  cannot be enough alone for the case of tunneling. We will explain why this is so, but now, we have to understand what is necessary to get full solution. By looking at the equation in (A.5), if we continue that equation on the position representation, we get

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V'(x_t)(x - x_t)\psi(x) = 0 \quad (\text{A.24})$$

where  $x_t$  represents the turning points and using the definition of  $z$  in (A.12) while, we get

$$\frac{\partial^2 \psi(x)}{\partial z^2} + z\psi(x) = 0 \quad (\text{A.25})$$

and this is nothing but the differential form of the Airy functions. As you notice that, this is a second order differential equation, and we have focused on only one solution which is (A.14). The other solution is known as in the form

$$\psi(x) = \int_0^\infty \left( e^{-j^3/3 - zj} + \sin j^3/3 - jz \right) dj \equiv Bi(-z) \quad (\text{A.26})$$

Using this solution, and again following the same steps which we have done while dealing with  $Ai(-z)$  above, we would get for  $Bi(-z)$  in the case of  $V'(x_1) > 0$

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' - \pi/4\right), & x < x_1 \\ \frac{1}{\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_1}^x q(x') dx'}, & x > x_1 \end{cases} \quad (\text{A.27})$$

and for in the case of  $V'(x_2) < 0$ ,

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_2}^x p(x') dx' + \pi/4\right), & x > x_2 \\ \frac{1}{\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_2}^x q(x') dx'}, & x < x_2 \end{cases} \quad (\text{A.28})$$

since we are dealing with the tunneling case, barrier region remains finite, and therefore, resulting  $\psi(x)$  from using  $Bi(-z)$  cannot diverge as  $x \rightarrow \pm\infty$ . However, unlike the case of tunneling, if it is the case of boundary states, then one lets  $x \rightarrow \pm\infty$  which diverges the corresponding  $\psi(x)$ . This property of  $Bi(-z)$  in boundary state problem, forces one to set the coefficient corresponding this function to zero, then  $Bi(-z)$  vanishes. As a result, we conclude that, in the tunneling case, it is appropriate to use also  $Bi(-z)$ .

Now, we know that, solution for the wave-function  $\psi(x)$  is (A.1), and we have found that, to find these coefficients, solution must include a linear combination of the two independent solutions  $Ai(-z)$  and  $Bi(-z)$  for all regions: region I, region II, and region III. Therefore, for the case of  $V'(x_2) < 0$ ,

$$\psi(x) \approx K Ai(-z) + L Bi(-z) \quad (\text{A.29})$$

is the expected solution. For region III, and then taking the  $x > x_2$  solutions both from the  $Ai(-z)$  and  $Bi(-z)$ , we get

$$\psi(x) = \frac{K}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_2}^x p(x') dx' - \pi/4\right) + \frac{L}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_2}^x p(x') dx' + \pi/4\right) \quad (\text{A.30})$$

if we set  $L = iK$ , then combining this linear combination results as

$$\psi(x) \approx \frac{K}{\sqrt{p(x)}} e^{\frac{i}{\hbar} \int_{x_2}^x p(x') dx' - \pi/4} \quad (\text{A.31})$$

and we have to compare this solution above with the  $x \geq x_2$  case in (A.1), what we have found is that

$$T = K e^{-i\frac{\pi}{4}} \quad (\text{A.32})$$

For the region II, which we have to consider  $x < x_2$  in this case, and hence, again by looking at solutions both from  $Ai(-z)$  and  $Bi(-z)$ , we have

$$\psi(x) \approx \frac{K}{2\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_2}^x q(x') dx'} + \frac{L}{\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_2}^x q(x') dx'} \quad (\text{A.33})$$

again if we set  $L = iK$ , then result becomes

$$\psi(x) \approx K \left( \frac{1}{2\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_2}^x q(x') dx'} + \frac{i}{\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_2}^x q(x') dx'} \right) \quad (\text{A.34})$$

and when we compare this solution with  $x_1 \leq x \leq x_2$  in (A.1), then using (A.32), what we obtain is

$$C = \frac{K}{2} = \frac{T}{2} e^{i\frac{\pi}{4}} \quad (\text{A.35})$$

and

$$D = iK = iT e^{i\frac{\pi}{4}} \quad (\text{A.36})$$

we have done our analysis for the case of  $V'(x_2) < 0$ . Now, we should investigate the  $V'(x_1) > 0$  case, which solution of the form is expected now

$$\psi(x) \approx N Ai(-z) + M Bi(-z) \quad (\text{A.37})$$

then for the region II, we have to consider now  $x > x_1$  cases for both  $Ai(-z)$  and  $Bi(-z)$  which

$$\psi(x) \approx \frac{N}{2\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_1}^x q(x') dx'} + \frac{M}{\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_1}^x q(x') dx'} \quad (\text{A.38})$$

from here, to make this equation look similar to the solution above (A.34), we have to rearrange integrals, if we define

$$\Phi = \frac{1}{\hbar} \int_{x_1}^{x_2} q(x) dx \quad (\text{A.39})$$

and then if we separate integrals

$$\int_{x_1}^x q(x') dx' = \int_{x_1}^{x_2} q(x) dx + \int_{x_2}^x q(x') dx' = \hbar\Phi + \int_{x_2}^x q(x') dx' \quad (\text{A.40})$$

then using this property of integral in (A.38), we get

$$\psi(x) \approx \frac{N}{2\sqrt{q(x)}} e^{-\frac{1}{\hbar} (\hbar\Phi + \int_{x_2}^x q(x') dx')} + \frac{M}{\sqrt{q(x)}} e^{\frac{1}{\hbar} (\hbar\Phi + \int_{x_2}^x q(x') dx')} \quad (\text{A.41})$$

then one gets

$$\psi(x) \approx \frac{N e^{-\Phi}}{2\sqrt{q(x)}} e^{-\frac{1}{\hbar} \int_{x_2}^x q(x') dx'} + \frac{M e^{\Phi}}{\sqrt{q(x)}} e^{\frac{1}{\hbar} \int_{x_2}^x q(x') dx'} \quad (\text{A.42})$$

then, we have to compare this equation with the (A.34), and (A.1). Comparing with (A.34) is necessary because unlike the other cases which there exists one to one correspondence between region I, and region III in terms of Airy solutions and WKB solutions (A.1) as we see above, here, for the region II, we have to understand two different solutions must represent one unique solution in this region.  $V'(x_1) > 0$  where  $x > x_1$ , and  $V'(x_2) < 0$  where  $x < x_2$  cases are the solutions corresponding to same wave-function, therefore, according to this fact, since we have already set  $C$  in (A.1) corresponds to  $K$  which is the coefficient of  $Ai(-z)$  in (A.29), and set  $D$  in (A.1) corresponds to  $iK$  which is the coefficient of  $Bi(-z)$  in (A.29), we must compare  $C$  and  $D$  coefficients in (A.1) with the coefficients of  $Ai(-z)$  which is  $N$ , and coefficient of  $Bi(-z)$  which is  $M$  for this case now. This change of sign of

the integral in this case ( $V'(x_1) > 0$  where  $x > x_1$ ) according to the previous case ( $V'(x_2) < 0$  where  $x < x_2$ ) are already encoded in their related airy functions  $Ai(-z)$ , and  $Bi(-z)$ , and therefore, instead of determining coefficients by looking at their integral signs as we did for previous cases, we must compare these coefficients by looking at their corresponding airy functions. Then, this statement leads to a solution for the coefficients

$$\frac{Ne^{-\Phi}}{2} = C = \frac{K}{2} = \frac{T}{2}e^{i\frac{\pi}{4}} \quad (\text{A.43})$$

and

$$Me^{\Phi} = D = iK = iTe^{i\frac{\pi}{4}} \quad (\text{A.44})$$

which then leaving  $N$  and  $M$  alone gives

$$N = Te^{i\frac{\pi}{4} + \Phi} \quad (\text{A.45})$$

and

$$M = iTe^{i\frac{\pi}{4} - \Phi} \quad (\text{A.46})$$

we are now in the last part of this calculation. We have to consider region I, which we need to look at the solutions of both  $Ai(-z)$  and  $Bi(-z)$  for the case of  $x < x_1$ . Therefore, again using the expected solution (A.37),

$$\psi(x) \approx \frac{N}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' + \pi/4\right) + \frac{M}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' - \pi/4\right) \quad (\text{A.47})$$

writing these cosine functions in terms of their exponential equivalent form

$$\psi(x) \approx \frac{N}{\sqrt{p(x)}} \left( \frac{e^{i(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' + \pi/4)} + e^{-i(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' + \pi/4)}}{2} \right) + \frac{M}{\sqrt{p(x)}} \left( \frac{e^{i(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' - \pi/4)} + e^{-i(\frac{1}{\hbar} \int_{x_1}^x p(x') dx' - \pi/4)}}{2} \right) \quad (\text{A.48})$$

then if we rearrange above,

$$\psi(x) \approx \frac{1}{\sqrt{p(x)}} \left( \frac{Ne^{i\frac{\pi}{4}} + Me^{-i\frac{\pi}{4}}}{2} \right) e^{i \int_{x_1}^x p(x') dx'} + \frac{1}{\sqrt{p(x)}} \left( \frac{Ne^{-i\frac{\pi}{4}} + Me^{i\frac{\pi}{4}}}{2} \right) e^{-i \int_{x_1}^x p(x') dx'} \quad (\text{A.49})$$

comparing this result with the  $x \leq x_1$  case in (A.1), what we get for the coefficient  $A$  is

$$A = \frac{Ne^{i\frac{\pi}{4}} + Me^{-i\frac{\pi}{4}}}{2} \quad (\text{A.50})$$

then putting (A.45) and (A.46), result becomes

$$A = \frac{Te^{i\frac{\pi}{4} + \Phi} e^{i\frac{\pi}{4}} + iTe^{i\frac{\pi}{4} - \Phi} e^{-i\frac{\pi}{4}}}{2} = \frac{Te^{i\frac{\pi}{2} + \Phi} + iTe^{-\Phi}}{2} \quad (\text{A.51})$$

and if we write  $e^{i\frac{\pi}{2}} = i$ , then

$$A = \frac{iTe^{\Phi} + iTe^{-\Phi}}{2} = iT \left( \frac{e^{\Phi} + e^{-\Phi}}{2} \right) = iT \cosh \Phi \quad (\text{A.52})$$

using the definition of transmission coefficient, which is

$$T_{trans} = \frac{|T|^2}{|A|^2} = \frac{|T|^2}{(iT \cosh \Phi)(-iT \cosh \Phi)} = \frac{1}{\cosh^2 \Phi} \quad (\text{A.53})$$

## APPENDIX B

### EXPERIMENTAL SET-UP IN TERMS OF ATOMIC UNITS

#### B.1. Hamiltonian Representation

First we have to write the standard representation of the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_e}\hat{\nabla}^2 - \frac{Ze^2}{4\pi\epsilon_0 x} - |e|Ex \quad (\text{B.1})$$

where  $m_e$  is the mass of the electron,  $\hat{\nabla}$  is the gradient operator,  $\epsilon_0$  is the vacuum permittivity,  $E$  is the applied electric field, and  $e$  is charge of the electron. From here, if we make a substitution to express above with dimensionless parameters such as

$$\xi = \frac{x}{a_0} \equiv \text{dimensionless} \quad (\text{B.2})$$

$$\mathcal{E} = \frac{E}{|e|/(4\pi\epsilon_0 a_0^2)} \equiv \text{dimensionless} \quad (\text{B.3})$$

where  $a_0$  is the Bohr radius. If we rewrite the Hamiltonian again in terms of these dimensionless parameters

$$\hat{H} = -\frac{\hbar^2}{2m_e a_0^2}\hat{\nabla}_\xi^2 - \frac{e^2 Z}{4\pi\epsilon_0 a_0 \xi} - |e|a_0 \frac{|e|}{4\pi\epsilon_0 a_0^2} \left( \frac{E}{|e|/(4\pi\epsilon_0 a_0^2)} \right) \xi \quad (\text{B.4})$$

which is

$$\hat{H} = -\frac{\hbar^2}{2m_e a_0^2}\hat{\nabla}_\xi^2 - \frac{e^2 Z}{4\pi\epsilon_0 a_0} \left( \frac{Z}{\xi} + \mathcal{E}\xi \right) \quad (\text{B.5})$$



now, to take all expression into one parenthesis, we have to do some algebra on  $\frac{\hbar^2}{2m_e a_0^2}$  term above

$$\frac{e^2}{4\pi\epsilon_0} \times \left( \frac{1}{\frac{e^2}{4\pi\epsilon_0}} \times \frac{\hbar^2}{2m_e a_0^2} \right) = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \times \frac{e^2}{(4\pi\epsilon_0) 2a_0^2} \quad (\text{B.6})$$

since first term of the result above is Bohr radius  $a_0$ , we immediately get

$$\frac{\hbar^2}{2m_e a_0^2} = \frac{e^2}{2(4\pi\epsilon_0 a_0)} \quad (\text{B.7})$$

therefore, if we put above into the Hamiltonian (B.5), we get

$$\hat{H} = \frac{e^2}{4\pi\epsilon_0 a_0} \left( -\frac{1}{2} \hat{\nabla}_\xi^2 - \left( \frac{Z}{\xi} + \mathcal{E}\xi \right) \right) \quad (\text{B.8})$$

here,  $\frac{e^2}{4\pi\epsilon_0 a_0}$  is the Hartree energy, and it is  $4.36 \times 10^{-18} J$  or  $27.211 eV$ . This Hartree energy is considered as  $1 a.u.$ . Therefore, we have just found the atomic unit representation of the Hamiltonian, which is

$$\hat{H} = -\frac{1}{2} \hat{\nabla}_\xi^2 - \left( \frac{Z}{\xi} + \mathcal{E}\xi \right) \quad (\text{B.9})$$

## B.2. Turning Points

To calculate turning points which make momentum to vanish  $\hat{p} = 0$ , first

$$\hat{H}\psi = -E_I \psi \quad (\text{B.10})$$

where  $E_I$  is the ionization energy of the He atom. However, we have to make  $E_I$  dimensionless, using the Hamiltonian (B.8),

$$\hat{H} = \frac{e^2}{4\pi\epsilon_0 a_0} \left( -\frac{1}{2} \hat{\nabla}_\xi^2 - \left( \frac{Z}{\xi} + \mathcal{E}\xi \right) \right) \psi = \frac{e^2}{4\pi\epsilon_0 a_0} \left( -\frac{E_I}{\frac{e^2}{4\pi\epsilon_0 a_0}} \right) \psi \quad (\text{B.11})$$

dividing and multiplying  $E_I$  with  $\frac{e^2}{4\pi\epsilon_0 a_0}$  gives us dimensionless  $\hat{E}_I$  which

$$\hat{E}_I = \frac{E_I}{\frac{e^2}{4\pi\epsilon_0 a_0}} \quad (\text{B.12})$$

and since first ionization energy of the He is in SI units  $E_{I_{SI}} = 24.59\text{eV}$ , we immediately get  $\hat{E}_I = 0.8941$  in terms of Hartree energy. From here, using the equality in (B.11),

$$\frac{\hat{p}^2}{2} - \left(\frac{Z}{\xi} + \mathcal{E}\xi\right) = -\hat{E}_I \quad (\text{B.13})$$

then what we get for the momentum in terms of atomic units is

$$\hat{p} = \sqrt{2 \left| \frac{\hat{p}^2}{2} - \left(\frac{Z}{\xi} + \mathcal{E}\xi - \hat{E}_I\right) \right|} \quad (\text{B.14})$$

hence, one finds turning points as

$$\frac{Z}{\xi} + \mathcal{E}\xi - \hat{E}_I = 0 \quad (\text{B.15})$$

if we multiply this equation with  $\xi$  and then solve this second order polynomial, we get turning points as

$$\xi_{L,R} = \frac{\hat{E}_I \pm \sqrt{\hat{E}_I^2 - 4\mathcal{E}Z}}{2\mathcal{E}} \quad (\text{B.16})$$

where  $Z = 2$  for He atom.

### B.3. Laser Intensity

Laser intensity is

$$\text{Laser Intensity} = L_I = \frac{1}{2}\epsilon_0 c E^2 \quad (\text{B.17})$$

where  $c$  is the speed of light. Using the dimensionless form of the applied electric field in (B.3), then we get

$$L_I = \frac{1}{2} \epsilon_0 c \left( \frac{e}{4\pi\epsilon_0 a_0^2} \right)^2 \mathcal{E}^2 \quad (\text{B.18})$$

if we divide and multiply the  $e$  term in parenthesis with  $4\pi\epsilon_0\hbar c$ ,

$$L_I = \frac{1}{2} \epsilon_0 c \left( \frac{\frac{e^2}{4\pi\epsilon_0\hbar c} 4\pi\epsilon_0\hbar c}{(4\pi\epsilon_0 a_0^2)^2} \right) \mathcal{E}^2 \quad (\text{B.19})$$

then, using the definition of fine structure constant  $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$ , we get

$$L_I = \frac{1}{2} \alpha \frac{1}{4\pi} \frac{\hbar c^2}{a_0^4} \quad (\text{B.20})$$

if we put their numerical values, what we get for the laser intensity in atomic units 1 a.u. is

$$L_I = 3.5152 \times 10^{20} \text{W/m}^2 \cdot \mathcal{E}^2 = 3.5152 \times 10^{16} \text{W/cm}^2 \cdot \mathcal{E}^2 \quad (\text{B.21})$$

we know that, in this experiment, laser intensity range is given as

$$L_{I_{exp}} = (0.73 - 7.5) \times 10^{14} \text{W/cm}^2 \quad (\text{B.22})$$

therefore, in terms of atomic units, this interval must give

$$(0.73 - 7.5) \times 10^{14} \text{W/cm}^2 = 3.5152 \times 10^{16} \text{W/cm}^2 \cdot \mathcal{E}^2 \quad (\text{B.23})$$

as a result, peak electric field interval is found in terms of atomic units as

$$\mathcal{E} = (0.0456 - 0.1461) \text{a.u.} \quad (\text{B.24})$$