Tunneling Times

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ABSTRACT

The tunneling time problem was a very popular problem at the end of the 20th century. In Quantum Mechanics only observables can be measured, i.e. these observables are real quantities. From mathematics it is well known that only hermitian operators have real eigenvalues, therefore we associate observables as eigenvalues of Hermitian operators. Until now no Hermitian operator for the time was not found. Therefore many approaches in order to determine the time a particle spends in a region or needs to travel across a region are developed. Based on this the Bohmian Dwell Time, the Büttiker Landauer Time, the Larmor Clock, and the minimal tunneling time are presented and discussed in this thesis.

Keywords: Quantum Mechanics, Traversal Time, Tunneling Time, Larmor Clock, Dwell Time

Öz

Tünelleme zamanı problemi yirminci yüzyılın sonunda çok popüler araştırma alanıydı. Kuantum mekanikte sadece görünebilirler ölçülebilir, yani bu görünebilirler reel bir değerdir. Matematikten bilinir ki Hermityan opertörlerin özdeğerleri reel sayıdır, ve bundan dolayı görünebilirleri Hermityan operatörlerin özdeğerleri ile ilişkilendirilir. Şimdiye kadar kuantum fiziksel zaman kavramı için Hermityan operatör bulununamadı. Dolayısı ile kuantum mekanite zaman kavramını, yani bir parçacığın bir bölgede geçirdiği veya bir bölgeyi geçmek için harcadığı zamanı, tanımlamak amacı ile farklı yaklaşımlar geliştirildi. Buna bağlı olarak Bohm kalma zamanı, Büttiker Landauer zamanı, Larmor saatı, ve minimal tünelleme zamanı yaklaşımları bu tezde veriliyor ve tartışılıyor.

Anahtar Kelimeler: Kuantum Mekanik, Geçme Zamanı, Tünelleme Zamanı, Larmor Saati, Kalma Süreci

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INTRODUCTION

In Quantum Mechanics the time plays a mystic role. This can be easily seen when the interested reader follows the discussion on superluminal tunneling experiments carried out by Günter Nimtz [14] in Germany or by Raymond Chiao [8] at Berkley. As we know from the standard quantum mechanics lecture all observables are the eigenvalues of Hermitian operators. If time is an observable, then there must be a Hermitian time operator. Unfortunately until now there is no hermitian time operator. Therefore physicists tried to invent different approaches to the tunneling time problem. Starting from a semiclassical approaches to variational approaches. As the hot discussions on the superluminal tunneling shows that the community of physicists still is very sensitive to the time problem in quantum mechanics.

Many different approaches for the definition of the tunneling time or traversal time respectively have been given. A review of various tunneling times was given by Hauge [10]. One of the first fruitful approaches to the time problem was given by Baz' and Rybachenko [2, 15] by proposing the Lamor clock as a measure of traversal time. This method is reviewed in chapter 4. Büttiker defined first the Dwell time, which can be seen as a semiclassical approach. Leavens developed the idea of the Dwell time using Bohmian trajectories as shown in chapter 2.1. The Dwell times for rectangular barrier as well as for two δ-spike potentials is calculated. In chapter 3 the Büttiker Landauer time is presented. The tunneling time is calculated for a constant localized barrier with a small time varying periodic perturbation. Finally the concept of the minimal tunneling time is put forward. The minimal tunneling time is based on a variational principle approach [4]. Exemplarily the minimal tunneling time for the symmetric constant barrier is calculated and compared to the corresponding Dwell time calculated in chapter 2.2.2. Furthermore the minimal tunneling time is used to determine the level splitting in the symmetric quadratic double well potential.

Chapter 2

DWELL TIME

2.1 Bohmian Dwell Time

Following C. Richard Leavens Bohmian trajectory approach to timing electrons in [13], we will now develop the idea of the Bohmian Dwell time.

Lets consider the one dimensional stationary quantum motion. We consider a continuous double degenerate spectrum of eigenstates $\psi_E(x)$ of the stationary Schrödinger equation.

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right)\psi_E(x) = E\psi_E(x) \tag{2.1}$$

With the solution of the Schrödinger equation (2.1) we can determine the probability current in one dimension $j(x)$, as following:

$$j(x) = \frac{\hbar}{m}\mathrm{Im}\left(\psi_E(x)^*\frac{\partial}{\partial x}\psi_E(x)\right) \tag{2.2}$$

As we are interested in determining the time of a quantum particle spent in the interval $a < x < b$ we may come up with the following definition of the traversal time:

$$\tau_D = \frac{1}{|j(\psi_E(x)|}\int_a^b |\psi_E(x)|^2 dx \tag{2.3}$$

Where does this come from? In the Bohmian ontological interpretation of quantum theory, the characteristic times for quantum particles will be discussed in terms of real trajectories, rather than virtual paths like in the Feynman's path integral formalism [9]. Let's consider a single quantum point-like particle propagating in the potential $V(x,t)$ accompanied by the wave function $\psi_E(x,t)$, examining the potential at each point in space-time and guides the particle's motion accordingly, such that the particle has a deterministically well defined position $x(t)$ and velocity $v(t)$ at each instant of time t. Bohm postulates in [3] that the particles equation of motion is given as:

$$v(t) = dx(t)/dt, \quad \text{and} \quad \rho(x,t)v(x,t) = j(x,t) \tag{2.4}$$

where

$$\rho(x,t) = \psi_E(x,t)^* \psi_E(x,t)$$

is the single particle probability density and

$$j(x,t) = \frac{\hbar}{m} \mathrm{Im} \left(\psi_E^*(x,t) \frac{\partial}{\partial x} \psi_E(x,t) \right)$$

denotes the probability current density. Here we have to note that the velocity $v(x,t)$ can never exceed the vacuum speed of light c.

In analogy to classical statical mechanics we have to to define first the probability distribution for a particle property f, which is defined for all trajectories as following:

$$\Pi(f) = \int_{\text{all spaces}} \rho(x^{(0)},0)\delta(f - f(x^{(0)})dx^{(0)} \tag{2.5}$$

where $f(x^{(0)})$ is the value of the property of a particle following the trajectory $x(x^{(0)},t)$ and $x^{(0)}$ denotes the initial position of the particle.

We now consider the complete set of trajectories that start at $x^{(0)}$ for the trajectory $x(x^{(0)},t)$ and reaches the final destination X at least once at the time $t > 0$. As in the Bohmian trajectory theory the trajectories do not cross or touch each other, this set must consist of a continuous interval $[x_a^{(0)}, x_b^{(0)}]$. Because of the nonintersection property of the trajectories there is only one $x^{(0)}$ in the interval $[x_a^{(0)}, x_b^{(0)}]$ for which the trajectory $x(x^{(0)},t)$ reaches the final point X at a particular time T. So if we want to calculate the arrival time distribution we get

$$\Pi(T) = \int_{x_a^{(0)}}^{x_b^{(0)}} \rho(x^{(0)}, 0)\delta(T - T(x^{(0)}))dx^{(0)}. \tag{2.6}$$

As one can see easily $T(x^{(0)})$ depends on the starting position $x^{(0)}$. The relation between $\delta(T - T(x^{(0)})$ and $\delta(x(x^{(0)}, t) - X)$ is given by:

$$\delta(x(x^{(0)}, t) - X)\Big|_{t=T} = \frac{\delta(t - T(x^{(0)}))}{|dx(x^{(0)}, t)/dt|}\Bigg|_{t=T} = \frac{\delta(t - T(x^{(0)}))}{|v(x(x^{(0)}, t), t)|}\Bigg|_{t=T} = \frac{\delta(T - T(x^{(0)}))}{|v(X, T)|} \tag{2.7}$$

Inserting now (2.7) into (2.6) the probability distribution for the arrival time yields to:

$$\Pi(T; X) = |v(X, T)| \int_{x_a^{(0)}}^{x_b^{(0)}} \rho(x^{(0)}, 0)\delta(x(x^{(0)}, T) - X)dx^{(0)} \tag{2.8}$$

This integral is just the probability density $\rho(X, T)$. So (2.8) reduces to:

$$\Pi(T; X) = |v(X, T)|\rho(X, T) = |j(X, T)| \tag{2.9}$$

Normalizing this probability distribution gives:

$$\Pi(T; X) = \frac{|j(X, T)|}{\int_0^\infty |j(X, t)|dt} \tag{2.10}$$

(2.10) is the probability distribution of all arrival times for all particles reaching X at any time $t > 0$. $\Pi(T; X)$ is not defined in the case if the integral in the denominator becomes 0. This actually is the case if no particle arrives X at a time $t > 0$. Also it is not defined is the numerator becomes infinite, i.e. if there is a periodic motion of particles described by the set of trajectories passing forever periodically $x = X$.

If the particle arrives at $x = X$ at the time $t = T$ from the left the velocity field $v(X, T) > 0$ is positive, and therefore according to (2.4) the probability current density

$j(X,T) > 0$ is also positive. We will denote this case with $(+)$. In the case where the particle arrives from the left obviously the velocity field $v(X,T) < 0$ is negative and analogously according to (2.4) $j(X,T) < 0$ is also negative. This case is denoted by $(-)$. So finally we will write (2.10) as following:

$$\Pi(T;X) = \Pi_+(T;X) + \Pi_+(T;X) \tag{2.11}$$

with

$$\Pi_\pm(T;X) = \pm \frac{j_\pm(X,T)}{\int_0^\infty (j_+(X,t) - j_-(X,t))\, dt} \tag{2.12}$$

where

$$j_\pm(x,t) = j(x,t)\Theta(\pm j(x,t)). \tag{2.13}$$

From (2.4) it is obvious that $\Pi_\pm(T;X) \geq 0$ for all X and T.

2.1.1 Transmission and reflection times

For the discussion of the transmission and reflection times we have to set up a gedanken experiment in order to model the system mathematically. We consider the one dimensional scattering experiment of a particle coming from the left of the localized barrier $V(x,t) = \Theta(x(x-d))V(x,t)$. In the following we will only consider positive valued potentials. If we assume that the wave function $\psi_E(x,t)$ is normalized and located far to the left at the time $t = 0$. If we now integrate the probability density $\rho(x,0)$ from zero to infinity:

$$P_0 = \int_0^\infty \rho(x,0)dx$$

and compare this with the transmission probability P_T

$$P_T = \int_d^\infty \rho(x,t_\infty)dx, \tag{2.14}$$

where t_∞ denotes the time when the scattering process is completed, we see that the relation between P_0 and P_T is given as

$$P_T \gg P_0.$$

This relation is important, in order not to get any significant contribution to the transmission probability from the wave function at the starting point. As already denoted above the Hermitian time operator operator has not been found yet and therefore time can not be considered as an observable. Now we are extending our experimental set up to carry out many experiments with the same setup and the same intrinsic wave functions $\psi_E(x,0)$, and average the corresponding reflection and transmission times.

In the following we are going to consider many identically setup experiments of the type described above and determine the average transmission and reflection times correspondingly. We will denote this times as $\tau_T(a,b)$ and $\tau_R(a,b)$ respectively, indicating the average time the particle is spending in the region $a \leq x \leq b$ after the time $t = 0$. These particles are either transmitted or reflected. Recalling that the barrier $V(x,t)$ is not vanishing in the region $[0,d]$, the average transmission time $\tau_T(0,d)$ is obviously identified as the so-called tunneling time.

In order to determine the average transmission and reflection times for a point-like particle, with the initial position $x = x^{(0)}$ at the time $t = 0$, the particle spends in the region $[a,b]$ we can use the classical stopwatch expression:

$$t(a,b,x^{(0)}) = \int_0^\infty \int_a^b \delta\big(x - x(x^{(0)},t)\big)\,dx\,dt \tag{2.15}$$

The mathematical modeling of a classical stopwatch is very straightforward. As we are considering a point-like particle the probability density of this particle is trivially given as $\delta\big(x - x(x^{(0)},t)\big)$. Integrating this probability density over the interval $[a,b]$ gives us the time dependent probability. After integrating the time from zero to infinity we get the time that the particle started at the point $x^{(0)}$ at the time $t = 0$ spend in average in the interval $[a,b]$.

By averaging (2.15) over all starting points we get the so-called mean dwell-time:

$$\tau_D(a,b) = \int_{-\infty}^{\infty} t(a,b,x^{(0)})\rho(x^{(0)},0)\,dx^{(0)} \tag{2.16}$$

As all these integrals are considered to be Lebesgue integrable and the order of integration can be changed according the theorem of Fubini. Therefore we get for mean dwell-time

$$\tau_D(a,b) = \int_0^\infty \int_a^b \underbrace{\int_{-\infty}^\infty \rho(x^{(0)},0)\delta\big(x - x(x^{(0)},t)\big)\,dx^{(0)}}_{\rho(x,t)}\,dx\,dt. \tag{2.17}$$

The integral

$$\int_{-\infty}^\infty \rho(x^{(0)},0)\delta\big(x - x(x^{(0)},t)\big)\,dx^{(0)} = \rho(x,t)$$

is the distribution of particles $\rho(x,t)$ at the time t. So the dwell-time simplifies to:

$$\tau_D(a,b) = \int_0^\infty \int_a^b \rho(x,t)\,dx\,dt. \tag{2.18}$$

In order to write $\tau_D(a,b)$ also in terms of the probability current density we are going to use the equation of continuity

$$\partial_t \rho(x,t) + \partial_x j(x,t) = 0. \tag{2.19}$$

If we multiply the equation of continuity (2.19) by t and integrate the equation of continuity over the time from zero to infinity and the location from a to b we get:

$$\begin{aligned} \int_a^b \int_0^\infty t\partial_t \rho(x,t)\,dt\,dx &= -\int_a^b \int_0^\infty t\partial_x j(x,t)\,dt\,dx \\ \int_a^b \left[t\rho(x,t)\Big|_0^\infty - \int_0^\infty \rho(x,t)\,dt \right] dx &= -\int_0^\infty t \int_a^b \partial_x j(x,t)\,dx\,dt \end{aligned} \tag{2.20}$$

The expression

$$t\rho(x,t)\Big|_0^\infty = 0$$

becomes zero because at the time $t = 0$ the probability density is finite, at the time $t = \infty$ the probability density becomes zero at every point of the interval $[a,b]$, because the probability of the particle at the time $t = \infty$, i.e. at a time after the scattering process is completed, to be in the scattering region is also zero. Applying the fundamental theorem of calculus on the right hand side of the equation (2.20) we get:

$$
\begin{aligned}
-\int_a^b \int_0^\infty \rho(x,t)\, dt\, dx &= -\int_0^\infty t\left(j(b,t) - j(a,t)\right)\, dt \\
\int_0^\infty \int_a^b \rho(x,t)\, dx\, dt &= \int_0^\infty t\left(j(b,t) - j(a,t)\right)\, dt \qquad (2.21)
\end{aligned}
$$

Inserting now (2.21) into (2.18) we get for the dwell time:

$$
\tau_D(a,b) = \int_0^\infty t\left(j(b,t) - j(a,t)\right)\, dt \qquad (2.22)
$$

Up to now we have not differentiated between transmitted and reflected particles. As we are dealing here with Bohmian trajectories, we want to recall that the trajectories do not cross each other. So there is a trajectory $x_B(t) = x(x_B^{(0)}, t)$ that divides the trajectories into trajectories associated with transmitted particles ($x^{(0)} > x_B^{(0)}$) and trajectories associated with reflected particles ($x^{(0)} < x_B^{(0)}$) . In the following we will use $x_B^(t)$ to separate the contributions of the transmitted and reflected particles.

The probability for a transmitted particle is then:

$$
P_T = \int_{x_b(t)}^\infty \rho(x,t) \qquad (2.23)
$$

with

$$
\rho(x,t) = \rho_T(x,t) + \rho_R(x,t)
$$

and

$$
\begin{aligned}
\rho_T(x,t) &= \rho(x,t)\Theta(x - x_B(t)) \qquad (2.24) \\
\rho_R(x,t) &= \rho(x,t)\Theta(x_B(t) - x). \qquad (2.25)
\end{aligned}
$$

Inserting this into equation (2.18) we get:

$$
\tau_D(a,b) = P_T\tau_T(a,b) + P_R\tau_R(a,b) \qquad (2.26)
$$

with

$$P_T\tau_T(a,b) = \int_0^\infty \int_a^b \rho(x,t)\Theta(x - x_B(t))\,dx\,dt =$$
$$= \int_0^\infty t\left(j(b,t)\Theta(b - x_B(t)) - j(a,t)\Theta(a - x_B(t))\right)\,dt \quad (2.27)$$

and

$$P_R\tau_R(a,b) = \int_0^\infty \int_a^b \rho(x,t)\Theta(x_B(t) - x)\,dx\,dt =$$
$$= \int_0^\infty t\left(j(b,t)\Theta(x_B(t) - b) - j(a,t)\Theta(x_B(t) - a)\right)\,dt \quad (2.28)$$

The dwell, transmission, and reflection times are all positive, real valued, and additive, i.e.

$$\tau_D(a,c) = \tau_D(a,b) + \tau_D(b,c), \quad \text{with } a < b < c. \quad (2.29)$$

Analogously this expression is also true for τ_T and τ_R.

Because the reflection and transmission times $\tau_T(a,b)$ and $\tau_R(a,b)$ depend explicitly on the boundary trajectory $x_B(t)$, the integrands are not anymore bilinear in $\psi_E(x,t)$ as in (2.18), and are rather implicit functionals of $\psi_E(x,t)$ themselves. Therefore if we consider the transmission and reflection times for wave packets, we can not determine them as easily as using a Fourier transform. So there is no simple relationship between the $\tau_T(a,b)$ and $\tau_R(a,b)$ respectively and its stationary counterparts $\tau_T(a,b;k)$ and $\tau_R(a,b;k)$ respectively. So the general properties of the transmission and reflection times can not be transferred to the stationary case.

The stationary case will be elucidated in the next section where the Dwell time will be discussed in the framework of Büttikers [5]idea.

2.2 Dwell Time

If we consider now the scattering process in the stationary case where a particle will be described by the wave function

$$\psi(x,t) = \psi_k(x)e^{-iEt/\hbar}$$

and with $E = \hbar^2 k^2/2m$.

$$\tau_D(x_1, x_2; k) = \frac{1}{v(k)} \int_{x_1}^{x_2} |\psi(x;k)|^2 \, dx \tag{2.30}$$

where $v(k)$ is the incoming flux (which is in parallel to Smith's idea). So the dwell time can be seen as the ratio of the probability of a particle being found in the region between x_1 and x_2 over the incoming flux.

Analogously to of the straight forward approaches to the tunneling time problem was given by Smith in [16], where he introduced the lifetime for a one dimensional elastic collision, which is resembles the basic idea of Büttiker's definition of the dwell time τ_D [5].

2.2.1 Dwell Time for a localized barrier

If we consider the simple example of a one dimensional barrier $V(x)$ that is localized on the interval (b, a):

$$V(x) = \begin{cases} V(x) & \text{if } b \leq x \leq a \\ \\ 0 & \text{else} \end{cases} \tag{2.31}$$

The solution of the time independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x;k) = E\psi(x;k) \tag{2.32}$$

of the localized potential $V(x)$ as given in (2.31) is then:

$$\psi(x;k) = \begin{cases} e^{ikx} + \sqrt{R}e^{i\beta}e^{-ikx} & x < b \\ \chi(x;k) & b < x < a \\ \sqrt{T}e^{i\alpha}e^{ikx} & x > a \end{cases} \tag{2.33}$$

This situation is illustrated graphically in the figure 2.1 below.

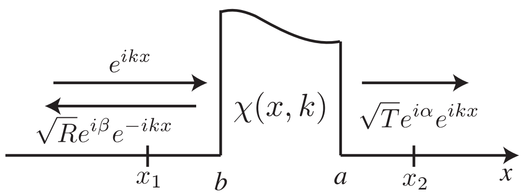

Figure 2.1: One dimensional potential barrier

Returning to Büttikers definition of the dwell time (2.30) we can see that in this definition there is no distinction between the reflected and transmitted components. Therefore it is obvious that this definition of the tunneling time averages over all scattering channels as already noted by Smith [16].

2.2.2 Dwell Time for the localized constant potential

Now let us calculate the dwell time for the potential barrier

$$V(x) = V_0 \Theta(x(d-x)) = \begin{cases} V_0 & \text{if } 0 < x < d \\ 0 & \text{else} \end{cases} \tag{2.34}$$

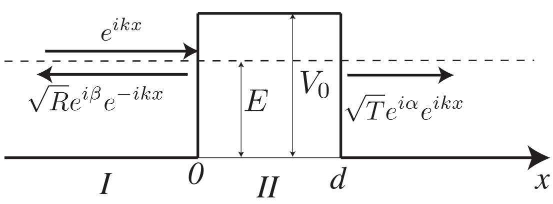

Figure 2.2: One dimensional rectangular potential barrier

The Solution of the Schrödinger equation in the regions I, II, III are given as following:

$$\psi_I(x;k) = e^{ikx} + Re^{-ikx} \tag{2.35}$$

$$\psi_{II}(x;\kappa) = Ae^{\kappa x} + Be^{-\kappa x} \tag{2.36}$$

$$\psi_{III}(x;k) = Te^{ikx} \tag{2.37}$$

where $k = \sqrt{2mE/\hbar^2}$ and $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$.

The wave function $\psi(x)$ has to be continuous and continuous differentiable at all points, therefore the wave function has to be continuous differentiable especially at the $x = 0$ and $x = d$. Therefore we have to fulfill the following continuity relations:

$$\psi_I(0;k) = \psi_{II}(0;\kappa) \tag{2.38}$$

$$\psi_{II}(d;\kappa) = \psi_{III}(d;k) \tag{2.39}$$

$$\psi'_I(0;k) = \psi'_{II}(0;\kappa) \tag{2.40}$$

$$\psi'_{II}(d;\kappa) = \psi'_{III}(d;k) \tag{2.41}$$

Using (2.35), (2.36), (2.37) results:

$$1 + R = B \tag{2.42}$$

$$Ae^{\kappa d} + Be^{\kappa d} = Te^{ikd} \tag{2.43}$$

$$ik(1 - R) = A\kappa \tag{2.44}$$

$$(A\kappa e^{\kappa d} - B\kappa e^{-\kappa d}) = ikTe^{ikd} \tag{2.45}$$

Solving (2.42)-(2.45) with respect to A, B, R, T gives:

$$T = \frac{4ik\kappa e^{d(\kappa - ik)}}{e^{2d\kappa}(k + i\kappa)^2 - (k - i\kappa)^2} \tag{2.46}$$

$$R = \frac{(k^2 + \kappa^2)\sinh(d\kappa)}{(k - \kappa)(k + \kappa)\sinh(d\kappa) + 2ik\kappa\cosh(d\kappa)} \tag{2.47}$$

$$A = -\frac{2k(k - i\kappa)}{e^{2d\kappa}(k + i\kappa)^2 - (k - i\kappa)^2} \tag{2.48}$$

$$B = \frac{ke^{d\kappa}(k + i\kappa)}{(k - \kappa)(k + \kappa)\sinh(d\kappa) + 2ik\kappa\cosh(d\kappa)} \tag{2.49}$$

Simplifying these equations for $\kappa d \gg 1$ we get:

$$T = \frac{4k\kappa}{k^2 + \kappa^2} e^{-(ik+\kappa)d} \exp\left\{\arctan\frac{k^2 - \kappa^2}{2k\kappa}\right\} \tag{2.50}$$

$$R = \exp\left\{-2i\arctan\frac{\kappa}{k}\right\} \tag{2.51}$$

$$A = -\frac{2k(k - i\kappa)}{e^{2d\kappa}(k + i\kappa)^2 - (k - i\kappa)^2} \tag{2.52}$$

$$B = \frac{k}{\sqrt{k^2 + \kappa^2}} \exp\left\{i\arctan\frac{\kappa}{k}\right\} \tag{2.53}$$

For

$$\psi_{II} = A\sinh\kappa x + B\cosh\kappa x$$

we can now calculate the Dwell time for the rectangular barrier as following. First we have to determine the absolute square of the wave function $\psi_{II}(x)$.

$$\begin{aligned} |\psi_{II}(x)|^2 &= (A^\star \sinh \kappa x + B^\star \cosh \kappa x)(A \sinh \kappa x + B \cosh \kappa x) \\ &= |A|^2 \sinh^2 \kappa x + (A^\star B + A B^\star) \sinh \kappa x \cosh \kappa x + |B|^2 \cosh^2 \kappa x \end{aligned}$$

For the Dwell time we have to calculate now the integral $\int_0^d |\psi_{II}(x)|^2\, dx$:

$$\int_0^d |\psi_{II}(x)|^2\, dx = |A|^2 \int_0^d \sinh^2 \kappa x\, dx + |B|^2 \int_0^d \cosh^2 \kappa x\, dx +$$

$$+ (AB^\star + B^\star A) \int_0^d \sinh \kappa x \cosh \kappa x\, dx =$$

$$= |A|^2 \frac{-\kappa d + \cosh(\kappa d)}{2\kappa} + |B|^2 \frac{\kappa d + \cosh \kappa d \sin \kappa d}{2\kappa} + (AB^\star + B^\star A) \frac{\sinh^2(\kappa d)}{2\kappa} \tag{2.54}$$

Inserting now the coefficients A and B from (2.48) and (2.49) into (2.54) gives:

$$\begin{aligned} \tau_D &= \frac{2}{v} \frac{k^2 \left[2\kappa d\,(\kappa^2 - k^2) + k_0^2 \sinh(2\kappa d)\right]}{q\left[k_0^4 \cosh(2\kappa d) - (-k^2 - 2\kappa k + q^2)(-k^2 + 2\kappa k + \kappa^2)\right]} \\ &= \frac{2}{v} \frac{k^2}{\kappa} \frac{2\kappa d\,(\kappa^2 - k^2) + k_0^2 \sinh(2\kappa d)}{k_0^4 \cosh(2\kappa d) - k_0^4 + 8\kappa^2 k^2} \end{aligned}$$

After simplification we get:

$$\tau_D = \frac{k^2}{vq} \frac{2\kappa d\,(\kappa^2 - k^2) + k_0^2 \sinh(2\kappa d)}{k_0^4 \sinh^2(2\kappa d) + 4\kappa^2 k^2} \tag{2.55}$$

With the flux

$$v = j_{in} = \frac{\hbar k}{m}$$

we can now calculate the Dwell time for the rectangular barrier for $0 < E < V_0$ by inserting v into (2.55) and get finally:

$$\tau_D = \frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 - k^2\right) + k_0^2 \sinh\left(2\kappa d\right)}{k_0^4 \sinh^2\left(2\kappa d\right) + 4\kappa^2 k^2} \tag{2.56}$$

Now we need to calculate the Dwell time for the case $E > V_0$. We can directly get the result from (2.56) by substituting κ by $i\kappa$ and exploiting the identity

$$\sinh(ix) = i\sin x$$

we get for th Dwell time for $E > V_0$:

$$\begin{aligned}
\tau_D &= \frac{mk}{\hbar i\kappa}\frac{2i\kappa d\left(-\kappa^2 - k^2\right) + k_0^2 \sinh\left(2i\kappa d\right)}{k_0^4 \sinh^2\left(2i\kappa d\right) - 4\kappa^2 k^2} \\
&= \frac{mk}{\hbar i\kappa}\frac{2i\kappa d\left(-\kappa^2 - k^2\right) + k_0^2 i \sin\left(2\kappa d\right)}{-k_0^4 \sin^2\left(2\kappa d\right) - 4\kappa^2 k^2} \\
&= \frac{mk}{\hbar i\kappa}\frac{(-i)\left(2\kappa d\left(\kappa^2 + k^2\right) - k_0^2 \sin\left(2\kappa d\right)\right)}{-\left(k_0^4 \sin^2\left(2\kappa d\right) + 4\kappa^2 k^2\right)} \\
&= \frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 + k^2\right) - k_0^2 \sin\left(2\kappa d\right)}{k_0^4 \sin^2\left(2\kappa d\right) + 4\kappa^2 k^2}
\end{aligned}$$

Finally we have to determine the Dwell time for the case $E = V_0$. This case can be dealt by taking the limit as $\kappa \to 0$. So we get:

$$\lim_{\kappa\to 0}\frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 + k^2\right) - k_0^2 \sin\left(2\kappa d\right)}{k_0^4 \sin^2\left(2\kappa d\right) + 4\kappa^2 k^2} = \frac{mb}{\hbar k_0}\frac{1 + k_0^2 b^2/3}{1 + k_0^2 b^2/4} \tag{2.57}$$

Summarizing the results for the Dwell time in all three cases we get:

$$\tau_D = \begin{cases}
\frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 - k^2\right) + k_0^2 \sinh(2\kappa d)}{k_0^4 \sinh^2(2\kappa d) + 4\kappa^2 k^2} & \text{for } E < V_0 \\
\frac{mb}{\hbar k_0}\frac{1 + k_0^2 b^2/3}{1 + k_0^2 b^2/4} & \text{for } E = V_0 \\
\frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 + k^2\right) - k_0^2 \sin(2\kappa d)}{k_0^4 \sin^2(2\kappa d) + 4\kappa^2 k^2} & \text{for } E > V_0
\end{cases} \tag{2.58}$$

2.2.3 Solution of the Schrödinger Equation for the Double Spike Potential

We want to solve the Schrödinger Equation for the double spike potiential, i.e.

$$V(x) = V_0 \left[\delta(x - b/2) + \delta(x + b/2)\right]. \tag{2.59}$$

Shown in the figure below.

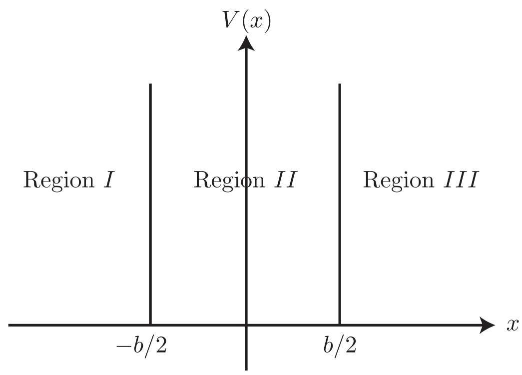

Figure 2.3: Double Spike potential.

Therefore we make the Ansatz:

$$\psi(x) = \begin{cases} \psi_I(x) = e^{ikx} + Re^{-ikx} & \text{for } \infty < x < -b/2 \\ \psi_{II}(x) = Ae^{ikx} + Be^{-ikx} & \text{for } -b/2 < x < b/2 \\ \psi_{III}(x) = Te^{ikx} & \text{for } b/2 < x < \infty \end{cases}$$

For the solution of the Schrödinger equation we have to comply with the following boundary conditions:

1. The wave function has to be continuous at $x = -b/2$ and $x = b/2$.
2. The derivative of the wave function has a jump at $x = -b/2$ and $x = b/2$.

Continuity conditions at $x = -b/2$ and $x = b/2$:

$$\psi_I(-b/2) = \psi_{II}(-b/2) \tag{2.60}$$

$$\psi_{II}(b/2) = \psi_{III}(b/2) \tag{2.61}$$

in detail this means:

$$e^{-\frac{1}{2}ibk} + Re^{\frac{ibk}{2}} = Ae^{-\frac{1}{2}ibk} + Be^{\frac{ibk}{2}} \tag{2.62}$$

$$Be^{-\frac{1}{2}ibk} + Ae^{\frac{ibk}{2}} = Te^{\frac{ibk}{2}} \tag{2.63}$$

First we have to motivate the jump condition in case of δ-potentials. Therefore we will integrate the Schrödinger Equation from $-\epsilon - b/2$ to $\epsilon - b/2$ and calculate the limit as $\epsilon \to 0$.

$$\lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m}\int_{-\epsilon-b/2}^{\epsilon-b/2}\psi''(x)\,dx + \int_{-\epsilon-b/2}^{\epsilon-b/2}V(x)\psi(x)\,dx\right] = E\lim_{\epsilon\to 0}\int_{-\epsilon-b/2}^{\epsilon-b/2}\psi(x)\,dx \tag{2.64}$$

considering the first term of the Schrödinger Equation:

$$\lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m}\int_{-\epsilon-b/2}^{\epsilon-b/2}\psi''(x)\,dx\right] = \lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m}\left(\psi'\left(\epsilon - \frac{b}{2}\right) - \psi'\left(-\epsilon - \frac{b}{2}\right)\right)\right] \tag{2.65}$$

As $-\epsilon - b/2$ is in region I and $\epsilon - b/2$ is in region II equation (2.65) gets

$$\lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m}\left(\psi'\left(\epsilon - \frac{b}{2}\right) - \psi'\left(-\epsilon - \frac{b}{2}\right)\right)\right] = -\frac{\hbar^2}{2m}\left[\psi'_{II}\left(-\frac{b}{2}\right) - \psi'_{I}\left(-\frac{b}{2}\right)\right] \tag{2.66}$$

As the potential is given by equation (2.59), the second term in equation (2.70) can be written as

$$\lim_{\epsilon\to 0}\left[\int_{-\epsilon-b/2}^{\epsilon-b/2} V(x)\psi(x)\,dx\right] =$$
$$\lim_{\epsilon\to 0}\left[\int_{-\epsilon-b/2}^{\epsilon-b/2} V_0\left(\delta(x-b/2)+\delta(x-b/2)\right)\psi(x)\,dx\right] =$$
$$V_0\psi(-b/2) = V_0\psi_I(-b/2) = V_0\psi_{II}(-b/2) \quad (2.67)$$

Finally we can verify easily that the right hand side of equation (2.70) vanishes. Using $\Psi(x)$ as antiderivative of $\psi(x)$ we get

$$E\lim_{\epsilon\to 0}\int\limits_{-\epsilon-b/2}^{\epsilon-b/2}\psi(x)\,dx = E\lim_{\epsilon\to 0}\left[\Psi\left(\epsilon-\frac{b}{2}\right)-\Psi\left(-\epsilon-\frac{b}{2}\right)\right] =$$
$$= E\left[\Psi\left(-\frac{b}{2}\right)-\Psi\left(-\frac{b}{2}\right)\right] = 0 \quad (2.68)$$

Using equations (2.67), (2.66), and (2.68) the condition of equation (2.70) can be summarized as

$$-\frac{\hbar^2}{2m}\left[\psi'_{II}\left(-\frac{b}{2}\right)-\psi'_I\left(-\frac{b}{2}\right)\right]+V_0\psi_I(-b/2)=0 \quad (2.69)$$

Analogously the same calculation can be carried out for

$$\lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m}\int_{-\epsilon+b/2}^{\epsilon+b/2}\psi''(x)\,dx+\int_{-\epsilon+b/2}^{\epsilon+b/2}V(x)\psi(x)\,dx\right] = E\lim_{\epsilon\to 0}\int_{-\epsilon+b/2}^{\epsilon+b/2}\psi(x)\,dx, \quad (2.70)$$

resulting in the boundary condition

$$-\frac{\hbar^2}{2m}\left[\psi'_{III}\left(\frac{b}{2}\right)-\psi'_{II}\left(\frac{b}{2}\right)\right]+V_0\psi_{III}(b/2)=0 \quad (2.71)$$

Introducing the abbreviation:

$$\kappa = \frac{2mV_0}{\hbar^2} - ik$$

the equations (2.69) and (2.71) yield to

$$
\begin{aligned}
-A\kappa e^{-ibk/2} + B\kappa^* e^{ibk/2} + ik\left(-e^{-ibk/2} + Re^{ibk/2}\right) &= 0 && (2.72)\\
-ik\left(Ae^{ibk/2} - Be^{-ibk/2}\right) - T\kappa e^{ibk/2} &= 0 && (2.73)
\end{aligned}
$$

$$
\begin{aligned}
R &= \frac{(k-i\kappa)(i\kappa^* + (2k+i\kappa)\cos(bk) + \kappa\sin(bk))}{e^{2ibk}k(k-i\kappa) + (k+i\kappa)^2 - ie^{ibk}(k-i\kappa)\kappa^*}, && (2.74)\\
A &= \frac{2k(k+i\kappa)}{e^{2ibk}k(k-i\kappa) + (k+i\kappa)^2 - ie^{ibk}(k-i\kappa)\kappa^*}, && (2.75)\\
B &= \frac{2k(k-i\kappa)}{(-ik-\kappa)\kappa^* + (2k^2 + ik\kappa - \kappa^2)\cos(bk) + (3k+i\kappa)\kappa\sin(bk)}, && (2.76)\\
T &= \frac{4k^2}{e^{2ibk}k(k-i\kappa) + (k+i\kappa)^2 - ie^{ibk}(k-i\kappa)\kappa^*} && (2.77)
\end{aligned}
$$

For the calculation of the Dwell Time we are only interested in the Reflection coefficient R and the Transmission Coefficient T (2.30). Therefore according to (2.30) we have to calculate first the integral of the absolute square of the wave function in region II, then we have to calculate the current density of the incident wave and get For the calculation of the Dwell Time we have to calculate first the integral of the absolute square of the wavefunction, i.e. for $\psi_{II}(x) = Ae^{ikx} + Be^{-ikx}$ we get:

$$
\int_{-b}^{b}\left|Ae^{ikx} + Be^{-ikx}\right|^2 dx = \int_{-b}^{b}\left(Ae^{ikx} + Be^{-ikx}\right)\left(A^*e^{-ikx} + B^*e^{ikx}\right)dx
$$

$$
\int_{-b}^{b}\left(|A|^2 + |B|^2 + AB^*e^{2ikx} + BA^*e^{-2ikx}\right)dx = \left(|A|^2 + |B|^2\right)2a + \mathrm{Re}\left(\frac{1}{2ik}AB^*e^{2ikx}\right)\Big|_{-a}^{a} =
$$

$$
= 2a\left(|A|^2 + |B|^2\right) + \frac{2\sin 2ka}{k}\mathrm{Im}(AB^*) \quad (2.78)
$$

The current density of the incident wave $\psi_I(x) = e^{ikx} + Re^{-ikx}$ is given as:

$$
j = \frac{\hbar}{m}\mathrm{Im}\left(\psi^*(x)\partial_x\psi(x)\right) = \frac{\hbar}{m}\mathrm{Im}\left(\left(e^{-ikx} + R^*e^{ikx}\right)ik\left(e^{-ikx} - R^*e^{ikx}\right)\right) =
$$

$$
= \frac{\hbar k}{m}\mathrm{Im}(i(1+|R|^2)) = \frac{\hbar k}{m}(1+|R|^2) \quad (2.79)
$$

So we get for the dwell time between the double spikes

$$\tau = \frac{2a\left(|A|^2 + |B|^2\right) + \frac{2\sin 2ka}{k}\mathrm{Im}(AB^*)}{\frac{\hbar k}{m}(1 + |R|^2)} \tag{2.80}$$

with A, B, R, T from the equations (2.74)- (2.77).

Chapter 3

BÜTTIKER-LANDAUER-TIME

Landauer and Büttiker analyzed in [6] the behavior of a particle tunneling through a time modulated barrier. In this work they verified that the particle interacts with the barrier and showed that the tunneling time depends on the modulation frequency. For low modulation frequencies the tunneling barrier looks static to the particle, whereas for high modulation frequencies the particle tunnels through the time-averaged barrier. This tunneling can also be inelastic loosing or gaining modulation quanta.

The time dependent barrier

$$V(x,t) = V_0(x) + V_1(x)\cos\omega t, \tag{3.1}$$

where $V_0(x)$ denotes the static part of the barrier, and $V_1(x)$ is the amplitude of a small modulation of the barrier. Incoming particles with the Energy E will interact with the perturbation $V_1(x)\cos\omega t$ and will therefore inelastically absorb or emit modulation quanta $\hbar\omega$. If the modulation frequency ω is low, i.e. that the interaction time $1/\omega$ much greater than the traversal time through the static barrier the barrier appears to the particle to be static. If the reciprocal of the modulation frequency is much smaller than the traversal time for the static barrier then the particle sees many cycles of oscillations. So the particle tunnels through a time averaged barrier. The effective barrier will not be larger or smaller than the static barrier. The only thing that changes is the Energy of the particles differ either because the particle absorbs or emits modulation quanta.

Particles with higher energy tunnel much easier through a barrier than particles with lower energy.

The interaction time of the transmitted particle can be given in semiclassical approximation using the following arguments. Let us start with the relation between momentum and velocity:

$$p(x) = mv(x),$$

where p denotes the momentum of the particle, m the mass of the particle, and v the velocity of the particle. Considering the units we can solve this equation with respect to $1/v$ and get

$$\frac{1}{v} = \frac{m}{p(x)}.$$

the unit of $1/v$ is s/m. If we now integrate both sided with respect to x we get:

$$\tau = \int_{x_1}^{x_2} \frac{1}{v(x)}\,dx = \int_{x_1}^{x_2} \frac{m}{p(x)}\,dx \tag{3.2}$$

from the correspondence principle for a free particle we know that $p(x) = \hbar\kappa(x) = \sqrt{2m(V_0(x) - E)/\hbar^2}$ we get for the interaction time, with x_1 and x_2 denoting the classical turning points.

$$\tau = \int_{x_1}^{x_2} \frac{m}{\hbar\kappa(x)}\,dx = \int_{x_1}^{x_2} \frac{m}{\hbar\sqrt{2m(V_0(x) - E)/\hbar^2}}\,dx = \int_{x_1}^{x_2} \sqrt{\frac{m}{2(V_0(x) - E)}}\,dx \tag{3.3}$$

τ is the semiclassical interaction time of a particle traveling in a one dimensional potential from x_1 to x_2. The Energy is below the barrier. The interaction time for energies above the barrier is given as $\tau = \int_{x_1}^{x_2} \sqrt{\frac{m}{2(E - V_0(x))}}\,dx$.

Coming back to the Büttiker-Landauer problem. For simplicity we will consider the spatially uniform Hamiltonian

$$H = \frac{p^2}{2m} + V_0 + V_1 \cos \omega t \tag{3.4}$$

describing the potential inside the barrier. Here V_0 and V_1 are considered constant. If we solve the time independent Schrödinger equation within the barrier for the time independent Hamiltonian $\tilde{H} = \frac{p^2}{2m} + V_0$ for $E < V_0$ we get

$$\tilde{H}\phi_E(x) = E\phi_E(x) \quad \Longrightarrow \phi_E(x) = Ae^{\kappa x} + Be^{-\kappa x}.$$

Therefore the solution of the time-dependent Schrödinger equation for (3.4)

$$H\psi(x,t;E) = i\hbar\partial_t\psi(x,t;E)$$

is

$$\psi(x,t) = \phi_E(x) \exp\left(-\frac{iEt}{\hbar}\right) \exp\left(-\frac{iV_1}{\hbar\omega} \sin \omega t\right). \tag{3.5}$$

using the identity 9.1.41 in [1], i.e.

$$\exp\left(z \cdot \frac{1}{2}\left(t - \frac{1}{t}\right)\right) = \sum_{n=-\infty}^{\infty} t^k J_n(z), \tag{3.6}$$

where $J_n(z)$ denotes the Bessel function of first kind for integer order n. We can now expand (3.5) using (3.6) by identifying $t = e^{-i\omega t}$ and $z = \frac{V_1}{\hbar\omega}$ in terms of Bessel functions of the first kind as following:

$$\psi(x,t) = \phi_E(x) \exp\left(-\frac{iEt}{\hbar}\right) \sum_{n=-\infty}^{\infty} J_n\left(\frac{V_1}{\hbar\omega}\right) e^{-in\omega t}. \tag{3.7}$$

This mathematical expansion can be interpreted also physically. The time modulation of the potential causes so-called sidebands, which can be interpreted as particles which absorbed ($n > 0$) or emitted ($n < 0$) modulation quanta. This becomes obvious if we take the time derivative of (3.7)

$$i\partial_t\psi(x,t) = \sum_{n=-\infty}^{\infty} \phi_E(x)\exp\left(-\frac{iEt}{\hbar}\right) J_n\left(\frac{V_1}{\hbar\omega}\right) e^{-in\omega t}(E+n\hbar\omega). \tag{3.8}$$

At the beginning of our discussion we considered the amplitude of the modulation of the potential as small. In this case we can observe that for $V_1/\hbar\omega \ll 1$ according to [1] 9.1.7,

$$J_n(V_1/\hbar\omega) \sim \left(\frac{V_1}{2\hbar\omega}\right)^n \cdot \frac{1}{\Gamma(n+1)} = \left(\frac{V_1}{\hbar\omega}\right)^n \cdot \frac{1}{2^n n!} \propto \left(\frac{V_1}{\hbar\omega}\right)^n$$

So the order of $V_1/\hbar\omega$ corresponds to the order of the sidebands.

In order to find the the solution for the oscillating potential we have to solve the time independent Schrödinger equation for the energies E and $E \pm \hbar\omega$ like in section 2.2.2.

The transmission coefficient T for the static barrier is according to (2.50) as:

$$T = \frac{4k\kappa}{k^2+\kappa^2} e^{-(ik+\kappa)d} \exp\left\{i \arctan\frac{k^2-\kappa^2}{2k\kappa}\right\}$$

As we consider the $V_1 \cos\omega t$ as small perturbation, we will assume for the following that $\hbar\omega \ll E$ and $\hbar\omega \ll V_0 - E$. Then the wave vectors for the sidebands

$$k_\pm = \sqrt{2m(E\pm\hbar\omega)/\hbar^2} = \sqrt{2mE/\hbar^2}\sqrt{1\pm\frac{\hbar\omega}{E}} \approx \sqrt{2mE/\hbar^2}(1\pm\frac{\hbar\omega}{2E})$$

with $k = \sqrt{2mE/\hbar^2}$ $k_\pm$ simplifies to

$$k_\pm \approx k \pm \frac{m\omega}{2\hbar k}.$$

Analogously $\kappa_\pm$ simplifies to :

$$\kappa_\pm \approx \kappa \mp \frac{m\omega}{2\hbar\kappa}.$$

then we get for the transmission coefficients multiplying the transmitted waves at the frequencies $E/\hbar \pm \omega$ for multiplying $\exp\left[ik_\pm - i(E\pm\hbar\omega)t/\hbar\right]$ as:

$$T_{\pm} = T\frac{V_1}{2\hbar\omega}\left(e^{\pm\omega\tau} - 1\right) \tag{3.9}$$

with

$$\tau = \frac{md}{\hbar\kappa}$$

τ can be directly calculated from (3.3) for $\kappa(x) = \kappa = \text{const.}$ and can be identified as traversal time through the constant barrier V_0. This traversal time is the time a particle needs to travel over a distance d with the velocity $v = \hbar k/m$.

The transmission probability gets then:

$$|T_{\pm}|^2 = |T|^2\left(\frac{V_1}{2\hbar\omega}\right)^2\left(e^{\pm\omega\tau} - 1\right)^2 \tag{3.10}$$

where $|T|^2$ is given as:

$$|T|^2 = \frac{16k^2\kappa^2}{(k^2+\kappa^2)^2}e^{-2kd} \tag{3.11}$$

For $\omega \ll 1/\tau$, i. e. the frequency of the barrier is small compared to the traversal time, the barrier looks static and the transmission probability for the two sidebands gets:

$$|T_{\pm}|^2 = |T|^2\left(\frac{V_1}{2\hbar\omega}\right)^2\left(1 \pm \omega\tau + O((\pm\omega\tau)^2) - 1\right)^2 = |T|^2\left(\frac{V_1\tau}{2\hbar}\right)^2 \tag{3.12}$$

In the high frequency limit, i. e. $\omega\tau \gg 1$ we can analyze the behavior of the transmission probability. In the case where the particle absorbs a quantum of $\hbar\omega$ and therefore has the energy $E + \hbar\omega$. This particle traverses the barrier which looks as an averaged barrier of the height V_0 more easily compared to the energies E and $E - \hbar\omega$. The transmission probability in this case becomes then

$$|T_+|^2 = |T|^2\left(\frac{V_1}{2\hbar\omega}\right)^2 e^{2\omega\tau}$$

This is the transmission probability of a particle that traverses the barrier at the higher energy, where the quanta $\hbar\omega$ can be absorbed everywhere along the traveling path of the particle.

Considering now $|T_-|^2$ we can see that in the high frequency limit, because of the exponential decay of the transmission probability gets:

$$|T_-|^2 = |T|^2 \left(\frac{V_1}{2\hbar\omega}\right)^2 \left(e^{-\omega\tau} - 1\right)^2 \approx |T|^2 \left(\frac{V_1}{2\hbar\omega}\right)^2$$

In this case we can see that the transmission probability strongly depends on the width of the barrier, decays according to (3.11) exponentially with respect to the barrier width.

Using the WKB approximation we can extend the discussion to more general barrier shapes. According to [11] the wave function

$$\psi(x,t) = Ae^{iS/\hbar}$$

is determined by the solution of the time-dependent Hamilton-Jacobi equation

$$\partial_t S(x,t) = \frac{1}{2m}\left(\frac{\partial S(x,t)}{\partial x}\right)^2 - V(x,t). \tag{3.13}$$

S denotes the classical action. The solution of (3.13) is given as $S(x,t) = S_0(x,t) + \sigma(x,t)$, where

$$S_0(x,t) = -Et + i\hbar \int \kappa(x)dx$$

is the solution for the static barrier $V(x) = V_0(x)$, whereas $\sigma(x,t)$ arises from the modulation ω and is given as:

$$\begin{aligned}\sigma(x,t) = i\frac{m}{2}\Bigg(e^{i\omega t}\int_{x_0}^{x}\frac{V_1(\xi)}{\hbar\kappa(\xi)}\exp\left\{-\int_{\xi}^{x}\frac{m\omega}{\hbar\kappa(\zeta)}d\zeta\right\}d\xi + \\ + e^{-i\omega t}\int_{x_0}^{x}\frac{V_1(\xi)}{\hbar\kappa(\xi)}\exp\left\{\int_{\xi}^{x}\frac{m\omega}{\hbar\kappa(\zeta)}d\zeta\right\}d\xi\Bigg]\end{aligned} \tag{3.14}$$

x_0 is the classical turning point at the left, where $\sigma(x,t)$ is assumed to be 0. If $V_1(x)$ is small, we have again only two sidebands. We can see from the first term in equation (3.14), that the damping for the higher sideband is lower compared to the damping of the lower sideband. This fact complies with our previous observations. Furthermore with $v(x) = \hbar\kappa(x)/m$ we can rewrite equation (3.14) as following:

$$\sigma(x,t) = i\frac{m}{2}\left(e^{i\omega t}\int_{x_0}^{x}\frac{V_1(\xi)}{\hbar\kappa(\xi)}\exp\left\{-\int_{\xi}^{x}\frac{\omega}{v(\zeta)}d\zeta\right\}d\xi + \right. \\ \left. + e^{-i\omega t}\int_{x_0}^{x}\frac{V_1(\xi)}{\hbar\kappa(\xi)}\exp\left\{\int_{\xi}^{x}\frac{\omega}{v(\zeta)}d\zeta\right\}d\xi\right] \quad (3.15)$$

In case of the lower side band the particle looses energy, so we can interpret this as dissipative tunneling. The traversal time in this case gives an estimate of the impact of friction effects on tunneling. The energy loss of a particle with velocity v and friction coefficient γ is then given by:

$$\Delta E = \gamma\int_0^d v(x)\,dx \quad (3.16)$$

As we don't have an exact idea what happens to the velocity inside the barrier, we can not calculate the energy loss based on (3.17) exactly. But for small dissipation, i.e. for $\Delta E \ll 1$ we can use the velocity of the unperturbed system $v_0(x)$. In this case the energy loss can be evaluated to:

$$\Delta E = \gamma\int_0^d \frac{\hbar\kappa(x)}{m}\,dx \quad (3.17)$$

In order to find the transmission probability for small dissipation we assume that the effective decay rate $\kappa = \sqrt{2m(V(x) - E(x))}/\hbar$ with $E(x) = E - \Delta E(x)$ is the energy corrected decay rate for the damped system. In this case according to [6] th toe first order in γ we find

$$\hbar\kappa = \hbar\kappa_0 + \frac{\gamma}{v_0(x)}\int_0^x v_0(\xi)d\xi.$$

Resulting in the phase integral for the exponential damping of the wave function:

$$S = \int \hbar\kappa\,dx = S_0 + \gamma\int_0^x \frac{d\xi}{v_0(\xi)}\int_0^{\xi} v_0(\zeta)d\zeta \quad (3.18)$$

For a smooth $v_0(x)$ we can find that the contribution in (3.18) is of the order γd^2, where d is the length of the barrier. So dissipation causes as expected decreased transmission. This property was predicted by Caldeira and Legget in [7].

Chapter 4

LARMOR CLOCK

One of the first approaches to the tunneling time problem was proposed by Baz' [2]. Rybachenko applied Baz's work to a one dimensional localized potential barrier [15]. This approach is based on the idea to use Larmor precession to measure the time a particle spends within the barrier. In order to employ Larmor precission we have to add a small magnetic field in z-direction as perturbation to the one dimensional localized barrier $V(x)$ as shown in figure 4.1.

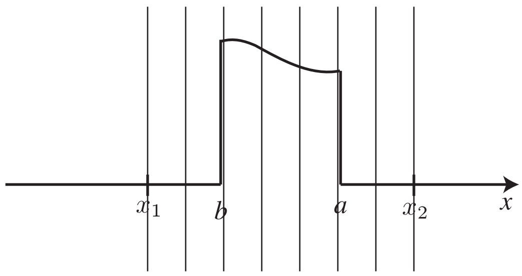

Figure 4.1: One dimensional localized potential barrier with small magnetic field $\mathbf{B} = \mathbf{e}_z B_0$ in the region $[x_1, x_2]$as perturbation.

The "infinitesimally small magnetic field" as Rybachenko [15] denoted this field is localized in the region $[x_1, x_2]$, which includes also the region of the localized potential $V(x)$. For $x < x_1$ and $x > x_2$ the magnetic field $\mathbf{B} = 0$. In order to have an interaction of the quantum particle with the magnetic field, we consider a quantum particle with spin $s = 1/2$ and therefore a magnetic moment of $\boldsymbol{\mu} = 2\mu\mathrm{s}$, where the spin is polarized along the x-axis. This is the same setup of the gedanken experiment employed by Baz

[2] to determine the average collision time. Now we will employ the same idea to determine the average transmission and reflection times of the particles spent in the region $[x_1, x_2]$.

$$\tau_{\text{refl}} = \frac{\theta_{\text{refl}}}{\omega}, \quad \text{and} \quad \tau_{\text{tr}} = \frac{\theta_{\text{tr}}}{\omega}, \tag{4.1}$$

where θ_{refl} and θ_{tr} denote the angle of the rotation of the spin for the particles reflected and transmitted respectively by the barrier $V(x)$. Furthermore $\omega = 2\mu B/\hbar$ denotes the Larmor frequency. As the magnetic field is infinitesimally small the times τ_{refl} and τ_{tr} are basically independent of the strength of the magnetic field. Now we have to solve the stationary Schrödinger equation including the magnetic field.

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \mu\mathbf{B}\hat{\sigma} + V(x)\right)\hat{\psi}(x) = E\hat{\psi}(x) \tag{4.2}$$

Here $\hat{\psi}(x)$ is an operator with respect to the to the spin variables. In absence of the magnetic field, i.e. $\mathbf{B} = 0$ the solution of equation (4.2) is given as:

$$\hat{\psi}(x) = \hat{I}\begin{cases} e^{ikx} + Re^{-ikx} & \text{for } x < x_1 \\ Te^{ikx} & \text{for } x > x_2 \\ \alpha\phi_1(x) + \beta\phi_2(x) & \text{for } x_1 < x < x_2 \end{cases}, \tag{4.3}$$

where $\phi_1(x)$ and $\phi_2(x)$ are the linearly independent solutions of (4.2) in absence of the magnetic field, and $\hat{I}$ denotes the identity matrix. We can identify R and T as the reflection and transmission amplitudes respectively.

As we have mentioned above the magnetic field in the region $[x_1, x_2]$ is infinitesimally small so we will take the infinitesimally small magnetic field into account by the energy shift $-\mu\mathbf{B}\hat{\sigma}$. This changes the wave functions $\phi_1(x)$ and $\phi_2(x)$ in the region $[x_1, x_2]$ as following:

$$\hat{\phi}_1(x + \mu\mathbf{B}\hat{\sigma}) - \hat{I}\phi_1(x, E) = -\mu\mathbf{B}\hat{\sigma}\frac{d\phi_1(x, E)}{dE} \tag{4.4}$$

$$\hat{\phi}_2(x + \mu\mathbf{B}\hat{\sigma}) - \hat{I}\phi_2(x, E) = -\mu\mathbf{B}\hat{\sigma}\frac{d\phi_2(x, E)}{dE} \tag{4.5}$$

Obviously the coefficients R, T, α, β change when the magnetic field is switched on. Actually our main interest is the effect of the perturbation by the magnetic field on the reflection and transmission amplitudes, which are given according to [15] as:

$$\hat{R}(E, \hat{\phi}_1, \hat{\phi}_2) = \hat{I}R(E, \hat{\phi}_1, \hat{\phi}_2) + \mu\mathbf{B}\hat{\sigma}\frac{\delta R}{\delta E} \tag{4.6}$$

$$\hat{T}(E, \hat{\phi}_1, \hat{\phi}_2) = \hat{I}T(E, \hat{\phi}_1, \hat{\phi}_2) + \mu\mathbf{B}\hat{\sigma}\frac{\delta T}{\delta E} \tag{4.7}$$

The differential operator $\delta/\delta E$ is a differential operator where only the functions $\phi_1(x)$ and $\phi_2(x)$ are varied, i.e.

$$\frac{\delta}{\delta E} = \frac{d}{dE} - \left(\frac{\partial}{\partial E}\right)_{\phi_1, \phi_2} \tag{4.8}$$

Applying now the operatores $\hat{R}$ and $\hat{T}$ on the spin wave function χ^0_{s,m_s} of the incident particle the spin wave function of the reflected and transmitted particles become:

$$\chi^{\text{refl}}_{s,m_s} = \left(1 + \mu B \frac{1}{R}\frac{\delta R}{\delta E}\sigma_z\right)\chi^0_{s,m_s} \tag{4.9}$$

$$\chi^{\text{tr}}_{s,m_s} = \left(1 + \mu B \frac{1}{T}\frac{\delta T}{\delta E}\sigma_z\right)\chi^0_{s,m_s} \tag{4.10}$$

These spin wave function we can identify as the rotation angles θ_{refl} and θ_{tr} for the rotation with respect to the z-axis.

$$\theta_{\text{refl}} = 2\mu B \text{Im}\left(\frac{1}{R}\frac{\delta R}{\delta E}\right) = 2\mu B \text{Im}\left(\frac{\delta \ln |R|}{\delta E}\right) \tag{4.11}$$

$$\theta_{\text{tr}} = 2\mu B \text{Im}\left(\frac{1}{T}\frac{\delta T}{\delta E}\right) = 2\mu B \text{Im}\left(\frac{\delta \ln |T|}{\delta E}\right) \tag{4.12}$$

Inserting (4.13) and (4.14) into (4.1) and exploiting the Larmor frequency $\omega = 2\mu B/\hbar$ we get:

$$\tau_{\text{refl}} = \frac{2\mu B}{\omega}\text{Im}\left(\frac{1}{R}\frac{\delta R}{\delta E}\right) = \hbar \text{Im}\left(\frac{\delta \ln |R|}{\delta E}\right) \tag{4.13}$$

$$\tau_{\text{tr}} = \frac{2\mu B}{\omega}\text{Im}\left(\frac{1}{T}\frac{\delta T}{\delta E}\right) = \hbar \text{Im}\left(\frac{\delta \ln |T|}{\delta E}\right) \tag{4.14}$$

In order to determine the reflection and transmission times we have to express the reflection amplitude R and the transmission amplitude T in terms of $\phi_1(x_1), \phi_2(x_1), \phi_1'(x_1), \phi_2'(x_1)$

and $\phi_1(x_2), \phi_2(x_2), \phi_1'(x_2), \phi_2'(x_2)$ explicitly to determine the partial derivatives $(\partial R/\partial E)_{\phi_1,\phi_2}$ and $(\partial T/\partial E)_{\phi_1,\phi_2}$ respectively. The constants α and β can be chosen arbitrarily $\neq 0$ to ensure the linear a proper linear combination of the solution ϕ_1 and ϕ_2.

Based on this we can now see that the Larmor clock gives us in general complex reflection and transmission times depending on the logarithmic derivatives of the reflection and transmission amplitudes $R(E, B)$ and $T(E, B)$ at $B = 0$. This linear response theory gives us 2 complex or 4 real time scales.

Chapter 5

MINIMAL TUNNELING TIME

In the following we want to define the minimal tunneling time $\tau_{\text{min}}(E)$ using a variational approach as discussed in [4]. As motivation we refer to chapter 2.1 where we ellucidated the Bohmian Dwell time approach. There we defined the Bohmian Dwell time τ_D in (2.3) as a functional of the wave function $\psi_E(x)$ (2.1). It is preferable to deal with a tunneling time that solely depends on the potential structure $V(x)$ and the energy of the particle then on the actual wave function. It seems to be advantageous to use the functional $\tau_D(\psi_E(x))$ as a time scale independent functional from the wave function $\psi_E(x)$. Therefore a simple variational principle is employed. The properties of this functional $\tau_D(\psi_E(x))$ are

- positive definite
- has a lower bound
- varies in the 2D space of the eigenfunctions $\psi_E(x)$

Consequently the dwell time $\tau_D(\psi_E(x))$ becomes minimal for some special solution of the Schrödinger equation (2.1) denoted by $\psi_E^{\text{min}}(x)$. The Dwell time for this wave function is then $\tau_D(\psi_E^{\text{min}}(x))$, which can be interpreted as the minimal tunneling time $\tau_{\text{min}}(E)$. This minimal tunneling time is the minimal tunneling time in the potential $V(x)$ for the interval $a < x < b$.

$$\tau_{\text{min}} = \min_{H\psi=E\psi} \left(\frac{1}{j(\psi_E)} \int_a^b |\psi_E(x)|^2 \right) \tag{5.1}$$

The eigenstate $\psi_E^{\min}(x)$ minimizes equation (5.7), and can therefore be seen as the minimal wave function of the barrier $V(x)$ in the region $a < x < b$. From equation (5.7) we can see that there is no maximum for the Dwell time functional $\tau_D(\psi_E(x))$, because the Dwell time diverges for solutions $\psi_E(x)$ that carry no current, i.e. the current density $j(\psi_E) \equiv 0$. The current density becomes zero e.g. in the case when the solutions of the Schrödinger equation (2.1) are are real. If we take a closer look at the variational principle we can see that the minimal solution refers to the origin of the time scale in a variational procedure. The tunneling time (5.7) is not universally the minimal tunneling time that can be found by all different tunneling time approaches. But this is another valid approach to define a tunneling time. The additivity of Dwell times as depicted in (2.29) can obviously not be resembled in (5.7). So we can deduce from equation (5.7) the inequality:

$$\tau_{\min}(a,b;E) \geq \tau_{\min}(a,c;E) + \tau_{\min}(c,b;E) \tag{5.2}$$

In the limit of the classical motion the equality should hold. Another interesting property of the minimal tunneling time is that $\tau_{\min}(E)$ is determined as a local quantity, whereas most other approaches depend on global quantities, as we can see directly e.g. in the case of the Smith Dwell time.

5.1 Explicit Expressions

In the following based on the the variational principle (5.7) we want to determine $\tau_{\min}(E)$ and the corresponding wave function $\psi_E^{\min}(x)$. Let us consider the two real linearly independent solutions of the Schrödinger equation (2.1) $c(x)$ and $s(x)$ for the energy E. In this general treatment we only require the Wronskian of the solutions to be normalized, i.e.

$$\mathcal{W}(s(x), c(x)) = s'(x)c(x) - s(x)c'(x) = 1 \tag{5.3}$$

By scaling of $s(x)$ we can always satisfy this property. Also note that the normalization using the wronskian is independent of the boundaries a and b. Now in order to find the minimal tunneling time and the minimal wave function we have to insert the general solution of (2.1)

$$\psi_E(x) = \alpha c(x) + \beta s(x) \tag{5.4}$$

into (2.3) and perform the variation of the complex parameters α and β and we get

$$\tau_{\min}(E) = \frac{2m}{\hbar}\left(\int_a^b c(x)^2 dx \int_a^b s(x)^2 dx - \int_a^b s(x)c(x)dx\right)^{1/2}. \tag{5.5}$$

$\tau_{\min}(E)$ is according to the Cauchy-Schwartz inequality for integrals [1] positive definite and independent of the of the basis functions $c(x)$ and $s(x)$. The only requirement is the satisfaction of equation (5.3). [4] proposes one possible pair of conjugate complex wave functions $\psi_E^{\min}(x)$

$$\psi_E^{\min}(x) \propto c(x) - \left(\frac{\int_a^b c(\xi)^2 dx}{\int_a^b c(\xi)^2 dx}\right)^{1/2} \exp\left\{\pm i \arccos \frac{\int_a^b s(\xi)c(\xi)d\xi}{\sqrt{\int_a^b c(\xi)^2 d\xi \int_a^b s(\xi)^2 d\xi}}\right\} \tag{5.6}$$

For the special case of a symmetric potential barrier, i.e. $V(-x) = V(x)$ and $a = -b$ the expressions for the minimal tunneling time and the minimal wave function simplifies. Selecting one eigenstate as even parity, i.e. $c(-x) = c(x)$ and one eigenstate as odd parity, i.e. $s(-x) = -s(x)$ we get for the minimal tunneling time and the corresponding wave function:

$$\tau_{\min}(E) = \frac{4m}{\hbar}\sqrt{\int_0^b c(x)^2 dx \int_0^b s(x)^2 dx} \tag{5.7}$$

$$\psi_E^{\min}(x) \propto \sqrt{\int_0^b s(\xi)^2 d\xi}\, c(x) \pm i \sqrt{\int_0^b c(\xi)^2 d\xi}\, s(x) \tag{5.8}$$

5.2 Minimal Tunneling Time for the Square Barrier

Let us calculate the minimal tunneling time for the symmetric rectangular barrier

$$V(x) = V_0\Theta(x - b/2)\Theta(b/2 - x) \tag{5.9}$$

Then the wave number κ in the barrier is given as

$$\kappa = \frac{1}{\hbar}\sqrt{2m|E - V_0|}. \tag{5.10}$$

Taking into account the condition (5.3) then we find the fundamental solutions $c(x)$ and $s(x)$ in the barrier region as:

$$c(x) = \cos(\kappa x), \quad s(x) = \frac{1}{\kappa^2}\sin(\kappa x) \tag{5.11}$$

These are the fundamental solutions for $E < V_0$. For $E < V_0$ the trigonometric functions will be replaced by its hyperbolic counterparts, then we obtain for $\tau_{\min}(E)$:

For $E > V_0$:

$$\begin{aligned}
\tau_{\min}(E) &= \frac{4m}{\hbar}\sqrt{\int_0^b \cos(\kappa x)^2 dx \int_0^b \frac{1}{\kappa^2}\sin(\kappa x)^2 dx} \\
&= \frac{4m}{\kappa\hbar}\sqrt{\frac{1}{2}\int_0^b (1 + \cos(2\kappa x))dx \, \frac{1}{2}\int_0^b (1 - \cos(2\kappa x))dx} \\
&= \frac{m}{\kappa\hbar}\sqrt{\left(b + \frac{1}{2\kappa}\sin(2\kappa b)\right)\left(b - \frac{1}{2\kappa}\sin(2\kappa b)\right)} \\
&= \frac{m}{\kappa\hbar}\sqrt{\left(b^2 - \frac{1}{4\kappa^2}\sin(2\kappa b)^2\right)} \\
&= \frac{m}{2\kappa^2\hbar}\sqrt{(2\kappa b)^2 - \sin(2\kappa b)^2} \\
&= \frac{m}{\kappa^2\hbar}\sqrt{(\kappa b)^2 - \sin(\kappa b)^2}
\end{aligned}$$

Analogously we can calculate the minimal tunneling time for $E < V_0$. In this case as mentioned above we have to take the corresponding hyperbolic functions for $c(x) =$

$\cosh(\kappa x)$ and $s(x) = \sinh(\kappa x)/\kappa$ in order to calculate the minimal tunneling time for $E < V_0$. Analogously we get for $E < V_0$:

$$\begin{aligned} \tau_{\min}(E) &= \frac{4m}{\hbar}\sqrt{\int_0^b \cosh(\kappa x)^2 dx \int_0^b \frac{1}{\kappa^2}\sinh(\kappa x)^2 dx} \\ &= \frac{4m}{\hbar}\sqrt{\int_0^b \frac{1}{4}(\cosh(2\kappa x)+2)dx \int_0^b \frac{1}{\kappa^2}\frac{1}{4}(\cosh(2\kappa x)-2)dx} \\ &= \frac{m}{\kappa^2\hbar}\sqrt{\sinh(\kappa b)^2 - (\kappa b)^2} \end{aligned}$$

In the case $E = V_0$, i.e. $\kappa = 0$ we can determine the minimal tunneling time by the limiting process

$$\tau_{\min}(E = V_0) = \lim_{\kappa\to 0} \frac{m}{\kappa^2\hbar}\sqrt{\sinh(\kappa b)^2 - (\kappa b)^2} = \frac{mb^2}{\sqrt{3}\hbar}$$

Finally putting all results together we get for the minimal tunneling time $\tau_{\min}(E)$:

$$\tau_{\min}(E) = \begin{cases} \frac{m}{\hbar\kappa^2}\sqrt{\sinh^2\kappa b - \kappa^2 b^2} & \text{for } E < V_0 \\ \frac{mb^2}{\sqrt{3}\hbar} & \text{for } E = V_0 \\ \frac{m}{\hbar\kappa^2}\sqrt{\kappa^2 b^2 - \sin^2\kappa b} & \text{for } E > V_0 \end{cases} \tag{5.12}$$

The corresponding Dwell time was already calculated in chapter 2.2.2, which is defined only for $E \geq 0$.

$$\tau_D = \begin{cases} \frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 - k^2\right) + k_0^2\sinh(2\kappa d)}{k_0^4\sinh^2(2\kappa d) + 4\kappa^2 k^2} & \text{for } E < V_0 \\ \frac{mb}{\hbar k_0}\frac{1 + k_0^2 b^2/3}{1 + k_0^2 b^2/4} & \text{for } E = V_0 \\ \frac{mk}{\hbar\kappa}\frac{2\kappa d\left(\kappa^2 + k^2\right) - k_0^2\sin(2\kappa d)}{k_0^4\sin^2(2\kappa d) + 4\kappa^2 k^2} & \text{for } E > V_0 \end{cases} \tag{5.13}$$

The minimal tunneling time is compared to the dwell time in the following figure 5.1

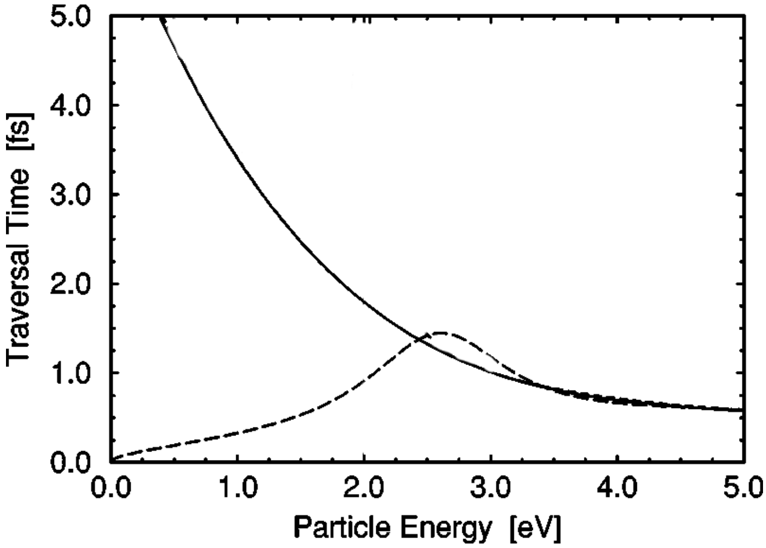

Figure 5.1: Traversal times for a rectangular barrier of width $d = 6$Å and height $V_0 = 2$eV. The solid line denotes the minimal tunneling time τ_{min}, whereas the dashed line denotes the Dwell time.

5.3 Energy Splitting in Symmetric Double Well Potential

5.3.1 Solution for the parabolic symmetric double well potential

We are considering now the symmetric double well potential.

$$U(x) = \begin{cases} \frac{m\omega^2}{2}(x+b)^2 & x < -c = -\frac{b}{2} \\ \frac{m\omega^2}{2}\left(\frac{b^2}{2} - x^2\right) & -c < x < c \\ \frac{m\omega^2}{2}(x-b)^2 & x \rangle c = \frac{b}{2} \end{cases} \tag{5.14}$$

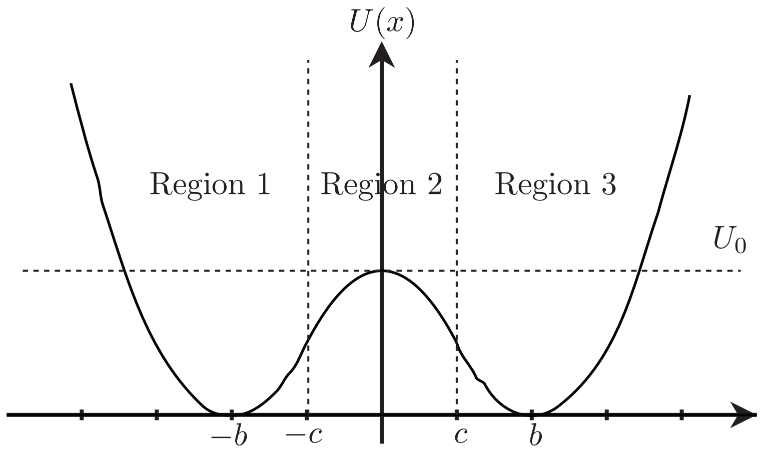

Figure 5.2: The symmetric double well potential $U(x)$.

First we have to solve the Schrödinger equation (2.1) for this symmetric potential, i.e. we have to solve the following two differential equations:

$$\left[E + \frac{\hbar^2}{2m}\partial_x^2 - \frac{m\omega^2}{2}\left(x \pm b\right)^2\right]\psi_{1,3}\left(x\right) = 0 \tag{5.15}$$

$$\left[E + \frac{\hbar^2}{2m}\partial_x^2 - \left(\frac{m\omega^2 b^2}{2} - \frac{m\omega^2}{2}x^2\right)\right]\psi_2\left(x\right) = 0 \tag{5.16}$$

In order to transform the Schrödinger equations to a known equation, we change the variables:

$$\xi = \sqrt{\frac{2m\omega}{\hbar}} \quad \Longrightarrow \quad \frac{\partial}{\partial x} = \sqrt{\frac{2m\omega}{\hbar}}\frac{\partial}{\partial \xi}$$

using the abbreviations

$$\beta = \sqrt{\frac{2m\omega}{\hbar}} b, \quad U_0 = \frac{m\omega^2 b^2}{4} = \frac{\hbar\omega\beta^2}{8}$$

the Schrödinger equations (5.15) and (5.16) transform to:

$$\left(\frac{\partial^2}{\partial \xi^2} - (\xi \pm \beta)^2 + \frac{E}{\hbar\omega} \right) \psi_{1,3}(\xi) = 0 \tag{5.17}$$

$$\left(\frac{\partial^2}{\partial \xi^2} + \frac{\xi^2}{4} + \left(\frac{E}{\hbar\omega} - \frac{\beta^2}{8} \right) \right) \psi_2(\xi) = 0 \tag{5.18}$$

Let us compare the resulting differential equations with the parabolic cylinder function in [1] 19.1.2 and 19.1.3.

For the oscillator: $\left(\frac{\partial^2}{\partial \xi^2} - \frac{\xi^2}{4} - a \right) Y_a(\xi) = 0$

For the inverse oscillator: $\left(\frac{\partial^2}{\partial \xi^2} + \frac{\xi^2}{4} - a \right) Y_a(\xi) = 0$

For $a = -\frac{E}{\hbar\omega}$ or $a = \frac{\beta^2}{8} - \frac{E}{\hbar\omega}$. For the regular solution in the third region we have to fulfill the requirement of the wave function to vanish in the limit as $\xi \to \infty$. Then we get for $\psi_3(\xi)$ according to [1] 19.8.1:

$$\psi_3(\xi) = U \left(-\frac{E}{\hbar\omega}, \xi - \beta \right) \tag{5.19}$$

$U(a, x)$ is the parabolic cylindrical function. Now we have to take the logarithmic derivatives at $x = c$, i.e. $\xi = \beta/2$. Before we do this, we will exploit the recurrence relation for the parabolic cylinder function [1] 19.6.2.

$$U'(a, x) = \frac{1}{2} x U(a, x) - U(a - 1, x) \tag{5.20}$$

we get for the derivative $\partial_\xi \psi_3(\xi)$:

$$\begin{aligned}\partial_\xi \psi_3(\xi)\Big|_{\beta/2} = \partial_\xi U\left(-\frac{E}{\hbar\omega}, \xi - \beta\right)\Big|_{\beta/2} = \\ = \frac{1}{2}(\xi - \beta) U\left(-\frac{E}{\hbar\omega}, \xi - \beta\right) - U\left(-1 - \frac{E}{\hbar\omega}, \xi - \beta\right)\Big|_{\beta/2} = \\ = -\frac{\beta}{4} U\left(-\frac{E}{\hbar\omega}, \frac{\beta}{2}\right) - U\left(-1 - \frac{E}{\hbar\omega}, -\frac{\beta}{2}\right)\end{aligned} \tag{5.21}$$

So we get for the logarithmic derivative

$$\frac{\partial_\xi \psi_3(\xi)}{\psi_3(\xi)}\Big|_{\xi=\beta/2} = -\frac{\beta}{4} - \frac{U\left(-1 - \frac{E}{\hbar\omega}, -\frac{\beta}{2}\right)}{U\left(-\frac{E}{\hbar\omega}, -\frac{\beta}{2}\right)} \tag{5.22}$$

with $a = \frac{\beta^2}{8} - \frac{E}{\hbar\omega}$.

The even solution in region II is given as:

$$\psi_2(\xi) = e^{-i\xi^2/4} M\left(\frac{1}{4} - \frac{ia}{2}, \frac{1}{2}, \frac{i\xi^2}{2}\right) \tag{5.23}$$

Note that $M(a, b, z)$ is the Kummer Hypergeometric function. The derivative of $\psi_2(\xi)$ is then:

$$\psi_2(\xi)' = -\frac{i}{2}\xi\psi_2(\xi) + i\xi e^{-i\xi^2/4} M\left(\frac{1}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i\xi^2}{2}\right)' \tag{5.24}$$

Using the identity [1] 13.4.12

$$M\left(\frac{1}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i\xi^2}{2}\right)' - M\left(\frac{1}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i\xi^2}{2}\right) = -\left(\frac{1}{2} + ia\right) M\left(\frac{1}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i\xi^2}{2}\right) \tag{5.25}$$

In the next step we will determine the even and odd solutions in the region 2. The even solution can be determined easily by substitution of a with ia and x with ix in the equations for the parabolic cylinder functions: So we get for the even solution in region 2:

$$\psi_2^{(e)}(\xi) = e^{-i\xi^2/4} M\left(\frac{1}{4} - \frac{ia}{2}, \frac{1}{2}, \frac{i}{2}\xi^2\right) \tag{5.26}$$

with $a = \dfrac{\beta^2}{8} - \dfrac{E}{\hbar\omega}$. Calculating the derivative of the even solution in region 2:

$$\psi_2^{(e)\prime}(\xi) = \frac{i}{2}\xi\psi_2^{(e)}(\xi) + i\xi e^{i\xi^2/4} M\left(\frac{1}{4} - \frac{ia}{2}, \frac{1}{2}, \frac{i\xi^2}{2}\right)' \tag{5.27}$$

using the identity (5.25) we get:

$$\psi_2^{(e)\prime}(\xi) = \frac{i}{2}\xi e^{-i\xi^2/4} M\left(\frac{1}{4} - \frac{ia}{2}, \frac{1}{2}, \frac{i\xi^2}{2}\right) - i\xi e^{-i\xi^2/4}\left(\frac{1}{2} + ia\right) M\left(\frac{1}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i\xi^2}{2}\right) \tag{5.28}$$

The odd solution in the region 2 is given as:

$$\psi_2^{(o)}(\xi) = \xi e^{-i\xi^2/4} M\left(\frac{3}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i}{2}\xi^2\right) \tag{5.29}$$

The derivative in of $\psi_2^{(o)}(\xi)$ is then

$$\frac{\partial}{\partial\xi}\psi_2^{(o)}(\xi) = \left(1 - \frac{i\xi^2}{2}\right) e^{-i\xi^2/4} M\left(\frac{3}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i}{2}\xi^2\right) + i\xi^2 e^{-i\xi^2/4} M\left(\frac{3}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i}{2}\xi^2\right)' \tag{5.30}$$

Using the identity [1] 13.4.13:

$$(b-a)M(a, b-1, x) = bM(a, b, x) + zM'(a, b, x) \tag{5.31}$$

we get for the derivative of of $\psi_2^{(o)}(\xi)$:

$$\frac{\partial}{\partial\xi}\psi_2^{(o)}(\xi) = e^{-i\xi^2/4} M\left(\frac{3}{4} - \frac{ia}{2}, \frac{1}{2}, \frac{i\xi^2}{2}\right) - \frac{i\xi}{2} e^{-i\xi^2/4} M\left(\frac{3}{4} - \frac{ia}{2}, \frac{3}{2}, \frac{i\xi^2}{2}\right) \tag{5.32}$$

Finally we have to determine the solutions in region 3 for $E = \frac{1}{2}\hbar\omega$:

The regular solution in this case is given as:

$$\psi_3^{(r)}(\xi) = e^{-(\xi-\beta)^2/4)} \tag{5.33}$$

The irregular solution in this case is given as:

$$\psi_3^{(i)}(\xi) = (\xi - \beta)e^{-(\xi-\beta)^2/4} M\left(\frac{1}{2}, \frac{3}{2}, \frac{1}{2}(\xi-\beta)^2\right) \tag{5.34}$$

which can also be written in the form:

$$\psi_3^{(i)}(\xi) = e^{-(\xi-\beta)^2/4} \int_{\beta}^{\xi} e^{-(x-\beta)^2/4} dx \tag{5.35}$$

5.3.2 Connection between the minimum tunneling time and level splitting

If we consider the potential illustrated in figure 5.2, showing a symmetric potential $U(x)$ composed of two potential wells separated by a potential barrier. If we consider the wells individually, each well has a discrete energy spectrum with the energies E_n. As we have here a symmetric structure the states on the left, as well as on the right are in resonance and the double degeneracy will disappear by the effect of electrons tunneling from region 1 to region 2, i.e. the potential wells can not be treated independently. The tunneling of electrons will cause a small energy shift ΔE_n, splitting the eigen energies into doublets $\tilde{E}_n \pm \Delta E_n/2$. Now let us consider a single well, e.g. the potential well on the right. The hamiltonian of this single potential well is denoted by H_{well}. Then the eigenstates of this potential well are given by the solutions of the stationary Schrödinger equation:

$$H_{\text{well}}\psi_n(x) = E_n\psi_n(x) \tag{5.36}$$

As a consequence of the existence of the second well, the eigenstates split into two states with definite parity, i.e. even and odd parity of the complete system:

$$\psi_n^{(e)}(x) \approx \alpha\left(\psi_n(x)+\psi_n(-x)\right) \tag{5.37}$$

$$\psi_n^{(o)}(x) \approx \beta\left(\psi_n(x)-\psi_n(-x)\right) \tag{5.38}$$

The pre-factors can be determined by the symmetry requirements,

$$\begin{aligned} \psi_n^{(e)}(x=0) &= 1 \\ \psi_n^{(o)}(x=0)' &= 1 \end{aligned}$$

The wronskian of both functions will be normalized at $x = 1$. Then we get for the eigenstates of the complete system, i.e. for the potential $U(x)$ including both wells:

$$\begin{aligned} H\psi_n^{(o)}(x) &= \left(\tilde{E}_n + \frac{\Delta E_n}{2}\right)\psi_n^{(o)}(x) \\ H\psi_n^{(e)}(x) &= \left(\tilde{E}_n - \frac{\Delta E_n}{2}\right)\psi_n^{(e)}(x) \end{aligned}$$

So the existence of the second potential well leads to a change in the eigen energies by $\tilde{E}_n - E_n$, which is exponentially small in the WKB approximation. The question of interest is now how the energy splitting is connected to the tunneling time through the potential barrier in the center of the potential. At the time $t = 0$ the system will be in the superposition of the states (5.37) and (5.38):

$$\psi_E^{(r)}(x,0) = \beta\psi_n^{(e)}(x) + \alpha\psi_n^{(o)}(x) \tag{5.39}$$

Now if we consider the time evolution of the complete system using (5.39) and (5.39) we get:

$$\psi_E^{(r)}(x) = 2\alpha\beta e^{-i\tilde{E}_n t/\hbar}\left(\psi_n(x)\cos\Omega_n t + i\psi_n(-x)\sin\Omega_n t\right) \tag{5.40}$$

with $\Omega_n = \Delta E_n/\hbar$. We can see that the electrons are oscillating between the two wells with a period $T_n = 2\pi/\Omega_n$, i.e. that an electron travels through the central barrier in the time $T_n/2$. So we can assume that $T_n/2$ is the characteristic tunneling time for this setup. In the next step we have to show the relation of the characteristic tunneling time $T_n/2$ with the minimal tunneling time τ_{min}.

The wave functions $\psi_n^{(e)}(x)$ and $\psi_n^{(o)}(x)$ are orthogonal functions in the symmetric interval $-d < x < d$, therefore the number of particles $N(d)$ will be constant with respect to time in this interval,i.e.

$$N(d) = \int_{-d}^{d} |\psi_E^{(r)}(x)|^2 dx = \int_{-d}^{d} \psi_n^{(e)}(x)^2 dx + \int_{-d}^{d} \psi_n^{(o)}(x)^2 dx \tag{5.41}$$

The current density at the center of the barrier is then

$$j(x=0,t) = \frac{\hbar}{m} Im \left(\psi_E^{(r)}(x)^* \frac{\partial}{\partial x} \psi_E^{(r)}(x) \right). \tag{5.42}$$

Inserting equation (5.40) into (5.42) we get:

$$j(x=0,t) = -\frac{\hbar}{m} \sin \Omega t \left(\psi_n^{(e)}(x) \frac{\partial}{\partial x} \psi_n^{(o)}(x) - \psi_n^{(o)}(x) \frac{\partial}{\partial x} \psi_n^{(e)}(x) \right) \Bigg|_{x=0} \tag{5.43}$$

$$= \frac{\hbar}{m} \sin \Omega t \, \mathcal{W}\Big(\psi_n^{(e)}(x), \psi_n^{(o)}(x) \Big) \Big|_{x=0} \tag{5.44}$$

where $\mathcal{W}\Big(\psi_n^{(e)}(x), \psi_n^{(o)}(x) \Big) \Big|_{x=0}$ is the Wronskian of the odd and even function at the point $x = 0$. As we mentioned before that the normalization of the wave functions will be done using the wronskian of the even and odd wave functions, equation (5.44) simplifies to:

$$j(x=0,t) = -\frac{\hbar}{m} \sin \Omega t. \tag{5.45}$$

So now let us have a look at the following integral from [12] at page 99:

$$\int_0^\infty \psi_n^{(e)}(x) \psi_n^{(o)}(x) \, dx = -\frac{\hbar^2}{2m} \frac{\mathcal{W}\Big(\psi_n^{(e)}(x), \psi_n^{(o)}(x) \Big) \Big|_{x=0}^{\infty}}{E_n^{(o)} - E_n^{(e)}} \tag{5.46}$$

As $\psi_n^{(o)}(x)$ and $\psi_n^{(e)}(x)$ are both bound states, the Wronskian of these two functions vanishes as x approaches ∞. On the other hand as mentioned above the Wronskian at $x = 0$ is used for the normalization and is therefore 1. Since we know that $T_n = 2\pi\Omega_n = 2\pi\hbar/\Delta E_n$, equation (5.46) becomes:

$$\int_0^\infty \psi_n^{(e)}(x)\psi_n^{(o)}(x)\,dx = \frac{\hbar^2}{2m}\frac{1}{E_n^{(o)} - E_n^{(e)}} = \frac{\hbar}{4\pi m}T_n \tag{5.47}$$

rewriting this equation we get for the characteristic tunneling time in this system:

$$T_n = \frac{4\pi m}{\hbar}\int_0^\infty \psi_n^{(e)}(x)\psi_n^{(o)}(x)\,dx \tag{5.48}$$

Although the functions in the integrand depend implicitly on the tunneling time T_n, equation (5.48) is an exact statement. In order to get rid of the implicit dependency of the integrand on the tunneling time we will substitute the exact wave functions by the wave functions $c(x)$ and $s(x)$ of the unperturbed system, as in (5.4). This is justified by the fact that the deviation of the eigenenergy of the real system from the unperturbed system is exponentially small. Wo we obtain finally the approximation for T_n as:

$$T_n \approx \frac{4\pi m}{\hbar}\int_0^d c(x)s(x)\,dx \tag{5.49}$$

Now we can express the the characteristic time T_n in terms of the minimal tunneling time τ_{min} from (5.7) and get:

$$T_n \approx \pi\sqrt{\tau_{\text{min}}(-d,d,E_n)^2 - 4\tau_{\text{min}}(0,d,E_n)^2} \tag{5.50}$$

$\tau_{\text{min}}(0,d,E_n)$ is exponentially small compared to the minimum tunneling time $\tau_{\text{min}}(-d,d,E_n)$ for opaque tunneling barriers and may therefore be omitted, so T_n becomes:

$$T_n \approx \pi\tau_{\text{min}}(-d,d,E_n) \tag{5.51}$$

Numerical results for the energy splitting in the exact case and the energy splitting of the ground state using the minimal tunneling time were determined according to [4] using the the dimensionless measure $\gamma = \sqrt{2m\omega/hbar d}$ for the separation of both wells. We get from the exact solutions in section 5.3.1 and the solutions using the minimal tunneling time the following numerical results in the following table:

γ	U_0	ΔE_0 (exact)	ΔE_0 (using τ_{min})	relative error
3	1.125	4.86088×10^{-2}	5.32624×10^{-2}	9.57×10^{-2}
5	3.125	6.46587×10^{-5}	6.49829×10^{-5}	5.01×10^{-3}
7	6.125	1.97591×10^{-9}	1.97615×10^{-9}	1.23×10^{-4}
8	8.000	2.78036×10^{-12}	2.78040×10^{-12}	1.41×10^{-5}

Chapter 6

CONCLUSION

In this thesis various tunneling time approaches were discussed. First the Dwell time was discussed using Bohmian trajectories, then the Dwell time was also defined in the sense of Büttiker and Smith. Based on this the Dwell time was calculated for two examples explicitly, i.e. for a rectangular barrier and for symmetric double δ- Potential. Then the Büttiker Landauer time was discussed. In this framework the calculations showed the inelastic nature of this tunneling process, because of the interaction of the particle with the perturbing time varying barrier. The Larmor Clock was reviewed as one of the first approaches to establish a traversal time concept in Quantum theory. Finally the variational approach of the tunneling time, the Minimal Tunneling time, was presented. First the Minimal Tunneling Time for the rectangular barrier was calculated and compared with the the Dwell time, then the connection of the minimal tunneling time with the energy splitting in a harmonic double well potential was determined and the results were compared to the exact solutions of the Schrödinger equation.

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